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Ollscoil na hÉireann, Corcaigh
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Applications of Big Data and Machine Learning in Global Energy System Modelling

Thesis presented by
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for the degree of
Doctor of Philosophy

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Author's Declaration

This is to certify that the work I am submitting is my own and has not been submitted for another degree, either at University College Cork or elsewhere. All external references and sources are clearly acknowledged and identified within the contents. I have read and understood the regulations of University College Cork concerning plagiarism.

Siddharth Joshi

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Executive Summary

Global efforts to limit atmospheric warming well below 2°C above pre-industrial levels form the backbone of our response to mitigate the detrimental effects of climate change. The energy sector contributes circa 75% of global GHG emissions, amongst which the Electricity and Heat sectors each contribute ~40%, and the Transport sector contributes ~20% to the total global energy-related GHG emissions. The recent IPCC AR6 report finds that in nearly all possible emission scenarios considered, the world is heading towards a 1.5°C global temperature rise by the early 2030s. Pursuant to this, Energy Systems Models (ESMs) and Integrated Assessment Models (IAMs) are essential tools that provide energy system pathways to limit global warming below the temperature threshold. Thus, improving the accuracies of ESMs and IAMs will lead to measurable improvement in energy policy formulation and evaluation, thereby increasing the likelihood of meeting the commitments under the Paris Climate Agreement.

This thesis develops and applies novel frameworks and methods that use a big data and machine learning driven strategy to improve the technology potential assessment of global decentralised solar PV technology and projection of transport energy service demand. The frameworks and methods developed in this thesis are presented in a format of methodological design principles followed by a case study using them. Specifically, on the supply side, the thesis investigates the global high-resolution spatiotemporal technical potential of rooftop solar PV for 2015 and further growth in the technical potentials from 2020-2050. For this assessment case study, the developed framework utilises a suite of GIS derived geospatial metrics in conjunction with a custom machine learning framework to calculate the global rooftop area at a high spatial resolution. Further using an IAM, the role of decentralised solar PV in global future energy transitions is explored. On the demand side, the thesis introduces a new machine learning model called 'TribuNet' that is capable of high accuracy in estimating future energy service demand in the transport sector. The thesis thus provides the first development of machine learning and GIS based methods to improve the accuracy of global ESMs and IAMs. Particular attention is also paid towards the reproduction and transparency of the methods and the frameworks developed in this thesis for cross-disciplinary research.

The thesis contributes to the important task of climate change mitigation by providing a bridge between mature IAM and ESM modelling and emerging machine learning-big data-driven tools. In doing so, this thesis demonstrates how the emerging methods in conjunction with large geospatial open source data, can aid in improving the technology representation of variable renewable energy technology in energy systems. The thesis also lays the foundation for providing solutions to energy system related tasks that are currently limited by high computational costs and data. The datasets and analysis generated by this thesis are presently assisting in unlocking the global role of decentralised renewable energy technologies in future energy systems and are also encouraging shifts in national decarbonisation pathways.

Units and Abbreviations

\$	US dollar
3D	Three Dimension
AG	Air-Goods data series
ANN	Artificial Neural Network
AOI	Area Of Interest
AP	Air-Passenger data series
AR6	Sixth Assessment Report of IPCC
BA	Built-up Area
BF	Building Footprint
CAPEX	Capital Expenditure
CO ₂	Carbon Dioxide
COP	Conference Of Parties
CORINE	CoORdination of INformation on the Environment
CPU	Central Processing Unit
CP _{UT}	Current Policy - Utility Only
CP _{UTDC}	Current Policy - Utility+Decentralised
CV	Cross Validation
DCSPV	DeCentralised Solar PV
DR	Discount Rate
EJ	Exa Joule
ESM	Energy System Models
ESRI	Environmental Systems Research Institute
FN	Fish Net
GDP	Gross Domestic Product
GEE	Google Earth Engine
GHG	Green House Gases
GHSL	Global Human Settlement Layer

GIS	Geographic Information System
GLOBIOM	GLObal BIOsphere Model
GPU	Graphic Processing Unit
GW	Gigawatt
GWh	Gigawatt-hour
IAM	Integrated Assessment Model
IEA	International Energy Agency
IIASA	International Institute for Applied Systems Analysis
IPCC	The Intergovernmental Panel on Climate Change
IRENA	The International Renewable Energy Agency
ITF	The International Transport Forum
JRC	Joint Research Centre, European Commission
km	kilometre
kW	kilowatt
kWh	kilowatt-hour
kWp	kilowatt Peak
LC	Land Cover
LCOE	Levelised Cost Of Electricity
LiDAR	Light Detection And Ranging
MESSAGEix	Model for Energy Supply Strategy Alternatives and their General Environmental Impact
ML	Machine Learning
MSE	Mean Squared Error
M _{UT}	Mitigation Policy - Utility Only
M _{UTDC}	Mitigation Policy - Utility+Decentralised
MW	Megawatt
MWh	Megawatt-hour
NM	Non Masked
OECD	Organisation for Economic Co-operation and Development

OPEX	Operating Expenses
OSM	Open Street Maps
PKM	Passenger kilometre
PPLN	Population
PV	Photovoltaics
PW	Petawatt
PWh	Petawatt-hour
RaG	Rail-Goods data series
RaP	Rail-Passenger data series
ReLU	Rectified Linear Unit
RL	Road Length
RMSE	Root Mean Squared Error
RoG	Rail-Goods data series
ROI	Region Of Interest
RoP	Road-Passenger data series
RTSPV	Rooftop Solar PV
SDG	Sustainable Development Goals
SSP	Shared Socioeconomic Pathways
TKM	Tonne kilometre
TrebuNet	Trebuchet Network
TW	Terawatt
TWh	Terawatt-hour
UN	United Nations
UNCTAD	The United Nations Conference on Trade and Development
UNFCCC	The United Nations Framework Convention on Climate Change
UTSPV	UTility scale Solar PV
VRE	Variable Renewable Energy

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Chapter 1: Introduction

1.1 Background

Global energy systems are the backbone on which modern society is built upon. Since antiquity, the need for energy has shifted from providing warmth during colder seasons to charging one's smartwatch. With each advancement in the quality of life over centuries, humans have increased their energy consumption, and hence their reliance on the delivery of energy to the end-use sectors has also increased. We consume energy during our daily activities ranging from transportation to cooking food and everything in between. The Internet age or Industry 4.0 age is extensively dependent on using energy to augment our quality of life beyond basic survival needs, with many experiencing energy poverty.

With an increase in energy consumption over the past century, humans have also exposed themselves to the perils of climate change and global warming. It has been empirically proven that anthropogenic modifications^[1] over the past centuries have led to the current challenges attributed to global warming and consequently the changes in the climate and weather cycles. Acknowledging the detrimental effects of global warming, an agreement to limit global climate warming to below 2°C compared to pre-industrial levels was signed in 2015 in Paris under the UNFCCC, COP21. The "Paris Agreement"^[2] came into force in 2016, thereby providing a legal basis for the goal of reducing global warming to below 2°C and aiming for 1.5°C by 2100 compared to pre-industrial levels. Pursuant to this, it has been calculated that the energy sector alone contributes

circa 75% of global GHG emissions, amongst which the Electricity and Heat sector contributes ~40%, and the Transport sector contributes ~20% to the total global energy driven GHG emissions^[3]. In 2023 the first global stocktake of the Paris Agreement is scheduled where the progress towards the goal of 2°C rise in average global temperature will be evaluated.

In light of the ambitious goals of the Paris Agreement, the recent IPCC AR6 report provides a compendium of results from the on-ground observations. The report finds that in nearly all possible emission scenarios considered, the world is heading towards a 1.5°C global temperature rise by the early 2030s. At the same time, the report underscores the importance of renewable resource based energy generation and demand side energy consumption pattern changes in achieving the lowest overshoot from 1.5°C targets. Thus, it becomes pertinent that an accurate assessment of renewable resource potentials and estimation of future energy demands will form the backbone of future energy systems analysis. Figure 1.1 illustrates the potential of various emission mitigation options in the energy sector.

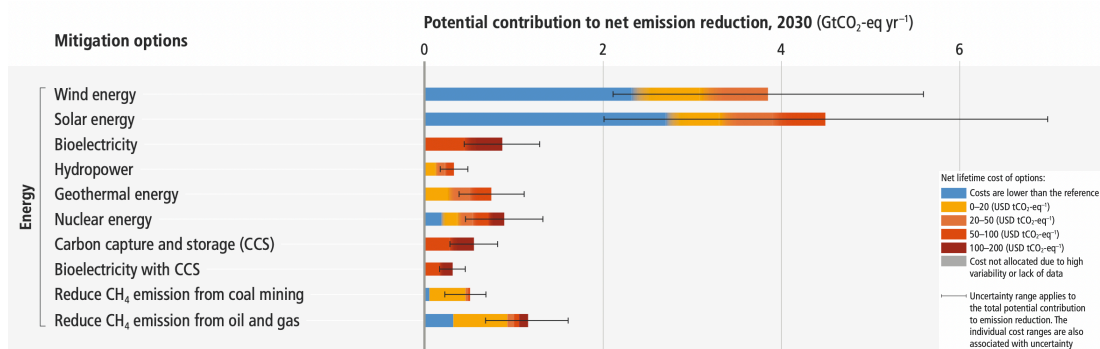


Figure 1.1 | Potentials of various mitigation options in the energy sector

Source: Reproduced from IPCC, 2022: Summary for Policymakers. In: Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change, Figure SPM.7

In parallel with the need to improve the accuracies of renewable energy potentials and energy service demand estimation, applications that use big data to enhance understanding of energy systems have gathered momentum^[4-13]. Complex analysis based on big data has provided valuable insights into improving our understanding of how energy systems interact with physical geography and vice versa. Since the 21st Century, development in machine learning methods, especially in the past decade, has unlocked the potential of how big data can aid in designing future energy systems that bolster climate change mitigation efforts^[14-21]. Examples are abundant in the field of earth observation^[22-29], resource planning^[30-33], quantifying the impact of natural hazards^[34-38], projection of weather patterns^[39-41], etc.

While contemporary literature is rich in the ancillary application of big data and machine learning in global energy systems, the direct application of these methods has recently started gaining cadence. This can partly be attributed to the reduction in barrier to entry for machine learning methods used for research and data analysis purposes and partly due to exponential growth in energy related big data in the past decade. The application of machine learning as a modelling tool in energy systems modelling is still a novel concept. Over the past decade, researchers have implemented the modelling concepts of machine learning to augment and complement the tasks of modelling an energy system^[42-45]. In its most basic form, an energy system modelling exercise is a mathematical representation of supply side and demand-side technologies with an objective function that links the two across spatial and temporal domains. The core objective of the energy system modelling exercise is thus to reduce the cost of the objective function while keeping the solution space within external constraints like emissions, merit order etc. Outside the modelling of energy systems, machine learning is enabling meta-analysis of the results from the runs of the energy system models (ESMs)^[46]. Integrated Assessment Models (IAMs) merge the energy system

models with climate, land, and macroeconomic modules to capture the cross-domain impacts of future energy systems. Here, machine learning has provided excellent results in climate modelling, land use and land change detection etc.^[21, 41, 47-49]. Thus it can be concluded that machine learning, although a novel modelling concept, has started enriching the way we design our energy systems.

Naturally, machine learning coupled with big data is expected to provide new insights into how we design future energy systems^[43, 50-53]. These methods can also improve the accuracy in the representation of energy demand and renewable supply in global IAM and ESMs, which can have a cascading effect on the solutions that IAM and ESMs can provide, and consequently improve the mobilisation of required policy levers to achieve climate change mitigation. Thus, it can be deduced that machine learning and big data derived methods for energy systems analysis are synergistic in achieving future global energy systems with the lowest overshoot from 1.5°C targets.

In this regard, Rolnick et al.^[44] published an overview of entry points for machine learning and big data-based applications in tackling the challenging goal of climate change adaptation and mitigation. They highlighted that some of the high-impact and high-value applications of machine learning and big data can be in the domain of supply side resource assessment and demand side projection. Here, Figure 1.2 illustrates the key entry points of big data and machine learning in IAMs and ESMs either as direct or ancillary applications. Within these entry points, this thesis explores the application of big data and machine learning in global energy systems by focusing on demand side and supply side applications.

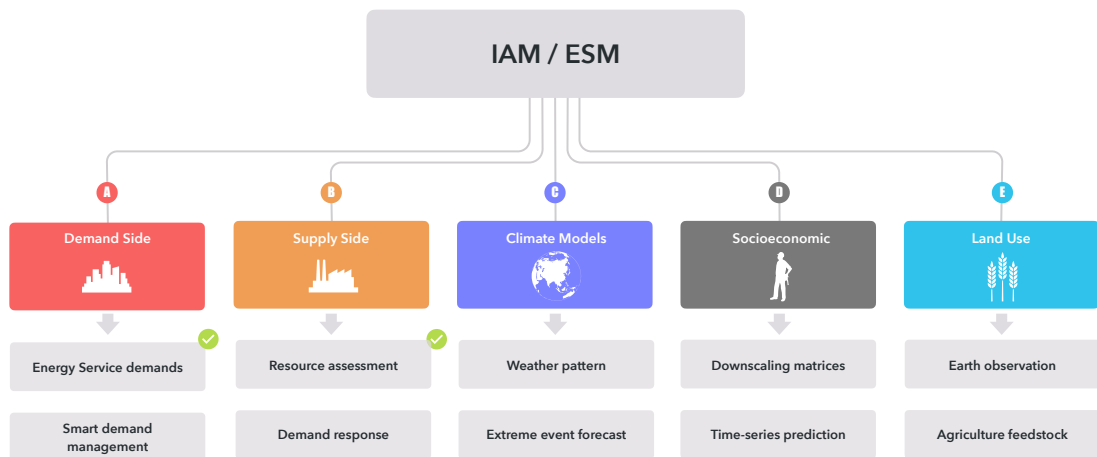


Figure 1.2 | Key entry points for big data and machine learning methods in IAM and ESMs

The focus of this thesis is on entry points A and B. The green ticks are the specific focus of this thesis.

1.2 Application areas

The IPCC AR6 report suggests that solar PV-based mitigation solutions will have the highest potential for emission reduction until 2030. Coupled with the steep decadal decline in solar PV costs, this renewable electricity generation technology has shown the highest net capacity increase in recent years. Amongst the global solar PV installed capacity in 2020, 40% contribution can be attributed to decentralised solar PV technology specifically rooftop solar PV^[54], Figure 1.3. Uptake of decentralised low-carbon and cost-effective renewable electricity generation (SDG 7) like rooftop solar PV has the potential to address the twin challenges of sustainable development and climate change (SDG 13) with co-benefits in advancing SDG 11 (sustainable human settlements) and SDG 15 (promoting sustainable life on land)^[55-58].

To enable the rapid uptake of decentralised solar PV technology and to understand its impact on energy security and energy justice, an accurate assessment of its global resource potential is pertinent^[59, 60]. This high-resolution assessment of global rooftop solar PV's technical potential has traditionally been a computationally extensive task^[61]. The complexity of the assessment develops

from the fact that the smallest unit of assessment is an individual household. Moreover, the households have geospatial causality like climatic zones, urban morphology, building practices etc.

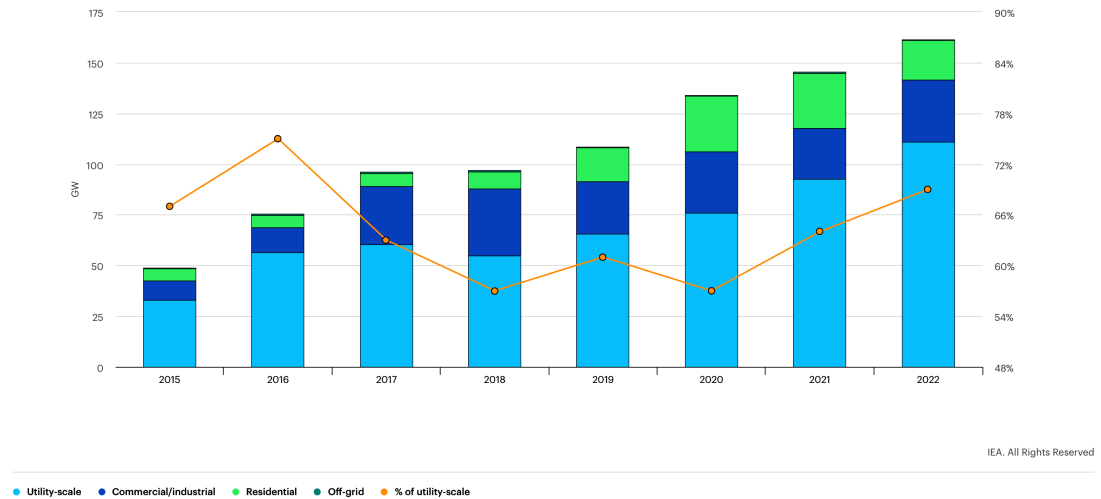


Figure 1.3 | Net installed capacity of solar PV by segment

Source: Reproduced from IEA (2021), Renewable Energy Market Update 2021, IEA, Paris <https://www.iea.org/reports/renewable-energy-market-update-2021>.

On one hand, the complexities of the global building archetype are the biggest impediment in the assessment of decentralised solar PV technology's technical potential, on the other hand, recent growth in open source building footprint data can aid in the mitigation of this impediment. Till a harmonised global dataset of building footprints is available for assessment, the challenge for an accurate global resource assessment will be to translate the learnings from big data that is available disproportionately for the developed countries onto the emergent countries. The global magnitude of this analysis is where big data and machine learning can provide invaluable insights in designing of global energy systems by aiding in accurate global resource assessment studies.

Similarly, machine learning-based approaches have shown breakthrough improvements in the accuracy of time-series forecasting^[62, 63] and energy demand forecasting^[64-67]. Time-series forecasting forms the backbone of future energy

demand projection. The global transport sector currently contributes to ~20% of the total global energy-driven GHG emissions. An accurate understanding of how global transport demand can change in short and medium-term will lead to better formulation and evaluation of policy levers used by national policymakers^[68]. The complexity in demand forecasting of the transport sector can be attributed to the interdependence of different modes of transportation e.g. rail, road and air and also due to bilateral/multilateral trade mechanisms between countries. Thus, improving demand forecasting for the transport sector would involve an accurate representation of demand and driver relationships for different transport modes and for countries in a region. Consequently, the application of machine learning in time-series forecasting can be beneficial to improving the accuracy of energy service demand forecasting for the transport sector.

1.3 Thesis aims

This thesis explores the application of big data and machine learning architectures with the aim of improving global energy system models. Further, this thesis explores the benefits of machine learning-based frameworks and novel methods introduced here for assessing the role of low-carbon technology in enabling global climate change mitigation efforts. To elucidate this, with an overall objective of improving the representation of supply-side renewable resources and energy service demand projections in global energy systems, the thesis explores the following specific research questions:

- (RQ-1)** What are the benefits and limitations of machine learning-based approaches in supply and demand side modelling of energy system models?
- (RQ-2)** How can machine learning-based frameworks aid in high-resolution spatiotemporal assessment* of current and future growth in global rooftop solar PV's renewable electricity generation potentials?
- (RQ-3)** How can the advancements in energy resource potential estimations elicited by the machine learning, GIS and big data-based frameworks improve the representation of decentralised solar PV in global Integrated Assessment Models?
- (RQ-4)** How do machine learning-based approaches improve the accuracy[§] of short, decadal, and medium-term transport energy service demand estimations?

The research questions stated above are designed to shed light on the various methodologies that can be specifically used to complete gaps in current literature and generate datasets/frameworks that can be used across disciplines. Although this thesis touches on the current state of the art for machine learning applications in global energy systems, it is not intended to provide conclusive answers to all possible questions as both the machine learning algorithms and the hardware they run on are improving at an exponential speed year over year. On the contrary,

* Here current is 2015 and future is 2020-2050

§ Here short term is single year and medium term is 2020-2050

this thesis aims to provide novel solutions and datasets to mitigate and advance the research gaps that have shown limited success using traditional methods. To this end, this thesis explores methodologies and frameworks that can be generalised in their application to broader research topics.

1.4 Thesis outline

This thesis contains four chapters and an Annex. Chapters 2, 3 and 4 are based on peer-reviewed publications. Chapter 5 documents the conclusions to the research questions asked in Section 1.3 and provides suggestions for further work. The Annex contains a report that is the direct policy application of the research conducted in this thesis. The chapters presented in this thesis attempt to answer multiple research questions in the format of an introduction of a novel methodology/framework followed by a case study that incorporates these methodologies. The structure and interlinkage of the thesis chapters with research questions are summarised in Figure 1.4, with each chapter documenting a separate chapter specific literature review.

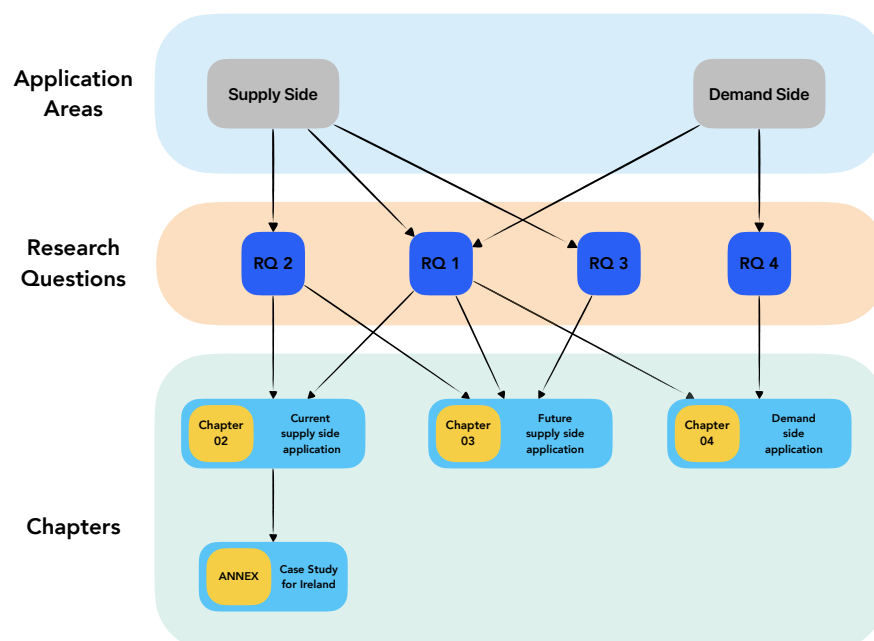


Figure 1.4 | Interlinkage between chapters and research questions

Chapter 2

Accurate assessment of rooftop solar PV potential at a global scale with high spatiotemporal resolution is a computationally complex and time-consuming problem that requires prohibitive computational hardware. As a result of this, assumptions around the potential of rooftop solar PV have driven the IAMs and ESMs- leading to the limited representation of rooftop solar PV in energy systems. This chapter introduces a novel machine learning and big data-driven framework that uses global geospatial landcover, population, and roads along with >300 million individual building footprint data to provide the first global high-resolution spatiotemporal assessment of rooftop solar PV's technical potential at scale ranging from city to continental levels. From this chapter, I conclude that aggregated yearly global potential for rooftop solar PV exceeds the yearly aggregated global demand for electricity. Here, I also demonstrate how multiple physical GIS-based metrics can be converted into the numerical domain for an efficient machine learning process that will benefit individual researchers in setting up their own research analysis without a need for complex hardware support. By way of a case study on the assessment of the global rooftop area, this chapter demonstrates the niche role of machine learning and big data in improving the accuracy of technical potential assessment of renewable supply-side technologies.

Chapter 3

Building on the learnings from Chapter 2, Chapter 3 introduces a novel framework to estimate the future growth in the global rooftop area and consequently the growth in the technical potential for decentralised electricity generation from rooftop solar PV. Here, I evaluate the growth in global rooftop areas for the five different worlds envisioned under the SSP narratives and conclude that the African continent will show the highest growth in rooftop areas across the different socioeconomic growth trajectories. I also demonstrate that the hotspots for future rooftop solar PV deployment will lie in developing economies. In this chapter, I

further evaluate the economic potential for decentralised rooftop solar PV at a global scale using current policy and stringent climate change mitigation policies using MESSAGEix-GLOBIOM IAM of IIASA. Based on the accurate representation of rooftop solar PV in global IAM, the chapter concludes that decentralised rooftop solar PV can account for more than 50% of the electricity generation from solar PV by 2050, hence making rooftop solar PV a capable policy lever for climate change mitigation objectives. In conclusion, this chapter demonstrates how big data and machine learning can provide state of the art tools to represent a decentralised renewable energy technology in a global IAM and hence aid in the accurate evaluation of global and local energy and climate mitigation policies.

Chapter 4

This chapter introduces a novel custom artificial neural network-based architecture that mimics the physical process of firing a trebuchet. Further, this architecture is used to project the energy service demands for air, road, and rail mode of transport for OECD countries. The chapter demonstrates how machine learning in combination with sparse time series data can improve the accuracy of energy service demand projection. Here, I validate the projections for short, decadal and medium-term time horizons and apply this framework to a global maritime freight transport case study. I conclude this chapter by objectively evaluating that machine learning-based frameworks can work very well with sparse data also and at the same time improve the accuracy of energy service demand projections which in turn drive the IAMs and ESMs.

Chapter 5

The final chapter, Chapter 5 provides answers to the research questions based on the conclusions that are drawn from Chapters 2, 3, and 4 and also provides recommendations for further work. To enable open-source uptake of the findings of this research - pseudocode, datasets and framework structures have been

released with this thesis. Figure 1.5 shows an overview of the theme and attributes of the thesis chapters.

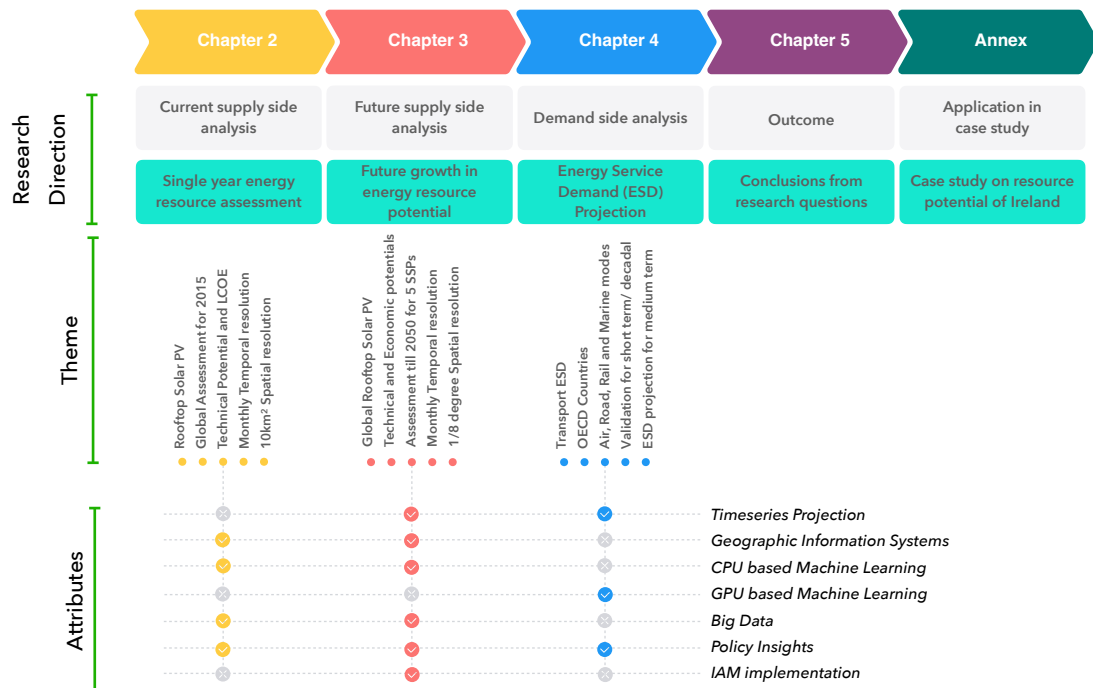


Figure 1.5 | Overview of chapter theme and attributes.

1.5 Contribution of the thesis

This thesis explores the application of big data and machine learning in global energy systems. It undertakes this exploration by developing new methodologies and frameworks that are custom tailored to the energy service demand estimation in the transport sector and assessment of rooftop solar PV's potential for renewable energy generation. In doing so, this thesis leverages open-source data and methodologies to create open-source frameworks to complete the stated research goals. Further, along with each research goal, this thesis delves into the best practices of incorporating machine learning workflows, the bottlenecks of current analysis platforms and solutions to circumvent these bottlenecks. The thesis also showcases how individual researchers and a team of researchers can leverage the machine learning workflows without overly relying on server-class hardware.

Specifically, this thesis undertakes the first-ever high-resolution global spatiotemporal assessment of rooftop solar PV's potential in 2015. Here, this thesis demonstrates an excellent use case for big data and machine learning for global energy systems. Leveraging the big data and machine learning framework developed in this thesis, it further researches the first global assessment of rooftop solar PV's future growth using SSP narratives. In doing so, this thesis utilises global IAMs and scenario analysis to explore the questions related to sustainable development and climate change mitigation. In its entirety, Chapters 2 and 3 showcase the best practices and workflows for applying big data and machine learning workflows to analyse a single decentralised renewable generation technology from the ground up and also quantitatively analyse the improvements this can accrue to IAMs and ESMs. Additionally, Chapter 4 of this thesis contributes significantly to the application of machine learning for time-series forecasting and demand forecasting, which can aid in increasing the accuracies of both short and medium-term time horizon ESMs.

Precipitating from the research conducted in this thesis, important conclusions were documented related to the spatial and temporal characteristics of decentralised solar PV vs utility-scale solar PV. To enable open-source uptake of the findings of this research - pseudocode, datasets and framework structures have been released with this thesis. To date, the main finds of this thesis have contributed significantly to the debate on energy security and climate change and formed part of the report presented in the Annex. The analysis and conclusions from the thesis have also formed the basis for energy-related policy formulation in the Republic of Ireland, where it has contributed to national energy autarky debates.

1.6 Methodology

This thesis utilises a suite of contemporary research methods and develops some novel methods of its own. Specifically, the development of new resource assessment frameworks and energy service demand projection model relies on the use of traditional machine learning methods to train the frameworks. Further in the thesis, the use of conventional energy systems analysis methods like energy system optimisation modelling using linear programming based least cost optimisation and scenario analysis is called upon. This section briefly documents the methodological basis of the techniques used to research new applications. Specific methodologies and state of the art in methods, their limitations and use cases are documented in detail in the methods sections of each chapter.

1.6.1 Development of a machine learning model

This thesis incorporates supervised learning in Chapters 2, 3, and 4. In supervised learning, the models are trained on known independent and dependent variables to minimise the prediction errors for dependent variables. Various error metrics like Mean Squared Error, Root Mean Squared Error, R^2 , etc., are often used to select the best fit for the machine learning model. The “best” model in the machine learning domain is a model that can adequately generalise its prediction for new independent variables. This could also mean that the best model may not be the one that realises the lowest error for a single error metric but the one that performs best for a combination of error metrics with the spread of error between predicted and true values following a bell curve around a mean. Within the supervised machine learning domain, this thesis aims at designing methods that target Regression tasks.

For a set of discrete or continuous independent variables $X_1, X_2, X_3, \dots, X_n$ and dependent variable Y (single output) or $Y_1, Y_2, Y_3, \dots, Y_n$ (multi-output), a supervised machine learning regression model $\psi : X \rightarrow Y$ will aim to reduce the error between

predictions $\psi(X)$, for all X , in comparison with actual values Y using loss metric Δ . Simply the main objective of training a machine learning regression model can be summarised as

$$\text{Select } \psi \text{ to minimise } \mathcal{E}(\psi) = \Delta(Y, \psi(X)), \text{ where } \mathcal{E}(\psi) \text{ are the errors} \quad (1.1)$$

The selection of ψ can be performed by rerunning (optimising) the model using different settings (formally known as hyperparameters of the model) to choose the best-performing model across different loss metrics. In general, the number of hyperparameter tuning optimising rounds can be decided based on when saturation in loss metric starts manifesting with each increasing iteration number. The selection of each next hyperparameter for each optimisation round can be based on different algorithms. One can rely on grid search algorithms that test the model for each combination of hyperparameters or random search algorithms that randomly choose a combination of hyperparameters. The grid search algorithm is time intensive and is suitable for the final selection of hyperparameters with a narrow hyperparameter search space. Random search algorithms are generally good for testing a wide hyperparameter search space with user-defined optimisation rounds. In this thesis, I use the Tree-Structured Parzen Estimator, which uses information from each hyperparameter optimisation round to decide on the next set of hyperparameters to be tested. This algorithm generally converges to the optimum hyperparameters quicker than the grid search algorithm. A flowchart for the steps involved in a machine learning workflow is shown in Figure 1.6

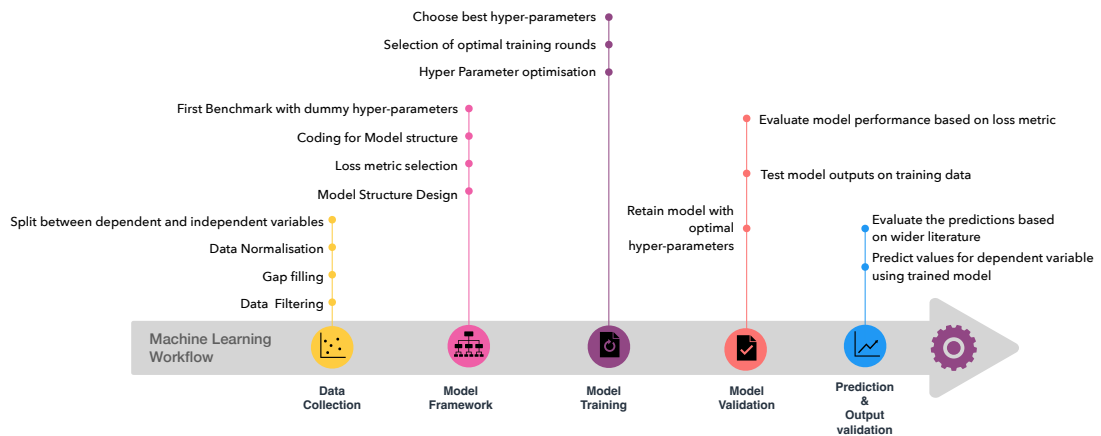


Figure 1.6 | A typical machine learning workflow

Training a machine learning model heavily depends on how the training data is exposed to the model during hyperparameter optimisation rounds. The traditional strategy for machine learning envisions dividing the training data into Train, Test and Validate sets. Each set will have a combination of dependent and independent variables. The Training set is used to train the model within each hyperparameter optimisation round. The Validation set is used to evaluate the model's performance by comparing the model's prediction using the Validation set's independent variable for each Validation set's dependent variable. The collection of hyperparameters that show the least prediction error is used to finalise the model. The final model is then evaluated for its generalising performance on the Test set. In summary, the Training set is used to "fit" the model, the Validation set is used to select the hyperparameters, and the Test set is used to evaluate the model performance.

This strategy is useful when dealing with big data in combination with the random selection of the three sets. The disadvantage of this strategy is that the model is biased towards information contained within the Training set and Validation set, while the information contained within the Test set is usually wasted due to non-exposure to the Test set while training the model. To mitigate this, a cross-validation (CV) strategy is used. In this, the data is first split into a combined Training+Validation set and Test set. The Training+Validation set is further split into

K-folds i.e. the set is split into K slices of data. The hyperparameter optimisation rounds then choose K-1 slices for training and one slice for validation. This is repeated for K times with different slices of data used for training and validation within a single optimisation round. The mean of the errors from the K folds is further used to determine the hyperparameter's performance. Figure 1.7 shows the K-fold CV strategy for 5-folds.

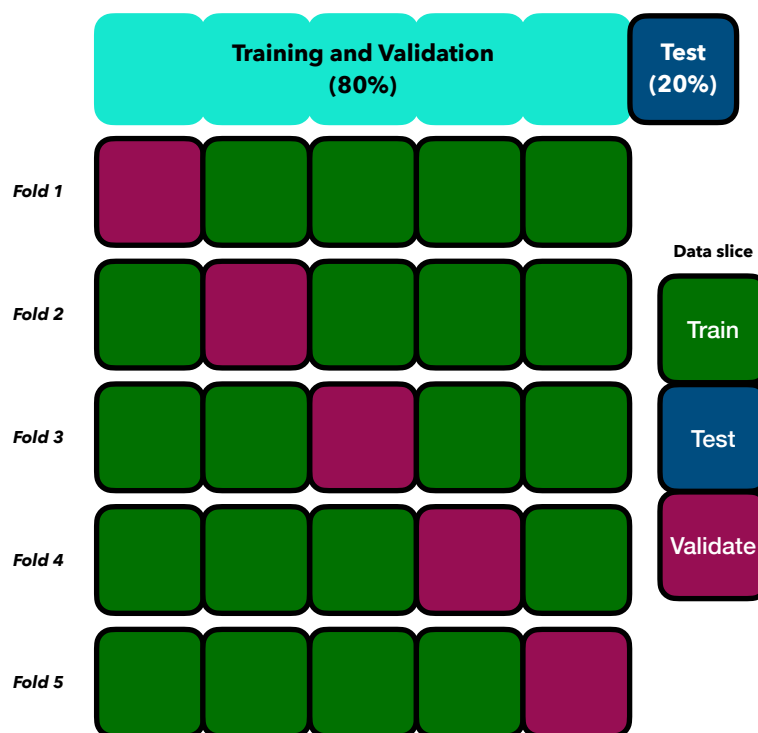


Figure 1.7 | A visualisation of a 5-Fold CV with Train/Validate/Test strategy

The K-fold CV method provides much-needed generalisation to the Train/Validate/Test strategy. K-fold CV also provides a virtual set of K datasets derived from a single dataset which in turn improves the training attributes of the model. While the method described above is a marked improvement over the Train/Validate/Test strategy, it still prevents a part of the data which is used as a Test set from being used for model training. A modified form of the Train/Validate/Test strategy is used in Chapter 4, where training is done on time-series data in which years can organically act as the division between the sets. In time series

forecasting, the independent and dependent variables change between years, hence this strategy is perfect for Chapter 4's case study. Splitting the dataset based on organic years aids in incorporating the complete year's data while training and validating, with unseen entire year's data being used for testing.

A further modification to the Train/Validate/Test strategy is implemented in Chapters 2 and 3, where a full set of data is used for K-fold CV. Here, the model trains on a full set of independent and dependent variables and then validates the model's performance again on the full set of data. The nudge towards generalisation in model performance is provided by using a 10-fold CV strategy. This strategy is useful as all data points are used for training the model, and similarly, all data points are used for evaluating the model performance. Additionally, a random sampling strategy is used to generate 10 slices of data to provide increased training opportunities to the model. An example of a 5-Fold CV strategy with a full set of training data is shown in Figure 1.8.

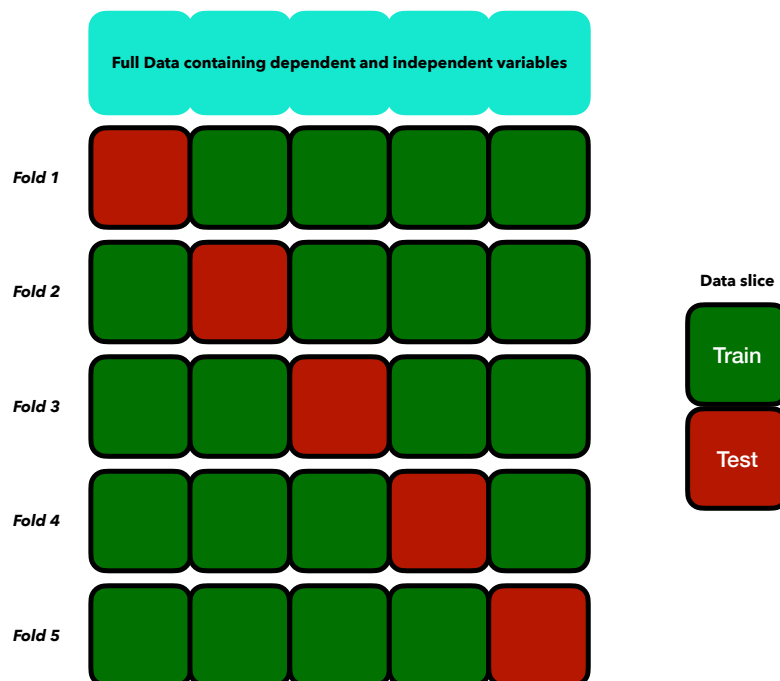


Figure 1.8 | A visualisation of 5-Fold CV with full set of training data

In this thesis, both CPU and GPU-based models are explored. Chapter 2 and 3 utilises the CPU-based Extreme Gradient Boosting machine learning methods to create a novel resource assessment framework. Chapter 4 utilises the concept of an Artificial Neural Network with Back Propagation of Errors to explore a novel architecture that can be used for regression tasks where the training data has a non-uniform variance. This custom architecture utilises the advancements in GPU-based machine learning workflows. Further information on the detailed methods is provided in the respective Methods section of each chapter.

1.6.2 GIS methods and multi-core processing

Global energy systems rely heavily on the geospatial characteristics of energy demand and supply. Current IAMs and ESMs that contribute to contemporary climate change research and energy policy analysis often demarcate their outputs based on a geographical boundary which can range from a city-level demarcation to regional aggregations like Africa, Europe etc. It is thus expected that any methodological advancement that can be accrued to machine learning and big data-based frameworks needs to incorporate the essence of GIS workflows. Chapters 2, 3, and Annex of this thesis rely on various GIS methods and techniques that enable the transformation and aggregation of independent and dependent variables.

In Chapters 2 and 3, GIS workflows like the clip, intersect, merge, buffer, zonal statistics etc. are utilised to convert big data derived building footprint, road, population and landcover data layers into Fishnet Grid tile structures. This splitting and aggregation of geospatial data layers via GIS methods aid in conversion of geospatial data into the numerical domain that can be used as training data for model development. In this thesis, extensive GIS workflows were executed on

ESRI's ArcGIS Pro software¹ and Google Earth Engine². Vector databases used in this thesis were primarily processed on ArcGIS Pro, whereas Raster datasets were processed on Google Earth Engine. Harmonisation across datasets was achieved by converting all dataset layers to a common Projected Coordinate System. Further details of the GIS methods that enable this thesis outcome are documented in the respective chapter's Methods section. A visual representation of the GIS methods used in this thesis is shown in Figure 1.9.

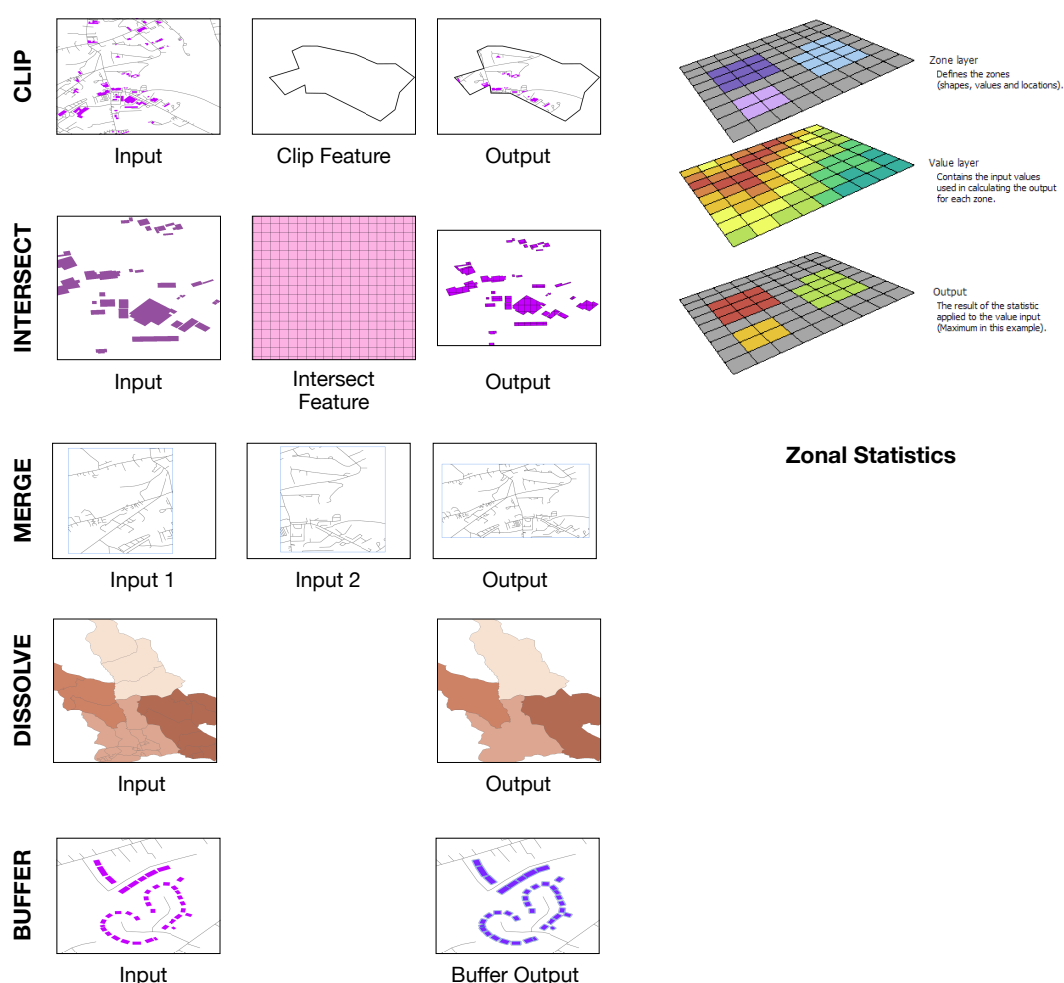


Figure 1.9 | A visual representation of GIS methods.

Source: Zonal Statistics reproduced from ArcGIS Pro online documentation. (<https://pro.arcgis.com/en/pro-app/latest/tool-reference/main/arcgis-pro-tool-reference.html>)

¹ (2022). ArcGIS Pro (Version 2.8). Esri Inc. <https://www.esri.com/en-us/arcgis/products/arcgis-pro/overview>.

² <https://earthengine.google.com/platform/>

One of the key methodological frameworks used in this thesis is the application of multi-core processing codes during various stages of the research. In Chapter 2, 3 extensive custom code is implemented to execute multi-core processing for 1) executing GIS workflows and 2) analysis and processing of data for model training. Chapter 4 implements a novel machine learning architecture based on utilising dual GPU hardware that shares the model training load between each other, thereby enabling the loading of large data into shared GPU memory space. In modern researchers' toolkits, CPU and GPU with multi-cores are becoming more common. This additional hardware resource is often left unused, leading to an increased research timeframe. The implementation of multi-core processing aids in reducing the time required for conducting research and in some cases makes the analysis computationally feasible within a reasonable timeframe. The details of the implementation of multi-core processing workflows and their application in this thesis are covered in the respective chapters, especially in Chapter 3. Along with Pseudocodes, the details in the methods section will aid in improving the reproducibility, transferability and transparency of the methods used in this thesis.

1.6.3 Integrated Assessment Modelling and scenario analysis

The role that an energy system will play in future depends on how the energy demand and supply will evolve within the constraints of just transition, sustainable development and climate change. To enable the policymakers, industries and citizens, insights pertaining to the future energy systems are derived from a combination of Integrated Assessment Modelling and scenario analysis. Integrated Assessment Modelling captures the effect of energy systems on emissions, land use, changing socioeconomic factors etc. and vice-versa. The IAMs often utilise the least cost optimisation linear programming within exogenous constraints methodology to find an optimum energy system state. The constraints here are commonly the emissions and global warming temperature thresholds. To conduct this analysis, scenarios are designed to understand the

different possible energy system states to achieve specific climate change mitigation or energy policy goals.

In this thesis, Chapter 2 incorporates the method of quantitate and qualitative analysis to document the global high-resolution spatiotemporal assessment of rooftop solar PV's technical potential in 2015. Chapter 3 builds upon the learnings of Chapter 2 and further documents the global growth of high-resolution spatiotemporal assessment of rooftop solar PV's technical potential between 2020-2050. The results of the future global growth in rooftop solar PV technical potential are analysed for its economic and climate change mitigation potential using global 11 region MESSAGEix-GLOBIOM IAM. Further scenario analysis is conducted to simulate current policy and climate policy goals within the IAM. Being built upon open-source training datasets and codes, the datasets generated in Chapters 2 and 3 have been made open source with a structure that enables its use across different IAMs and supports the adoption of machine learning frameworks to aid global energy systems. This thesis also documents pseudocode in Appendix B for easy replication of the methods used here.

1.7 Thesis outputs

1.7.1 Peer reviewed journal papers

- ❖ **Joshi, S.**, Mittal, S., Holloway, P., Shukla, P.R., Gallachoir, B.O., Glynn, J., "*High resolution global spatiotemporal assessment of rooftop solar PV's potential for renewable electricity generation*", Nature Communications (2021), <https://doi.org/10.1038/s41467-021-25720-2>

- ❖ **Joshi, S.**, Zakeri, B., Mittal, S., Mastrucci, A., Holloway, P., Krey, V., Shukla, P.R., Gallachoir, B.O., Glynn, J., "*Assessing the growing role of decentralised rooftop solar photovoltaics in the global energy transitions*" (Submitted at Scientific Data)

- ❖ **Joshi, S.**, Gallachoir, B.O., Glynn, J., "A nature-inspired deep learning framework to improve transport energy service demand estimates for future shared socioeconomic pathways", Scientific Reports (2023), <https://doi.org/10.1038/s41598-023-30555-6>

1.7.2 Conferences and invited talks

- ❖ **Joshi, S.**, *Energy Service Demands projections in the transport sector for SSPs.* IEA ETSAP Workshop, Paris, France. *June 2019*

- ❖ **Joshi, S.**, Application of Custom Neural Networks in Transport Sectors Energy Service Demand Estimation for SSPs. 12th Integrated Assessment Modelling Consortium (IAMC), Tsukuba, Japan. *December 2019.*

- ❖ **Joshi, S.**, Estimation of global Rooftop Solar PV potentials for medium-term growth envisioned in SSPs. International Institute for Applied Systems Analysis (IIASA) Young Scientist Summer Program (YSSP) colloquium. IIASA, Austria. *August 2021.*

- ❖ **Joshi, S.**, Role of Rooftop Solar PV in global energy transitions. 14th Integrated Assessment Modelling Consortium (IAMC). *December 2021*.
- ❖ **Joshi, S.**, The role of Rooftop Solar PV in global energy transitions. MESSAGEix Community Meeting. IIASA, Austria. *May 2021*.
- ❖ **Joshi, S.**, Assessing growing role of decentralised rooftop solar photovoltaics in global energy transition. 40th International Energy Workshop (IEW), Freiburg, Germany. *May 2021*.
- ❖ **Joshi, S.**, Global potential of solar rooftops. Sustainability Seminar Series, Ahmedabad University, India. *June 2021*.

1.7.3 Posters

- ❖ **Joshi, S.**, High resolution assessment of global rooftop solar PV's technical and economic potential using big data and machine learning. MaREI Symposium, Ireland (Video Poster). *November 2020*.
- ❖ **Joshi, S.**, High resolution assessment of global rooftop solar PV's technical and economic potential using big data and machine learning. 13th IAMC (Virtual Poster). *December 2020*.
- ❖ **Joshi, S.**, Application of Custom Neural Networks in Transport Sectors Energy Service Demand Estimation for SSPs. MaREI Symposium, Ireland. *November 2019*.

1.7.4 Awards

- ❖ **Joshi, S.**, ICF DGCLIMA Travel Grant. European Commission. *December 2019*.
- ❖ **Joshi, S.**, Best Poster Award. MAREI Symposium. *November 2020*.

- ❖ **Joshi, S.**, Best Poster Award. 13th Integrated Assessment Modelling Consortium (IAMC), *December 2020*.
- ❖ **Joshi, S.**, Mikhalevich Award for outstanding research during Young Scientist Summer Program (YSSP). International Institute of Applied Systems Analysis (IIASA). *January 2022*.
- ❖ **Joshi, S.**, Best student publication from the School of Engineering and Architecture for 2021. University College Cork, Ireland. *May 2022*.
- ❖ **Joshi, S.**, Individual Ph.D Student in Research Excellence Award, MAREI Symposium. *May 2022*.

1.7.5 Reports

- ❖ **Joshi, S.**, Role of Rooftop Solar Photovoltaics in Global Energy Transitions. IIASA YSSP Report. Laxenburg, Austria. *September 2021*. <https://pure.iiasa.ac.at/id/eprint/17497/>
- ❖ **Joshi, S. and Deane, P.**, Quantifying the potential for rooftop solar photovoltaic in Ireland. MAREI. Irish Solar Energy Association. *June 2022*. <https://www.marei.ie/solar-panels-could-power-quarter-of-irish-households/>

1.8 Role of collaborators

This thesis is documentation of the original work undertaken by me. Although the ideas and execution of the research questions were conducted by me, in essence this work would not have been as enriching without the collaborations with experts in the field of geography, energy policy and energy systems modelling from various universities and research groups. In this section, I have documented the role of collaborators in this thesis and credited others who have strengthened it.

Chapter 2 is based on an article submitted to a peer-reviewed journal of which I am the lead author. I wrote this chapter in its entirety while Professor Brian Ó Gallachóir and Dr James Glynn provided guidance and reviewed drafts.

Chapter 3 is based on a published peer-reviewed journal paper for which I am the lead author. I designed and developed the framework and model along with the codes. I along with Dr Shivika Mittal and Dr Paul Holloway designed the GIS and data analysis frameworks. I created the figures and wrote the manuscript. Prof Priyadarshi Ramprasad Shukla, Prof. Ó Gallachóir and Dr James Glynn provided valuable insights on the results and reviewed drafts.

Chapter 4 is based on an article submitted to a peer-reviewed journal of which I am the lead author. I designed and developed the framework and model along with the codes. I along with Dr Shivika Mittal, Dr Paul Holloway, Dr Behnam Zakeri and Dr Alessio Mastrucci designed the GIS and data analysis frameworks. I and Dr Behnam Zakeri developed the MESSAGEix-GLOBIOM implementation. Dr Shivika Mittal and Dr Behnam Zakeri supported the model analysis. I created the figures and wrote the manuscript. Prof Priyadarshi Ramprasad Shukla, Prof. Ó Gallachóir, Dr Volker Krey and Dr James Glynn provided valuable insights on the results and reviewed drafts. All authors discussed the results and contributed to the manuscript.

Annex is based on the direct outputs of Chapters 2 and 3. I am the lead author of the report. I along with Dr Paul Deane conducted the data analysis, scenario design and visual outputs. Dr Paul Deane drafted the report and conducted the scenario analysis. We received feedback from Mr Conall Bolger of the Irish Solar Energy Association during all phases of report design and publication.

Chapter 2: High resolution global spatiotemporal assessment of rooftop solar photovoltaics potential for renewable electricity generation

Joshi, S., Mittal, S., Holloway, P., Shukla, P.R., Gallachoir, B.O., Glynn, J., “High resolution global spatiotemporal assessment of rooftop solar PV’s potential for renewable electricity generation”, Nature Communications (2021), <https://doi.org/10.1038/s41467-021-25720-2>

2.1 Abstract

Rooftop solar photovoltaics currently account for 40% of the global solar photovoltaics installed capacity and one-fourth of the total renewable capacity additions in 2018. Yet, only limited information is available on its global potential and associated costs at a high spatiotemporal resolution. Here, we present a high-resolution global assessment of rooftop solar photovoltaics potential using big data, machine learning and geospatial analysis. We analyse 130 million km² of global land surface area to demarcate 0.2 million km² of rooftop area, which together represent 27 PWh yr⁻¹ of electricity generation potential for costs between 40-280 \$ MWh⁻¹. Out of this, 10 PWh yr⁻¹ can be realised below 100 \$ MWh⁻¹. The global potential is predominantly spread between Asia (47%), North America (20%) and Europe (13%). The cost of attaining the potential is lowest in India (66 \$ MWh⁻¹) and China (68 \$ MWh⁻¹), with USA (238 \$ MWh⁻¹) and UK (251 \$ MWh⁻¹) representing some of the costliest countries.

2.2 Introduction

Since powering the National Aeronautics and Space Administration (NASA's) Vanguard satellites in 1958 to lighting homes in sub-Saharan Africa, solar photovoltaics (PV) technology has come a long way. Rooftop Solar photovoltaics (RTSPV) technology as a subset of the solar photovoltaics electricity generation portfolio can be deployed as a decentralised system either by individual homeowners or by the large industrial and commercial complexes. Over the past decade, reduction in the deployment cost coupled with policy driven initiatives has led to a rapid uptake of RTSPV globally. Between 2006 and 2018, the installed capacity of the RTSPV has grown from 2.5 GW to 213 GW - an 85-fold increase globally^[69]. With an additional capacity installation of 41 GW, RTSPV currently account for 40% of global cumulative installed capacity of the solar PV and nearly one-fourth of the total renewable capacity additions in 2018 - surpassing the combined new installed capacities of both coal and nuclear. At the same time, RTSPV technology has demonstrated a steep decline in its deployment costs which ranged between 63-265 \$ MWh⁻¹ in the year 2019 – a reduction of between 42-79% over 2010 values^[70].

Globally, nearly 800 million people were without electricity in 2018, the majority of who are living in the rural areas^[71]. Here, the role of decentralised rooftop PV in advancing the ethos of the Sustainable Development Goals (SDG) 7 becomes very important. The fast installation time and low levelised cost of RTSPV can aid in mitigating the problem of energy access by making citizens or communities a prosumer. The prosumer can generate and consume electricity as per their requirements without depending exclusively on a centralised grid infrastructure. As the fastest deployable energy generation technology with the highest year on year growth rate^[72], solar PV technology is projected to supply 25-49 % of the global electricity needs by 2050 while providing employment for up to 15 million

people between 2018 and 2050^[73]. Out of this, RTSPV deployment will contribute up to 40% of the total solar PV derived electricity generation by 2050.

Increased deployment of RTSPV can support in displacing fossil fuels out of the current energy generation mix as can be observed in the successful implementation of rooftop photovoltaics in Germany. As the demand for electricity as an energy source increases in the future, RTSPV based generation sources will form a large part of the future renewable based generation portfolio. This shift in current generation mix coupled with the future low carbon generation capacity expansion can aid in reducing the energy derived greenhouse gas emissions and also aid in advancing the SDG13 goal of combating climate change with co-benefits for the SDG3. RTSPV technology can thus lead to consumer driven breakthrough in tackling climate change, reducing local air pollution, accelerating development and in providing affordable energy access to the areas lacking electrification.

To better understand the role that a RTSPV system can fulfil in the future, a global harmonised geo-mapped assessment of its technical potential and the costs associated with attaining the technical potential is pertinent especially when such assessments at a global level are lacking. RTSPV systems are deployed as a decentralised system contrary to the utility scale solar PV systems, which increases the complexity of its assessment as the smallest unit of deployment becomes a rooftop as opposed to a large plot of a green or brownfield site. Along with the complexities associated with accurately determining the rooftop area, assessment of seasonal variations of its potential is also important to understand the supply dynamics of variable renewable energy (VRE) technologies like RTSPV. This highlights the need for a high-resolution spatiotemporal assessment that accurately represent the geographical variability of the built environment along with impacts of seasonal changes in solar insolation.

Current research primarily focusses on utility scale solar PV resource assessment at a global scale. Similar assessment has not been done for decentralised RTSPV at a scale greater than regional/national levels^[19, 74-76]. As a result, energy system models and research informing climate change policy have not fully considered the role of solar PV in meeting the climate change mitigation goals^[59]. Assessment of RTSPV potential requires an underlying dataset of building footprints, solar insolation mapping, and technology specific information like panel size, conversion efficiency, and system losses. The current literature is adequate in providing global information on latter two categories, with the largest inaccuracies^[77] attributed to the demarcation and calculation of building footprints which require large data and costly information processing hardware to extract buildings from satellite imagery^[61].

Two major approaches are currently used to determine built-up area, or more specifically the extent and area occupied by building rooftops, Supplementary Table A.7. The first approach addresses the problem from a “Bottom-Up”^[78-88] perspective and is the most common approach currently implemented to calculate rooftop area at scale. Such approaches establish the relationship between building footprint data (cadastral, crowd sourced, satellite derived) and socio-economic metrics (Gross Domestic Product (GDP), Population) for a small sample set and then estimate the extent of building footprints across a wider scale. In the study by Jacobson et al.^[89], the authors have used the bottom up methodology to calculate available rooftop area for 179 countries by establishing relationship between population, GDP and floorspace area per capita based on sample data from USA and several European countries. For a full set of global countries, Gernaat et al.^[60] have used the relationship between population density, household expenditure and rooftop area to calculate available rooftop area per country. They have calibrated their relationship equations on World Bank’s data and realised a $R^2=0.66$. These methods are quick to implement and are relatively

accurate when predicting building footprint area in the neighbourhood regions, but inaccuracies arise when the analysis is upscaled towards country/regional levels. This reduction in accuracy^[90] can be attributed to the inaccuracies in coarse geospatial mapping of socioeconomic data^[91] and the heterogeneity of built-up landscape.

The second approach addresses the problem from a “Top-Down”^[92-103] perspective, utilising aerial imagery to determine built-up area along with building footprints contained in it. “Top-Down” methods include earth observation, drone mounted Light Detection and Ranging (LiDAR), and machine learning (ML) classification algorithms to detect buildings. On a country wide scale, Gagnon et al.^[11] have used LiDAR datasets for 128 US sample cities to calculate available rooftop area for the continental USA using statistical inferencing to extrapolate beyond their sample site. They have generated statistical measures to generalise rooftop orientation, slope and availability based on high resolution LiDAR imagery. Collecting, processing and analysing the aerial imagery is a costly and computationally intensive task requiring data-centre scale infrastructure. These shortcomings have led to limitations in the scale of studies using top down methods, where only a few commercial^[104-106] ventures have been able to provide country wide building footprints, and to date a global scale analysis has yet to be implemented. One solution to mitigate the processing and data bottleneck is to use predefined land cover classification^[47, 107-112] to demarcate global land areas which are artificially built-up and then downscale the built-up area to actual building footprint^[112] using simplifying assumptions. This hybrid approach was used in a study by Bodis et al.^[76], where they have established relationship between cadastral data of Netherlands, CORINE landcover and European Settlement Map to infer the rooftop area in other 27 EU countries.

The current state of art^[113-118] methods utilise ML based object detection algorithms to map individual buildings for Region of Interest (ROI) at city/country

level. However, none of the state of art methods have been applied to a global ROI assessment partly due to the amount of data processing required in ML based methods and partly due to the limitations of the ML algorithm in detecting similar objects that deviate from training sample sets.

Here, we directly address the gap in the current literature by developing a hybrid framework that integrates “Top-down” and “Bottom-up” methods using a ML model to provide a high-resolution global assessment of rooftop solar PV technical potential at a monthly temporal resolution (Figure 2.1). We divide the entire global landmass into multiple 10km² assessment units. In each assessment unit, we utilise a high-resolution population dataset (at 100m spatial resolution), road length and built-up area boundaries to estimate the rooftop area. The estimation algorithm built upon ML model is designed to learn the relationship between population, road length and built-up area boundaries and actual rooftop area from a large global sample set covering countries in various stages of socio-economic development and built-up topography. This way we utilise a comprehensive set of disparate built environment archetypes involving variable population densities in different landscape configurations to overcome the limitations imposed by the “Top-down” and “Bottom-up” methods used in previous studies. Along with the geo-mapping of the technical potential, we also map the associated Levelised Cost of Energy (LCOE) and regional supply cost curves for a global ROI covering >195 countries, spanning 130 million km² land area, containing buildings ranging from detached rural nucleated settlements to global conurbation dotted by multi-storied skyscrapers across varied geographies.

In our study, we define the “technical potential” of RTSPV as the maximum electricity generation that can be derived from a given rooftop area, where the rooftop area is kept consistent with 2015 year’s built-up extent and does not include additional building stock created after that. The results presented in this

study have considered a 100% rooftop availability at a 10% panel efficiency. To account for change in the potential due to different panel efficiencies and rooftop availability, we have documented global and regional potentials for a set of rooftop scaling factors and panel efficiencies (Supplementary Tables A.4, A.5). Additional boundary conditions of our study and the limitations in interpretation of the main results are documented in Methods Section.

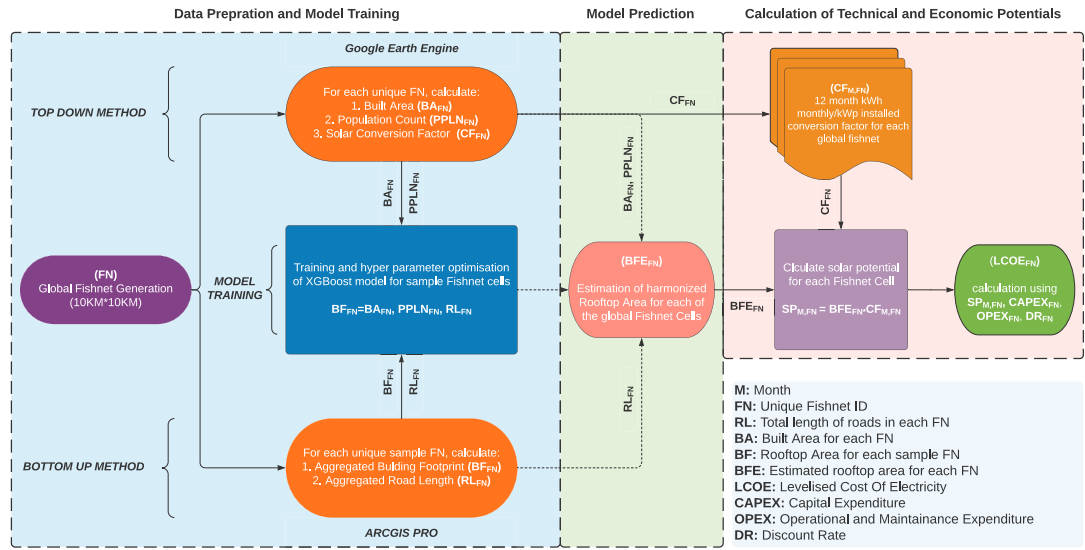


Figure 2.1 | Framework for assessment of RTSPV's global technical potential and costs

The framework developed in this study starts with data preparation and mapping of various geospatial metrics to both Top-down and Bottom-up pathways. Further, the machine learning model is trained and used to estimate BFE_{FN} values from BA_{FN} , $PPLN_{FN}$, and RL_{FN} values. Next, the BFE_{FN} values are used to calculate the technical potential (SP) with the aid of the conversion factors (CF). Finally, the calculated potential dataset is used to map the Levelised Cost of Electricity (LCOE) values using IRENA's renewable power generation cost data. The detailed framework is described in the "Results" and "Methods" sections. Model parameters and regional mappings are provided in Supplementary Tables A.6, A.8–10 and Supplementary Figure A.3a–d.

2.3 Results

2.3.1 Model design and validation

We started by dividing the global landmass into a Fishnet Grid (FN) containing a total of 3,521,120 unique squares of 10 km² size, where each FN has a unique id and is attributed to a unique country. Aggregation of the built area (BA_{FN}) within each FN was undertaken using built area sub classifications (100 m resolution) provided by the global landcover layer^[110] (LC) of Copernicus land monitoring

program. Being derived from a native 10 m resolution satellite imagery, the LC layer provided us with a significantly improved representation of built-up area over the current state of art methods that utilise coarser resolution landcover classification. The use of pre-built landcover classifications also aided in reducing the information processing overheads related to manually classifying petabytes of satellite imagery.

It is important to highlight that the BA_{FN} layer aggregations contain buildings along with roads, green area boundaries, footpaths, parking lots, etc. These additional built-up structures are not relevant to the current analysis and can occupy significant BA_{FN} area in a low-density built environment. Methodological uncertainties can also arise due to the heterogeneity of impervious landscapes and due to misclassification caused by similar spectral signature of other built structures on the ground, but at a global ROI, these errors form a very small percentage of the ground truth. This underscores the need to downscale the BA_{FN} layer globally to accurately represent a harmonised rooftop area.

To downscale the BA_{FN} layer, we started by generating a subset of global FN containing actual building footprint^[104, 106] (BF_{FN}), road length^[119] (RL_{FN}) and population count^[120] ($PPLN_{FN}$). For calculating building footprints (derived from Microsoft AI, Ecopia AI and Open Street Map-OSM datasets), we aggregated individual building footprints based on FN cells overlapping the individual buildings to generate a single building footprint area value per FN (Figure 2.2). In total, 37,115 km² of building footprint area and 11.4 million km² of total land area was covered by our samples FNs, accounting for >300 million individual buildings ranging from small outdoor sheds to mega factories. The building samples also provided us with a diverse set of building types in different geographies spanning a wide spectrum of socio-economic stages of development. These global sample

sets (Figure 2.3a, Supplementary Table A.1) are a marked improvement over the previous literature, where a narrow sampling strategy often at a city/country level is undertaken. Using heterogeneous global building samples enables the overall analysis to be more resistant to generalisation error which are introduced due to over reliance on a small set of similar built-up landscapes.

OSM provides a highly accurate open source global roads infrastructure dataset^[121], which we used for mapping road length (RL_{FN}). Our sample dataset showed a Pearson Correlation of 0.95 (Figure 2.4 a,b,c) between building footprint sample and road length sample. It can be observed that in the real world, development of roads is often associated with increasing population size and with increasing building stock. Road length has not been used in any previous studies and will increase the accuracy of downscaling over previous methods. In total, we processed >16 million km of roads for our sample FNs (Figure 2.3b).

For our population count aggregation, we utilised WorldPop's high resolution gridded population count. The high-resolution population dataset coupled with a high resolution BA_{FN} layer enabled us to accurately map the population count for each of our sample FN. Previous studies at country/regional scale have used coarse resolution (≥ 1 km resolution) population count which can lead to inaccuracies in downscaling due to over counting of population in a given FN. Aggregation and processing of big data like geospatial building and road datasets require a very high computation time and significant cost in hardware. To overcome this challenge, we used Google Earth Engine's (GEE) cloud computing platform to perform planetary scale analysis, where the datasets were split into smaller raster files based on each FN's geographical extent and finally aggregated to represent a single value (see methods section). It should be noted that GEE platform is lacking in processing of vector data like building and road polygons,

for which we utilised multi-core processing enabled by ArcGIS PRO desktop software.

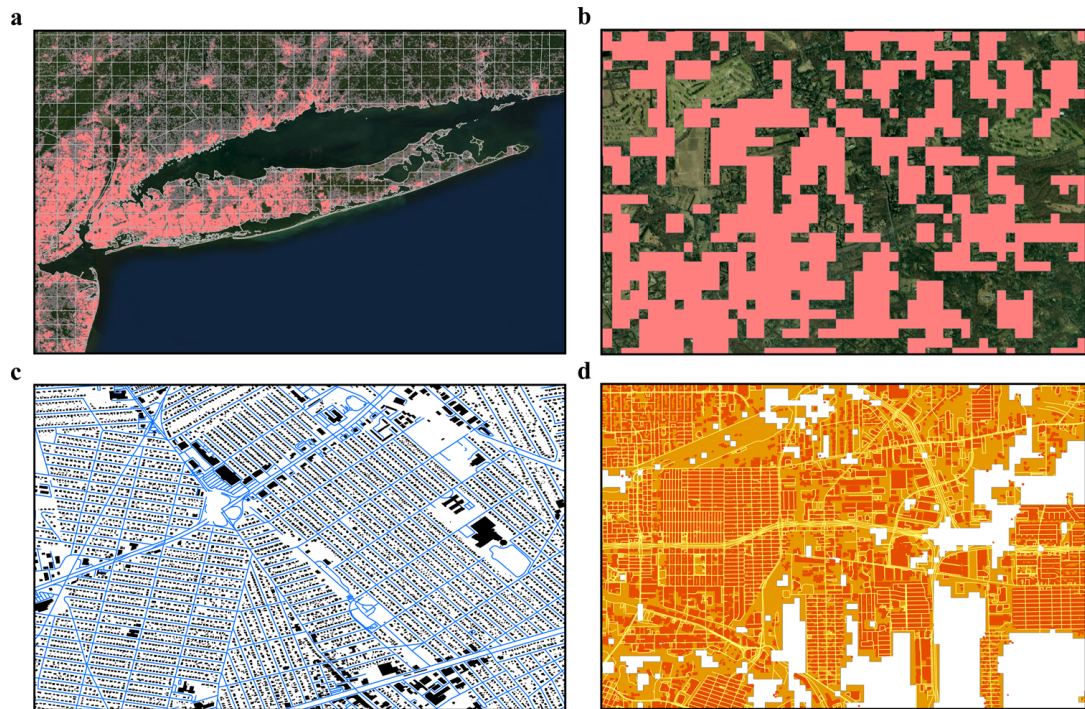


Figure 2.2 | Visual representation of a sample FN involved in Bottom-up methods

a The image is depicting an area over New York, USA. The gridlines are the geographical boundaries of Fishnet cells (FN), with each cell size of 10 km². The red area inside each FN is the built area (BA_{FN}). **b** The green areas in the image are the non-built-up geography in the year 2015, with red areas representing BA_{FN} as 100 m² blocks. Each block has a value of 0–100% based on the percent of built-up area in a block. **c** The black polygons are the building footprints (BF_{FN}) derived from big data sources, inside a sample FN. The blue lines are the roads (RL_{FN}) inside the sample FN, with white areas representing empty spaces that are not used in our analysis. **d** The image represents the four main categories of objects present inside each sample FN. The orange areas are the BA_{FN} blocks, with red areas representing the actual buildings, yellow lines representing roads, and white areas are the areas not considered in our study. Data Credits: Copernicus GLC Landcover, Microsoft Building Footprints, and Open Street Maps.

This combination of GEE for raster data (PPLN_{FN}, BA_{FN}) and ArcGIS PRO for vector data enabled us to process our datasets at a fraction of the time and cost. To our knowledge, this is the first attempt at merging two fundamentally different service platforms to assess global potentials, which could be useful for other planetary scale resource assessments. Links to the input datasets and their validation reports are documented in Supplementary Table A.2.

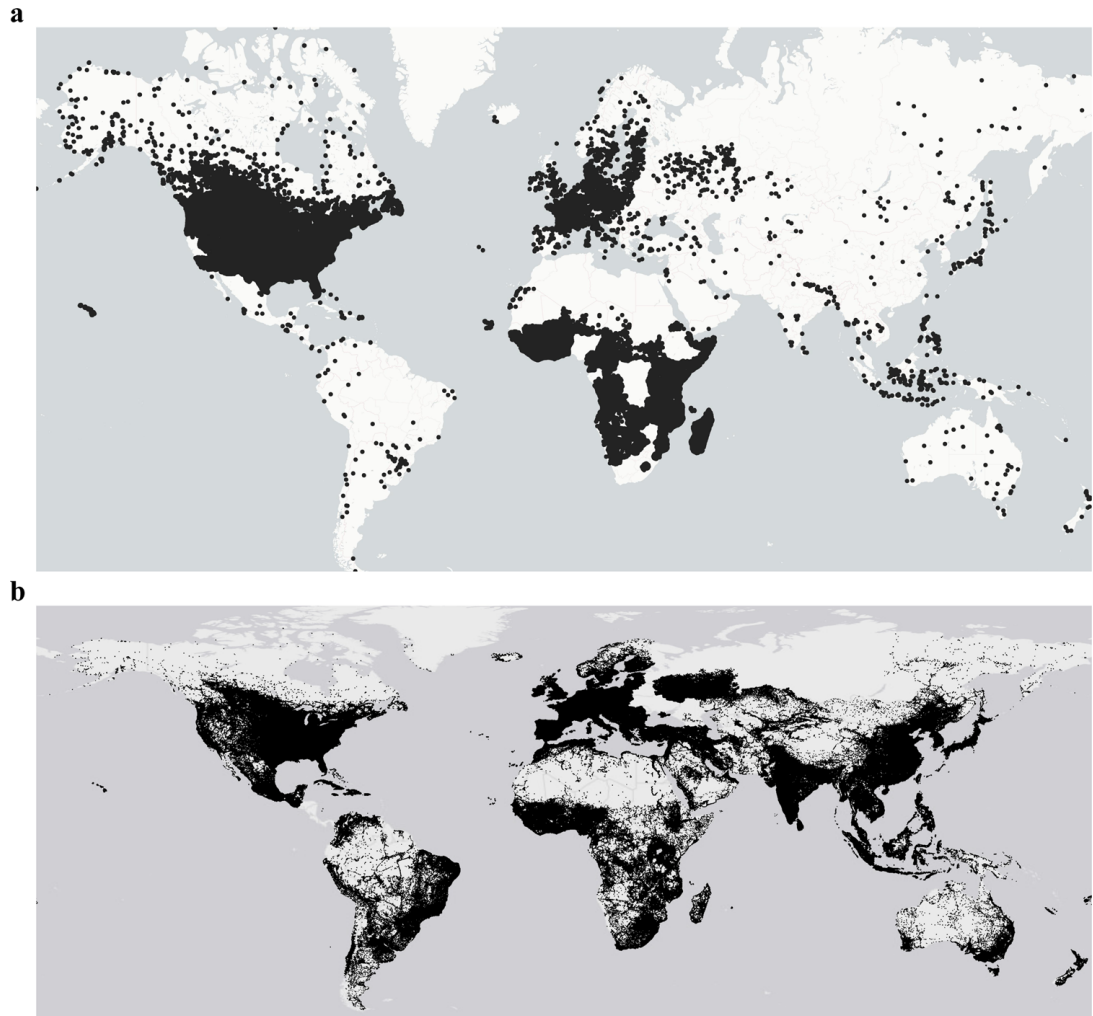


Figure 2.3 | Geographical distribution of global roads and sample Fishnet cells

a Global distribution of sample FN was generated in our study. Microsoft AI- based building polygons are used for the USA, Canada, and Tanzania, Ecopia AI-derived building footprint areas are used for the African countries. OSM- derived building polygons representing a total of 4000 sample FNs are used for the rest of the world. **b** Geographic location of all the global roads used in our analysis. OSM-derived global roads have near-global coverage, with each pixel on the map being for each road feature inside the country of reference. Data Credits: Figure 2.3, © OpenStreetMap contributors.

Next, we linked the aggregated BA_{FN} , $PPLN_{FN}$ datasets from Top-down methods and processed BF_{FN} , RL_{FN} datasets from Bottom-up method using a ML model that takes BA_{FN} , $PPLN_{FN}$, RL_{FN} datasets as independent variables and BF_{FN} as dependent variable. The ML model trains from the relationship between the independent and dependent variables for our sample FNs and estimates the aggregated building rooftop area for the rest of the non-sample FNs, effectively

downscaling BA_{FN} layer to an estimated area occupied by building rooftops (BFE_{FN}). For data gaps in $PPLN_{FN}$, RL_{FN} layer, we used an iterative imputing method to interpolate missing values in the dataset using multiple regression runs.

In our tests, the ML model built upon XGboost algorithm provided better accuracy (R^2 value) and better overall error reduction (considerably lower mean absolute error) in prediction of sample data as compared to multivariate regression (Supplementary Table A.3). To reduce overfitting of the ML model, a 10-fold cross validation strategy was used for tuning hyperparameters to generate best model (see Methods section). The ML model performed well (Figure 2.4 d,e) with $\pm 4 \text{ km}^2$ error in predicting total building footprint per 100 km^2 FN, with majority of errors lying between $\pm 0.25 \text{ km}^2$. Also, for a total of $37,000 \text{ km}^2$ of absolute building footprint area across our samples, a total of 4 km^2 of absolute error was recorded. On a regional level, slight left skewness/systematic underestimation of rooftop area was observed for the Asian Region (Supplementary Figure A.1). At the end of the downscaling step, a dataset containing 3,521,120 FN cells is generated, with each cell containing aggregated building rooftop area (BFE_{FN}).

Rooftop area to solar potential conversion was undertaken by using World Bank's conversion factor^[122] (CF_{FN}) for locations between 60^0N and 45^0S , covering over 99% of the world's population. The CF_{FN} layer is provided as a gridded raster dataset representing kWh produced by each kWp installed capacity per day. The locations outside the latitudes were assigned a constant CF value of 3.5 kWh/kWp/day (peak). Next, CF_{FN} values for each of the twelve months were used to generate monthly solar potential per FN ($SP_{FN,M}$). Further we aggregated monthly technical potentials to yearly technical potentials for each of the countries to generate a global RTSPV potential map, as shown in Figure 2.5. To represent the

costs associated with the technical potential, we used LCOE metric (see Methods). The capital expenditure (CAPEX) values range between 840-3,874 \$ kW⁻¹ of installed capacity for 17 countries in total, with rest of the world being allocated averages for the continent they are in. The operation and maintenance cost (OPEX) and discount rates (DR) were based on whether the country is OECD or Non-OECD. For each FN, LCOE costs were calculated based off CAPEX, OPEX, SP, and DR with a project lifetime of 25 years. Our technology cost data are based on IRENA² residential solar PV costs for 2019.

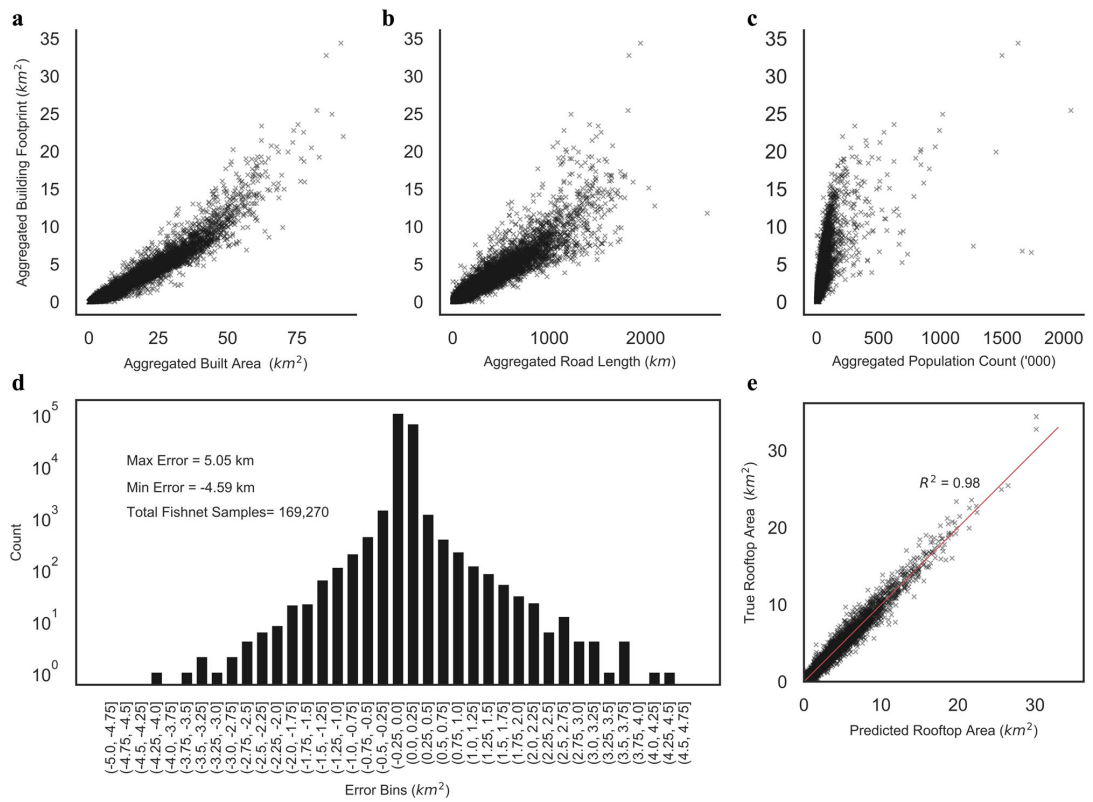


Figure 2.4 | Relationship between inputs, distribution of errors, and prediction accuracy of the downscaling model

The distribution of BA_{FN} (Built Area) **(a)**, RL_{FN} (Road Length) **(b)**, and PPLN_{FN} (Population) **(c)** in relation to the BF_{FN} (Building Footprint). The distributions have a Pearson Correlation of 0.97, 0.95, 0.72, respectively. The distribution of errors in prediction **(d)** has a bell shape when using the trained model to predict the sample dataset. Each bar is the count of FN that is in each error bin. The majority of errors lie in the -0.25 to $+0.25$ km² per FN range, with peak error capping at ± 5 km² per FN. The downscaling model built upon the machine learning model has shown adequate accuracy in prediction **(e)** with an $R^2 = 0.98$. Each cross represents the predicted value of each sample FN. The density of points is higher for low values as the majority of sample FN will have smaller built-up areas contained in them, with very few covering major cities due to the size of the FN used in this study.

2.3.2 Global technical potential and cost assessment

Our assessment shows a total global technical potential of 27 PWh yr⁻¹, of which Asia (13PWh yr⁻¹), North America (5.5 PWh yr⁻¹) and Europe (3.6 PWh yr⁻¹) represent a majority of the potential followed by Africa (2.9 PWh yr⁻¹) and South America (1.7 PWh yr⁻¹). The hotspots for the potential are concentrated in and around the densely populated nucleated settlements globally (Figure 2.5a). Nearly 20% (5 PWh yr⁻¹) of the global potential is located within the areas with a high population density (>1500 people/km²), with 55% (15 PWh yr⁻¹) of the potential being dispersed within the low-density areas (< 500 people/km²). Amongst the countries, China (4.3 PWh yr⁻¹), USA (4.2 PWh yr⁻¹), and India (1.7 PWh yr⁻¹) have the highest yearly potential (Table 2.1). A $\pm 1\%$ deviation can be observed in the yearly global potential due to the aggregation methodology of the CF factor (Supplementary Figure A.2).

Although the African region has a good solar insolation endowment, the RTSPV potential is assessed at being the third lowest due to low building stock. Amongst the African Region, the largest potential is concentrated in the West African region followed by the North African Region. The combined West and North African regions have more potential than India, highlighting the importance that low cost RTSPV can play in future energy systems. Future population growth and corresponding increase in the building stock may increase the overall RTSPV potential for Africa. Both North American and European regions have similar assessed rooftop areas (~30,000 km²), yet North America has nearly 1.5 times the potential of Europe due to higher solar insolation during the year especially during the winter months.

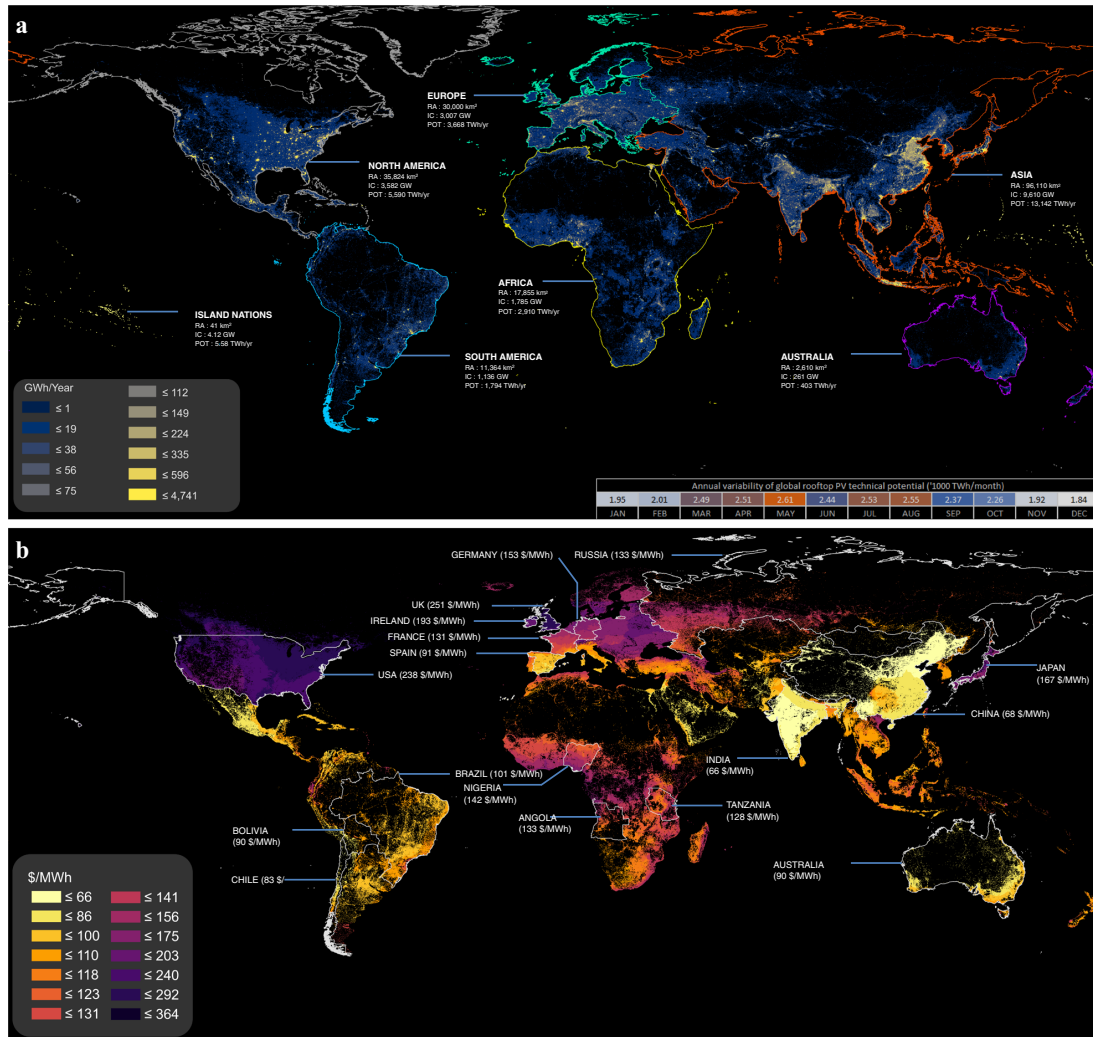


Figure 2.5 | Global Distribution of RTSPV technical potential and LCOE values

a The geographical distribution of global RTSPV technical potential generated in our study. Major world regions are highlighted in the image and data is provided for the total estimated rooftop area (RA), installed capacity (IC), and potential generation (POT) for each region. The global landmass is color-coded into 11 RTSPV potential bins. Seasonal variation in aggregated global potential is highlighted in the bottom right. **b** The geographical distribution of LCOE values generated in our study across the globe with major countries highlighted in each world region. Each highlighted country has a corresponding aggregated LCOE value for the whole country. The LCOE values are color-coded into 14 cost bins. Map boundary data from the Database of Global Administrative Areas (GADM: <https://gadm.org>).

Table 2.1 | 32 Region global distribution of rooftop area and technical solar potentials.

32 World Regions ^a	Land Area (‘1000 km ²)	BA _{FN} (km ²)	BFE _{FN} (km ²)	Potential (TWh/yr) ^b
AFE (Africa East)	4,355	6,921	1,246	214
AFN (Africa North)	5,485	18,631	3,398	592
AFS (Africa South)	5,537	18,132	2,443	413
AFW (Africa West)	13,130	59,604	8,613	1,317
ANZ (Australia and NZ)	7,971	15,581	2,610	404
ARG	2,780	9,330	1,749	285
ASC (Asia Central)	6,622	36,053	4,981	748
ASE (Asia South East)	2,334	62,144	9,568	1,354
ASO (Asia Other)	354	13,121	2,117	304
ASR (Rest of Asia)	1,642	8,942	1,561	219
BRA	8,533	31,962	6,386	997
CAN	9,904	13,851	2,394	327
CHN	9,380	273,585	35,156	4,375
ENE (Non-EU East)	1,035	34,634	4,111	499
ENW (Non-EU West)	466	4,199	630	75
EUE (Europe East)	1,138	47,700	5,457	648
EUW (Europe West)	2,984	134,286	17,467	2,210
GBR	244	15,798	2,400	238
IDN	1,899	35,710	6,163	878
IND	3,160	78,971	11,731	1,815
IRN	1,623	12,437	2,004	341
JPN	372	41,533	7,942	1,044
KOR	100	8,758	1,439	201
LAM (Latin America)	7,231	27,268	5,028	805
MEA (Middle East)	1,619	15,742	2,628	462
MEX	1,956	20,502	4,037	720
ROW (Rest of the world)	2,426	1,302	212	35
RUS	16,832	58,175	8,038	941
SAU	1,920	6,333	918	169
TUR	780	13,526	1,716	265
USA	9,457	160,479	27,585	4,247
ZAF	1,221	11,954	2,150	374
TOTAL	134,491	1,297,163	193,875	27,512

^a ISO alpha-3 codes are the region names for individual countries, group of countries as a region have names described in parenthesis.

^b Considering 100% rooftop availability at 10% panel efficiency.

Along with spatial variability due to on-ground building distributions, seasonal variability of the RTSPV potential is also observed due to the variation in intra annual solar insolation. The seasonal variability of the monthly global potential is between 1.84 and 2.61 PWh, with December and January representing the months with the lowest global potential (Figure 2.5a). Globally the highest seasonal variability of the potentials is observed above the 45 degree North latitude covering Europe, Russia, USA and Canada. Within regions, the highest intra annual variability of the potentials (Figure 2.6) is observed in West European region (EUW) with monthly potentials between 94 and 255 TWh. There is a variability of $\pm 40\%$ around the average monthly potential of 183 TWh in EUW, with the highest monthly potential being observed in the summer and the lowest monthly potentials in the winter. The lowest regional intra annual variability of potentials is observed in the West African region (AFW) with monthly potentials between 97 and 119 PWh. There is a variability of $\pm 1\%$ around the average monthly potential of 109 TWh in AFW region, with the maximum monthly potential observed in December and January.

To analyse the cost of attaining the potentials, we generated supply cost curves for seven world regions and also at an aggregated global level (Figure 2.7a). Nearly 10 PWh yr^{-1} (40%) of the global potential can be achieved below 100 \$ MWh yr^{-1} , with majority of the potential being realised below 200 \$ MWh $^{-1}$ (Figure 2.7b). At a global level, nearly 40% of the potential can be achieved with investment equivalent to 10% of the 2015 global GDP value and with investment equivalent to 30% of the 2015 GDP value, nearly 100% of the global potential can be realised (Figure 2.7c). We found that realisable potential doubles with each subsequent doubling of capital investment in RTSPV until invested capital is equivalent to 20% of the global GDP value in 2015. An increase of investment from 20 to 30% of the global 2015 GDP value increases the realisable potential by only 27% indicating the areas where the cost of implementation of RSTV is very high. These areas are

represented by large warehouse/industrial complexes in Alaska and Canada, where yearly solar insolation is low and CAPEX investment is high to cover the entire large rooftops with solar panels.

At a global level, spatial variability in the LCOE is also observed (Figure 2.5b). In the northern hemisphere, the LCOE values gradually increase from 40 \$ MWh⁻¹ to 280 \$ MWh⁻¹ with increasing latitude. Here North-East China is an exception which has shown a decrease in LCOE values with increasing latitudes. For Asia, a majority of the potential can be realized between 40 and 100 \$ MWh⁻¹ making the RTSPV competitive with fossil fuel technologies. The cost of attaining the country-specific potential is lowest in India at 66 \$ MWh⁻¹ compared to China (68 \$ MWh⁻¹).

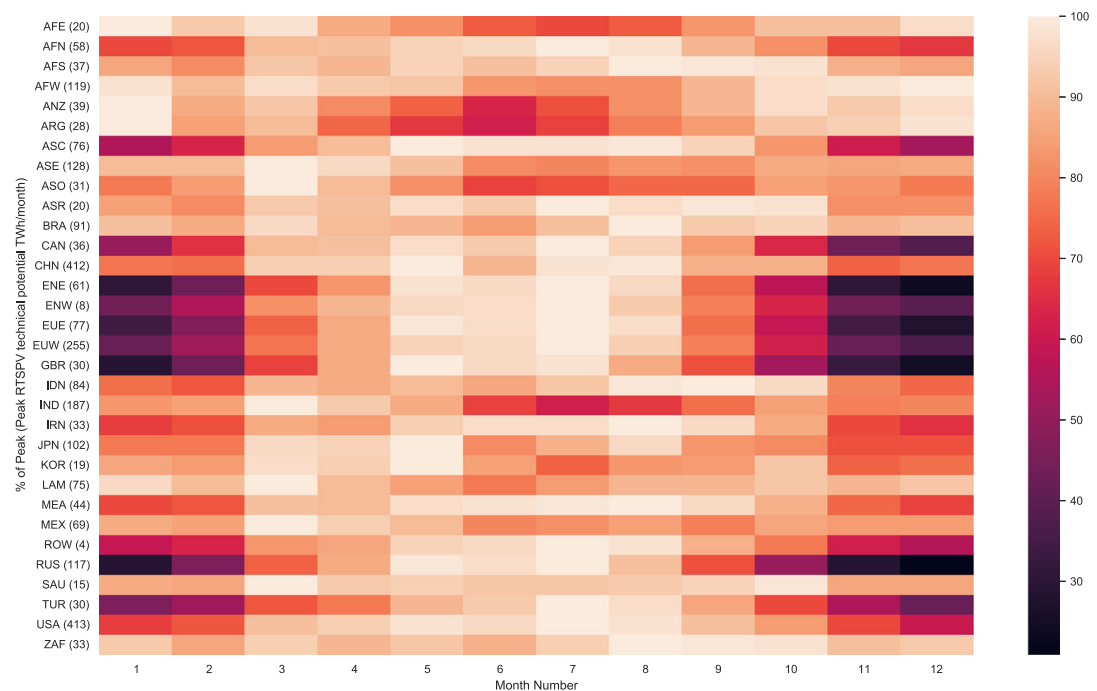


Figure 2.6 | Monthly potential variability for 32 world regions

The heatmap represents the monthly variability of regional potentials. The values in the parenthesis represent the highest monthly potential for the region. The color-coded heatmap represents % of the maximum monthly potential of the region. Europe (EUW, EUE) has shown high intra-annual variability of the potential, with the maximum potential being realised in the summer months. In the southern hemisphere, the maximum potential is realised in the winter months. Africa West (AFW) has shown the lowest variability in the monthly potential.

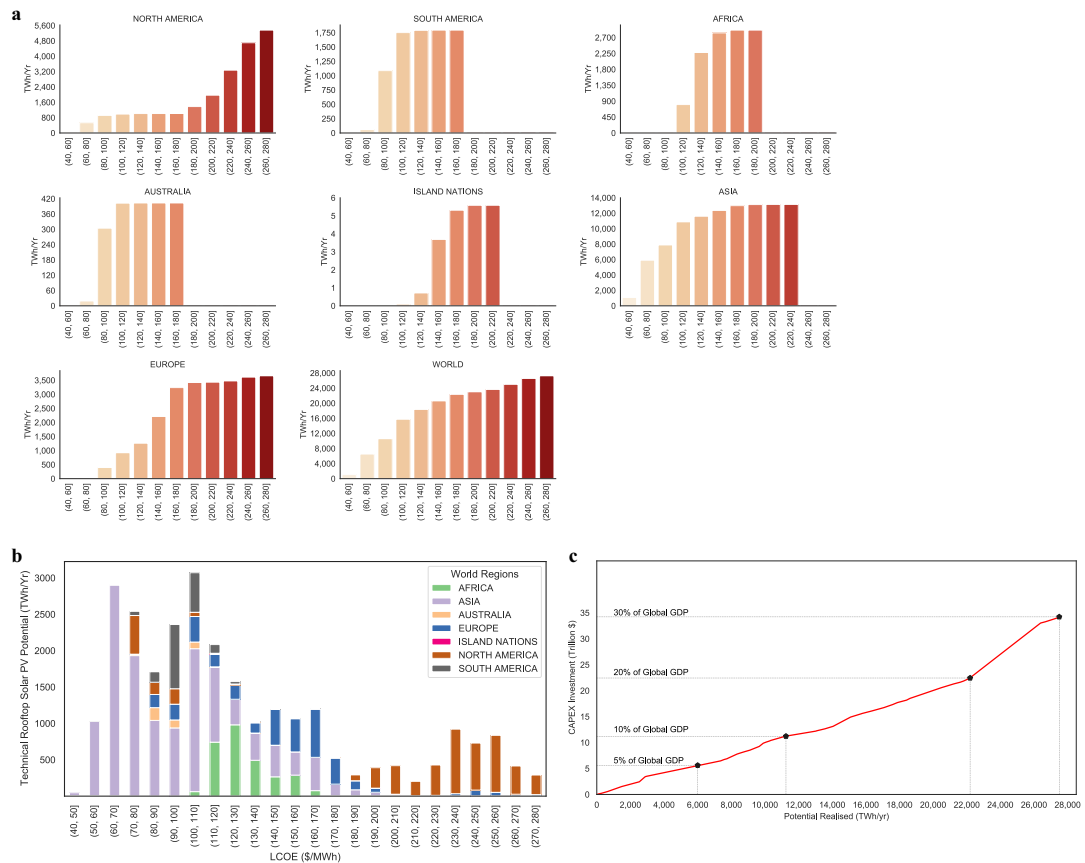


Figure 2.7 | Regional supply cost curves based on a 20 \$/MWh bin size and distribution of LCOE across regions

Regional Supply cost curves **(a)**, showing the cumulative technical potential for a given LCOE bin size. The absolute increase in the bar height represents the change in the added potential that can be realized in a given LCOE bin. Near constant bar heights for consecutive bins are representative of a very small additional potential being realised at an increasing cost. For a single bar, the height of the bar represents the cumulative potential that can be realised within a specific LCOE band. **b** Distribution of potentials across LCOE bins of 10 \$/MWh size. Potential extraction is the cheapest in Asia, followed by Africa and Europe. **c** CAPEX investment required to achieve a specific total potential as a percentage of global GDP in 2015. Nearly 50% of global potential can be achieved at investment equivalent to 15% of 2015 global GDP value.

For Europe, Africa, South America and Island Nations a majority of total potential can be realised below 180 \$ MWh⁻¹. Within Europe, Spain has the lowest LCOE cost of 90 \$ MWh⁻¹, with an increasing trend in cost being observed when moving towards the higher latitudes. Within each country of the European region, further variability in LCOE is also observed with some regions observing cheaper costs than neighbouring regions in the same latitude. In the African region, majority of the total potential can be realised between 110-160 \$ MWh⁻¹. Within Africa,

Nigeria, Gabon and Cameroon have the highest costs (around 150 \$ MWh⁻¹) to achieve their respective potentials.

North America, UK and Japan have shown the highest cost to realise the potential. This can be attributed to the high CAPEX costs in the countries, which is expected to reduce in the future due to technological innovations and reduction in import tariffs. In North America, Canada and north eastern states of U.S.A around the Great Lakes have the highest LCOE costs. The cost to achieve the potential in these countries ranges from 200-280 \$ MWh⁻¹. U.K (251 \$ MWh⁻¹) has the highest country specific costs to achieve its potential.

Globally, CAPEX required to access potential varies both with respect to the size of the GDP and with respect to the LCOE values (Figure 2.8a). To realise complete potential in their respective countries, low-income countries would need to invest capital which is multiple times (up to 3.5 times) their 2015 GDP value even at relatively low LCOE of between 80-150 \$ MWh⁻¹ to cover for high upfront costs. For similar LCOE values, high income countries (World Bank Income Classification) can achieve their complete potentials with capital investment equivalent to fraction (up to half) of their 2015 GDP value.

We categorised countries into groups based on their GDP per capita (GDPC) and on their yield factor (Figure 2.8b). In this study, we defined yield factor as the yearly potential that can be realised from 1 TW of installed capacity. Based on this categorisation, we found out that emerging economics including India, Brazil and Mexico have high yield factor (1.5-2) that would favour the deployment of RTSPV in these countries. Even though the LCOE difference between the two most populous countries (India and China) is minimal, with the greater solar endowment and with high yield factor, RTSPV technology rollout becomes more favourable in India compared to China. However, the uptake of RTSPV is still very low in these

countries due to lack of credit and inability to pay the high upfront cost of RTSPV system. This highlights the need for global cooperation, technology transfer and green financial instruments to accelerate the deployment of low carbon RTSPV technology in low- and medium-income countries.

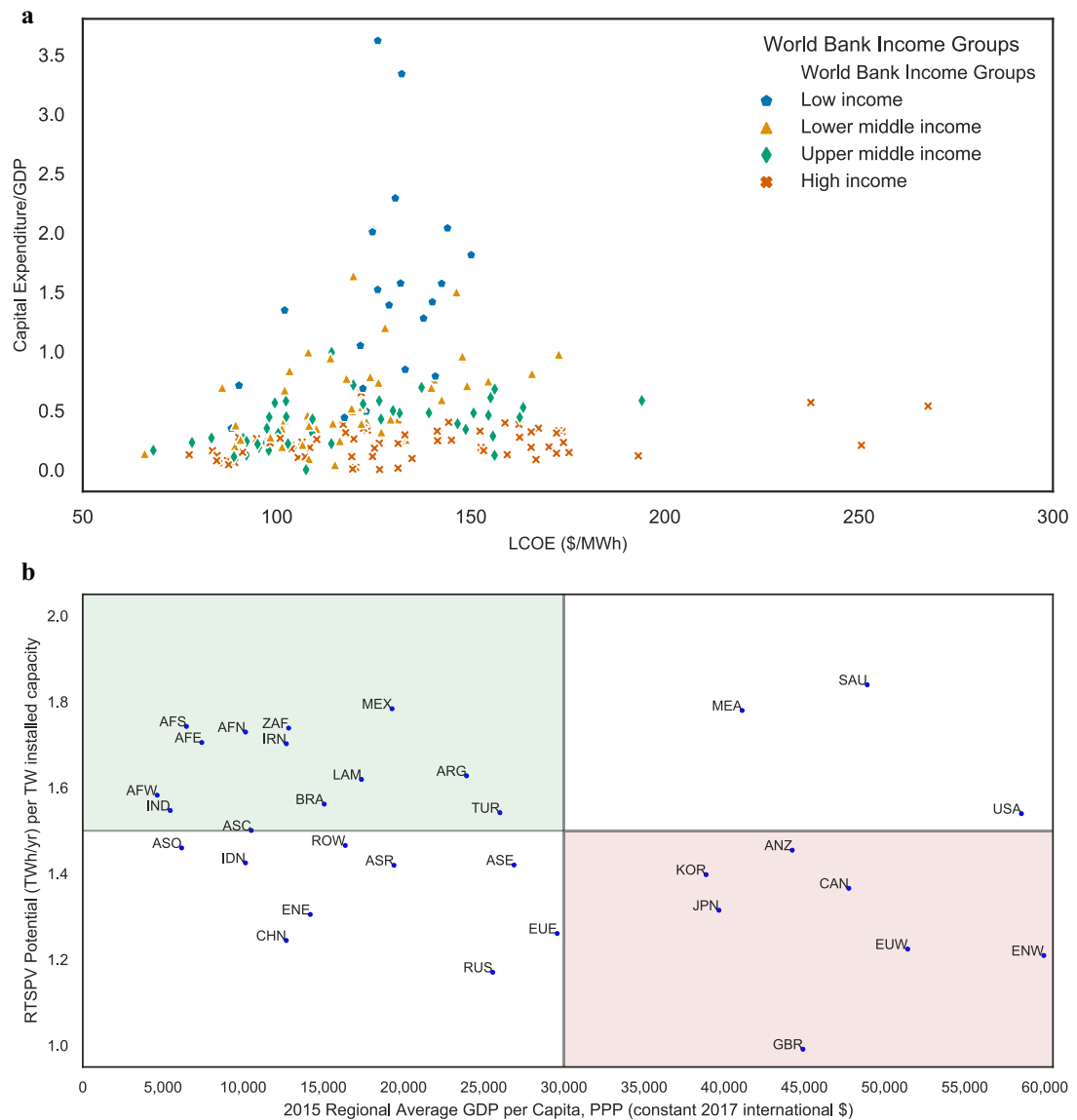


Figure 2.8 | Global economic and technical variation in accessing the potentials

a Disparity in achieving full potential, with low-income countries requiring capital investment greater than their respective 2015 GDP value to achieve full potential. **b** Distribution of 32 regions in relation to their relative yield factor and GDP per capita. The red region focuses on countries that currently have high rooftop PV rollout. The green region focuses on countries where RTSPV technology rollout will have maximum benefits.

2.4 Discussion

The study showcases how framework based on big data and a ML model in conjunction with cloud computing platforms can be used to undertake a planetary scale resource potential assessment. We analysed 130 million km² of global land surface area by utilising learnings from global samples containing 300 million buildings with 16 million km of roads. Using Google Earth Engine and ML model we demarcated 1.2 million km² of built-up area containing 0.2 million km² of rooftop area. As part of the assessment, we generated 1) a global rooftop area dataset 2) a global RTSPV potential dataset at a monthly temporal resolution, 3) costs of attaining the technical potential. The datasets were further used to generate high resolution global maps of the potential and costs. We have also advanced the current state of art by combining the top down and bottom up approaches at a global scale to develop a hybrid framework for resource potential assessment which can also be used in advancing the assessment of global wind and bioenergy potentials. The assessment shows that a sizeable RTSPV potential of 27 PWh yr⁻¹ exist at a global level that can be attained for costs between 40 and 280 \$ MWh⁻¹. The potential is highest in Asia followed by North America and Europe. A capital investment of around 7 trillion dollars is required at current prices to achieve a global RTSPV based electricity generation of 10 PWh yr⁻¹ below the LCOE of 100 \$ MWh⁻¹, covering 3.72 billion people globally.

At EU-27 regional level, our estimated rooftop area of 7,596.4 km² is similar to the 7,935 km² calculated in Bodis et al. study when incorporating rooftop scaling factor of 0.3. For the USA, our estimated rooftop area and annual potential of 8,827 km²/1.9 PWh yr⁻¹ compares well with the estimates of 8,130 km²/1.4 PWh yr⁻¹ presented in the Gagnon et al. study when incorporating a rooftop scaling factor of 0.32. On a city level basis, our potential of 1 TWh yr⁻¹ is in alignment with the 1 TWh yr⁻¹ calculated in a study by Hong et al.³⁶ where they have used advanced

hillshade analysis to capture the effects of building induced shadows in a dense urban topography. A detailed global/regional/country and city level comparison of our results with selected research work is documented in Supplementary Table A.7. From the comparison with other studies, we can conclude that the results from our framework demonstrate high veracity as they are within the margin of error of values present in the literature. Additionally, good estimation accuracy of our framework at high spatial resolution feeds into higher accuracies at aggregated lower resolutions.

Our assessment has important implications for addressing the twin challenges of sustainable development and climate change with co-benefits in advancing the SDG 3 and SDG 7. First, the analysis of spatial RTSPV potential presented in this study shows that 55% of the global RTSPV potential is spread across low density areas. This highlights an important aspect of solar transition, where the majority of its benefits in providing cost effective and fast deployable electricity can be realised in rural areas. RTSPV can thus aid in mitigating the energy poverty being experienced in the less developed and sparsely populated areas in a country where extensive grid integration maybe costly or where competition for land may exist. Nearly 20% of the global potential lies in the high-density areas where deployment of RTSPV can aid in displacing fossil fuel derived electricity with less polluting electricity generation thereby reducing local air pollution^[123]. Second, from a perspective of energy equality and “leaving no one behind” agenda of the SDG, the most disadvantaged areas with respect to access to electricity are currently the low-income countries^[71] which require rapid and cost effective deployment of clean electricity generation infrastructure. Our assessment shows that low-income countries may need significant capital investments as steep upfront RTSPV installation costs in order of magnitude 2-3 times their 2015 GDP value to achieve their country specific potentials. At current costs governments may need to provide subsidies and seek external investments to improve the

prospects of deployment of RTSPV in these areas. This highlights the vital role that the developed economies may play in enabling the deployment of RTSPV in these countries by the means of financial flows to realise the climate change co-benefits. With maturing of the technology and emergence of economy of scales, costs will further go down to enable a solar revolution in these areas and aid in their low carbon energy future.

Third, countries that are currently reaping their demographic dividends like India and China are better suited for rapid deployment of RTSPV. We showed that these countries have high potential with low seasonal potential variability along with low cost of deployment. As these countries have the largest population share globally with large building stocks, they can be the first movers in decarbonising their electricity generation infrastructure by substantially deploying decentralised electricity generation portfolio, further aiding in climate change mitigation. Along with climate mitigation, RTSPV deployment in these countries can gain a lot from the high workforce percentage in the population in the form of cost-effective manufacturing and operational maintenance. Fourth, the high-resolution assessment can aid the local governments in identifying suitable locations for rapid deployment of energy generation infrastructure. This way bottom-up formulation of energy policy can lead to inclusive designing of nationwide policies to provide energy justice to the citizens.

Fifth, businesses and financial institutions like World Bank and International Monetary Fund can analyse in-depth the investment opportunities and risks in implementing RTSPV infrastructures leading to local job creation and sustainable development of manufacturing industries. Sixth, the information contained in the assessment along with supply cost curves are a measurable step forward and fills in a significant information gap that is present in current integrated assessment models where solar PV potentials are often represented as aggregated potentials

for utility and rooftop installations. Our assessment provides insightful findings and technical potential datasets that will certainly aid in accurately modelling the future carbon neutral scenarios to inform national energy policies^[124-129]. This will no doubt aid in exploring sustainable and inclusive low carbon future possibilities.

Our study shows pronounced variability of seasonal potentials in the higher latitudes for countries covering Europe, North America and Australian regions. These regions have high electricity consumption per capita along with the financial capacity to introduce significant VRE in the electricity generation mix. To mitigate the variability of the potentials over the year, smart grids that optimise the generation portfolio and introduction of regulator driven mechanisms that balance the generation market becomes important. Further, introduction of new market mechanisms^[130] are needed to effectively integrate the prosumers and utility operators in competitive electricity generation markets. With falling prices of electricity storage technologies and smart management of interconnected grids, RTSPV technology will play a critical role in these markets by undertaking generation, storage and system balancing roles.

In conclusion, our assessment shows that the current electricity generation potential of RTSPV exceeds the current (2018) yearly aggregated global electricity demand^[131]. Our assessment also shows that a minimum of 50% of the total global rooftop area is required to meet the yearly global aggregated electricity demand. Due to the diurnal cycles of solar insolation and to balance the seasonal and daily variability of the RTSPV generation, the role of storage solutions to compliment RTSPV electricity generation is critical in realising the maximum potential of this technology and to meet the peak daily demand. Hence, the practical realisable potential of RTSPV will depend on the future cost trajectory of storage technologies, capital expenditure related to the technology and overall configuration of the energy system.

Even with its limitations and shortcomings the current assessment is still the state of art and provides researchers with global analysis datasets. The underlying methods and datasets have been peer reviewed and are of the highest quality currently available and represents a generation advancement over the datasets used in the current state of art methods. The current dataset can be improved by using a next generation 10 m resolution landcover dataset and with increase in the spatial resolution of the population and solar data at a global scale. Better data processing platforms can enable further work to be accomplished at a 1 km resolution providing 100 times increase in the spatial representation of the potentials. Additionally, inputs in the form of realistic regional variation in the rooftop availability will aid in narrowing down the uncertainty in potentials and cost and should be the next logical research step in model improvement.

2.5 Methods

2.5.1 Top-Down method

We generated a total of 3,521,120 fishnets using ArcGIS PRO desktop application for all the global landmass except for the continent of Antarctica. The FN grid is the lowest unit of data aggregation in our method. The FN's at the boundary of two countries have a common Fishnet identifier but unique country attribution with FN being split at the boundary. Next, the fishnet polygons were uploaded to Google Earth engine platform^[132] (GEE) to calculate satellite derived Built Area (BA_{FN}), Population ($PPLN_{FN}$) and conversion factors (CF_{FN}) for each fishnet cell.

We utilised the global landcover (LC) layer from Copernicus Global Land Service v2.0 to calculate BA_{FN} values within each FN. This landcover classification layer was chosen for its robustness and near global coverage and it is backed by exhaustive testing and validation. The LC has many categories of classifications, amongst

which built-up area is one of the classifications. The built-up classification is in turn derived from European Space Agency's World Settlement Footprint 2015 layer that is derived from a 10 m resolution sentinel mission's radar and optical imagery. To calculate the total built-up area in each Fishnet cell, the LC raster file was first cut into smaller size based on each fishnet's geographical bounds. The individually cut LC dataset was then aggregated using the following:

$$BA_{FN} = \sum (PX_V * PX_A) \quad (2.1)$$

where, BA_{FN} is the Built-up area in each fishnet cell, PX_V is the pixel value (0-100) representing percent of built area in each pixel, PX_A is the area occupied by each pixel.

To map the number of people living in each fishnet cell, we utilised a global population raster file at 100 m resolution provided by WorldPop project. The population raster disaggregates the recorded United Nation's population counts in an administrative unit to a finer resolution using ML based methodology. The population raster file was split into smaller entities based on each fishnet cell's geographical bounds. Then, a masking file containing areas covered by LC layer within each fishnet cell is used to mask the population outside the bounds of the BA_{FN} area in each fishnet. The individual small population dataset was aggregated for each fishnet cell using the following:

$$PPLN_{FN} = \sum PX(NM)_V \quad (2.2)$$

where, $PPLN_{FN}$ is the total count of people living in each fishnet and $PX(NM)_V$ is the pixel value of each pixel that is not masked by overlay LC layer. The population raster file was masked to remove any population count data that is not part of the

LC pixel. The masked population raster pixel can be attributed to artefacts induced due to the downscaling algorithm in the original dataset or extra built-up areas that were external to the LC layer. To maintain homogeneity in the analysis, LC layer was taken as the base for all analysis and any area not covered by (BA_{FN}) was assumed to be not present on the ground, even if it actually exists as ground truth.

The CF factors were calculated using World Bank's SolarGIS raster datasets. The dataset is provided as a 1 km resolution raster dataset with each pixel providing daily kWh generation for each kWp (peak) installed capacity within that pixel at a monthly resolution. The dataset has been generated using extensive simulation and validation of solar insolation, power conversion losses, effects of atmosphere and panel ageing using 20 years of documented data. For each fishnet cell, the CF factors were aggregated using the following:

$$CF_{M, FN} = \frac{1}{n} \sum_1^n PX_V \quad (2.3)$$

where, CF_{M, FN} is the CF factor for each month for each FN, n is the number of CF pixels in the FN and PX_V is the pixel value of each pixel in the FN geographical bound. All the three datasets (PPLN_{FN}, CF_{FN}, BA_{FN}) and FN geometries were first processed on ArcGIS Pro desktop application to harmonise coordinate reference systems and then uploaded to GEE platform for processing. On GEE, we split the datasets based on individual FN geometries and aggregated the three datasets based on the rules highlighted above. GEE's cloud computing architecture can process a large number of datasets in relatively shorter time frame and outputs a tabulated dataset for further processing.

2.5.2 Bottom-Up method

To generate ground truth building footprints, we collected building polygon shapes as vector layer from big data sources. For building footprint samples, we used AI generated building footprints by Microsoft AI and Ecopia AI teams. These two datasets cover the entire USA, Canada and 39 African countries. The samples from Microsoft AI and Ecopia AI (>300 million individual buildings) were split up based on the FN layer for each FN cell overlapping the sample countries, further masked to remove building footprints outside of the BA_{FN} layer. The unmasked building footprints were aggregated based on following:

$$BF_{FN} = \sum BP(NM)_V \quad (2.4)$$

where, BF_{FN} is the aggregated building footprint for each sample FN and $BP(NM)_V$ is the unmasked individual building footprint polygon area within the FN that is overlapping the BA_{FN} layer. The masking removed buildings constructed after the 2015 reference year. Although, the BA_{FN} layer cover entire extent of built-up area globally, it can still miss some built-up areas due to artefacts in satellite imagery. However, this is negligible and for the purpose of our study considered as the reference layer with which to base our analysis on. Overlapping building footprints were dissolved into a single polygon before splitting and polygons being intersected by a FN boundary was split up at the line of intersection. For the rest of the world, OSM derived building footprints (accessed April 2020) were analysed and aggregated based on equation (2.4). A total of 4000 global FN samples were selected from OSM building dataset. The sampling strategy to generate the 4000 OSM samples was to extract buildings bound by FNs that had BF_{FN}/BA_{FN} ratio of between 0.15 and 0.11. These ratios correspond to the 75th percentile and 50th percentile of data processed from Microsoft AI and Ecopia AI datasets. In total, we were able to successfully collect samples from nearly all the

global countries covering different stages of socio-economic development, cultural spread and geographical locations.

The road length metric was derived entirely from the OSM datasets. To process the RL dataset, OSM's planetary dataset file (accessed April 2020) was used. The planetary file has roads represented in the form of lines attributed by the different types e.g., residential, highway, footpath etc. The line feature was split up based on each global FN, masked using BA_{FN} layer, and aggregated based on following:

$$RL_{FN} = \sum L(NM)_V \quad (2.5)$$

where, RL_{FN} is the aggregated road length for each global FN and $L(NM)_V$ is the individual length of all the roads within each FN overlapping BA_{FN} layer. It was observed during the aggregation of the RL_{FN} dataset, that road endpoints in OSM dataset overlap in some locations, these overlaps were dissolved into single line feature prior to aggregation. Also, some roads extend beyond the BA_{FN} layer within each FN. These roads were clipped at the BA_{FN} boundary to maintain a homogenous extent for the region of interest for all the datasets used in the analysis. In total, we were successful in processing the road infrastructure for nearly all the countries of the world.

Loading, splitting and geometry processing for the building footprints and the road lines were performed using ArcGIS PRO's multicore support. The aggregation of the datasets and mapping of the aggregated dataset with FN boundaries was performed using custom python scripts built on DASK^[133] parallel compute module. Due to the sheer size of the data being processed, we found that multicore architectures and parallel computing frameworks developed in the recent years can be of great use in designing and executing planetary scale

analysis with minimal cost and time requirements.

We have used cloud computation in the form of Google Earth Engine platform. In general, parallelisation of the data processing was performed in four ways, first when disaggregating global raster datasets and mapping the aggregated values to our global FNs. We did this task for 12 monthly solar rasters, 1 Landcover raster and finally for global population raster. Here, we ran all the raster algebra and mapping codes on Google Earth Engine where the backend data processing was split into multi parallel streams and executed on google cloud infrastructure. This led to speeding up of the data crunching as raster algebra is highly parallel in its execution where each raster cell can be worked on independently.

Second, when disaggregating global vector datasets and mapping the aggregated values to our global FNs. As of the time of the writing this article, Google Earth Engine was less efficient in undertaking vector analysis. The reason for this is that instead of pixel raster surface which can be computed in a parallel fashion, vector datasets need specialised algorithms. Here, we utilised the multi core parallel processing architecture of ARCGIS Pro where vector datasets in the form of building footprints and roads can be effectively processed by splitting the map into different regions and processing each region on a single core. This task is performed in the backend using apache spark.

Third, when doing data aggregation and manipulation inside desktop python environment. Large components of the data processing ranging from calculating rooftops to LCOE calculations were performed using DASK framework. In this framework, dataframes can be broken down into small chunks and processed in parallel. This provided us with a significant reduction in processing times.

Fourth, when training ML model. Custom scripts were written on python to perform hyperparameter optimisation and 10-fold cross validation in a parallel fashion. Each of the 10-folds of the cross validation were assigned to independent core of our 12-core machine which led to faster convergence of the hyperparameters to an optimal solution.

2.5.3 Downscaling model

The ML model was trained on $PPLN_{FN}$, RL_{FN} , BA_{FN} as independent variable and BF_{FN} as the dependent variable for each sample FN. The first step in model preparation was to impute the missing data in the independent variables. The imputations are necessary as some FNs have either missing population or road length data due to global scale of the analysis. This discrepancy is expected and is present due to OSM roads not being mapped for every road on the planet and also due to the downscaling methodology used in generating the original population raster by WorldPop.

Data imputation was handled using a custom python script utilising Scikit-Learn^[134] module's iterative impute function. Further, we generated the downscaling model using XGBoost^[135] framework. When choosing between Neural Network based framework or Gradient boosting frameworks, we used the latter as XGBoost framework has shown superior performance, while using considerably less computation time to reach an optimum model state. Also, being run on CPU only architecture, XGBoost framework can generate repeatable results in each subsequent run, which is difficult to achieve on a GPU based framework like Neural Networks due to inherent uncertainty induced by massive parallel compute architecture of a GPU.

The base XGBoost model was customised for our task by hyper-tuning the parameters of the model using 5-fold cross validation. Each fold of the cross-

validation generated a mean square error (MSE) loss metric at the end of its run. The mean of all five MSE was chosen as the metric to reduce during the hyper-tuning process (final model parameters are present in Supplementary Table A.6). The trained model was then used to estimate building footprint values for each global FN cell using $PPLN_{FN}$, RL_{FN} , BA_{FN} values. The final output of the downscaling (BFE_{FN}) was stored as a global 10 km resolution raster file where each pixel represents the estimated aggregated building footprint for each FN.

2.5.4 Technical potential estimation

To calculate RTSPV potential from BFE_{FN} , we made some generalising assumptions to maintain the uniformity in our calculations. We assumed that the estimated building footprint is representative of the available rooftop area in each FN i.e 100% of the estimated rooftop is available for solar panel installation. To install 1 kWp of roof mounted solar PV, 10 m² of rooftop area is required, which is in line with the thin film technology currently in use. The roof mounted solar PV are installed at the optimum angle for each latitude and are sun facing and shade free to generate maximum electricity output. The building rooftops are flat in design leading to utilisation of entire rooftop for installation of solar panels.

Based on the assumptions i.e. 10 m² area for a 10% efficient panel, the technical solar potential is calculated for all the global FNs for 12 months using the following:

$$SP_{M,FN} = BFE_{FN} * CF_{M,FN} * \frac{Days_M}{10} \quad (2.6)$$

where, SP is the technical solar potential, BFE_{FN} is the estimated roof area in m², CF is the conversion factor, M is the month and FN is the unique fishnet cell, and $Days_M$ is the number of days in the respective month. The World Bank's solar conversion factors are available for the regions between 60°N and 45°S. For

regions beyond 60°N and 45°S, we assumed a constant conversion factor of 3.5 kWh/kWp/day. This has led to a slight over assessment of potential for countries like Sweden, Norway. However, as the density of built-up area reduces significantly beyond the 60°N and 45°S, the total global error due to this assumption remains small. The calculations for generating the solar potential are processed using custom python scripts using DASK module to handle massive arithmetic operations. Further, the processed solar potential raster dataset is stored as a geopackage file for visualisations and economic calculation.

2.5.5 Cost calculation

LCOE provides an easy and robust method to compare economic viability of a project within a specific FN. It was assumed that the capital cost of the installation (CAPEX) will be staggered to the first year of commissioning and the installed panels will have a lifetime of 25 years. The geo-mapping for CAPEX, operating expenditure (OPEX) and discount rate (DR) was sourced from IRENA's renewable energy cost report 2019. The LCOE for each FN is calculated using following:

$$LCOE_{FN} = \frac{\frac{\sum_{t=1}^{25} CAPEX_{FN} + OPEX_{FN,t}}{(1 + DR)^t}}{\frac{\sum_{t=1}^{25} \sum_{M=1}^{12} SP_{M,FN}}{(1 + DR)^t}} \quad (2.7)$$

where, $CAPEX_{FN}$ (2019 \$/kW) is the capital expenditure in installing the RTSPV system for the given FN, $OPEX_{FN,t}$ (2019 \$/kW) is the operational and maintenance expenditure for the given FN and for the specific year (t), t is the year number, DR is the discount rate, M is the month number, and $SP_{M,FN}$ (kWh/month) is the potential generation for the given month and FN. We have used CAPEX data for 17 different countries and allocated average CAPEX value to the rest of the countries based on the continent they are in. OPEX and DR have values based on OECD and Non-OECD country classifications. Country-wise aggregation of

LCOE, SP from each FN from their respective high resolution intra country values has been done using the following rule

$$LCOE_{country}: \left\{ \begin{array}{l} CAPEX: aggregation_of_individual_FN_values \\ OPEX: aggregation_of_individual_FN_values \\ SP: aggregation_of_individual_FN_values \\ DR: mean_of_individual_FN_values \end{array} \right\} \quad (2.8)$$

It should be noted that we did not consider the cost of additional grid expansion or storage infrastructure to attain the full technical rooftop solar PV potential. Also, the cost of decommissioning and scrap metal value of the installation was not considered at the end of the 25-year lifetime of the projects. While calculating the SP and LCOE, it was assumed that no rooftop solar PV installation exists globally, and all the additional capacities will start their commissioning from year 2019.

2.5.6 Limitations

Our assessment is based on the accuracy of global landcover layer, which with its 100 m resolution can in some locations overestimate the built-up area extents. Additionally, the landcover classifies roads, parking lots, boundaries of green areas, tennis courts and archaeologically significant areas as built-up areas with misclassification varying between different regions. Our assumption that the rooftops being flat, shadow free and sun facing with full rooftop available for installation adds into the methodological limitations. Next, the big data related to building footprints and global roads have inherent methodological limitations like the simplified representation of a complex rooftop with a square polygon, overlapping roads etc.

For technical potential calculations, we assumed that 100% of the estimated rooftop is available for installing solar panels i.e., orientation and slope of the building is not accounted for the 100% rooftop availability assumption-based results in our main analysis. These assumptions can lead to limitations in real world

interpretation of main results as a fraction of rooftop maybe available for installation of solar panels. To account for this, we have documented regional change in potential as an uncertainty analysis for a combination of rooftop scaling factors and panel efficiencies. In the current literature, reduction of total rooftop area to available rooftop area is generally done through a rooftop scaling factor which is a proxy for loss of rooftop area due to orientation, slope, and roof super structures like chimneys etc. Although, some studies exist at country level where the rooftop scaling factor is documented, on a global scale no authoritative dataset exists that can demarcate country wise rooftop scaling factors. Further work is required to document the country specific rooftop scaling factors which is outside the scope of the research aim of this study.

Our cost assumptions cover 17 different countries across continents with average values for rest of the countries. These assumptions can assign increased or decreased LCOE values to a certain region like Africa and South America. Another limitation of the cost assumptions is the inability of the LCOE metric to capture intra country variation of LCOE to a high degree due to lack of high-resolution cost data. Also, cost variability due to additional grid rollout, tariff mechanisms and global change in prices due to trade protectionism practices are beyond the scope of the current assessment. Finally, we calculated all the cost and potential metrics assuming that no installed capacity exists for the ROI, where in the present time horizon, some installed capacity does exist.

A majority of limitations can be attributed to the underlying data used in our assessment, which can be improved with subsequent advancement in the methodology of the data providers. Further research can be undertaken to reduce the methodological limitations that are currently bootstrapped by the data availability and lack of homogenous global data.

Chapter 3: Assessing the growing role of decentralised rooftop solar photovoltaics in the global energy transitions and co-benefits for sustainable development

Joshi, S., Zakeri, B., Mittal, S., Mastrucci, A., Holloway, P., Krey, V., Shukla, P.R., Gallachoir, B.O., Glynn, J., "Assessing the growing role of decentralised rooftop solar photovoltaics in global energy transitions" (Submitted Scientific Data)

3.1 Abstract

Net Zero scenarios to contain global warming to below 1.5°C envisage a significant role of solar photovoltaics (PV), but they are often very limited in evaluating the role of decentralised rooftop solar PV within the solution space. Considering decentralised rooftop solar PV installed capacity contributed 42% of global installed solar photovoltaics capacity in 2020 with the benefit of avoided land use and sustainable development implications, analysing its role in future energy transitions is imperative. We address this gap with the aid of machine learning based analysis and Shared Socioeconomic Pathway narratives, showing that global rooftop area will grow by 20-52% between 2020-2050, with the highest growth in the emerging economies. We find that by 2050 decentralised solar PV can account for >50% of total PV generation under stringent climate targets leading to an increase of 23% in solar PV generation over Utility solar PV only implementation. This will lead to avoiding 30,000 km² of land area and create 141 million jobs by 2050.

3.2 Introduction

The UN Sustainable Development Goals (SDG) which were adopted along with Paris agreement offers a window of opportunity for emerging economies to shift their energy transition pathways towards sustainability^[2, 136]. Accelerating the deployment of low carbon and cost-effective renewable electricity generation (SDG 7) has the potential to address the twin challenges of sustainable development and climate change (SDG 13) with co-benefits in advancing the SDG 11 (sustainable human settlements). Current electricity generation from renewable energy sources is primarily derived from wind, hydro and solar. Amongst these, solar photovoltaics (PV) is the fastest growing technology, growing 16 times from 40.3 GWp to 709 GWp^[137] while recording a decline in global utility scale weighted average cost by 85% between 2010-2020^[138], making utility solar PV (UTSPV) currently the cheapest renewable source of electricity in history^[139].

It is anticipated that solar PV will form a sizeable part of mid-term low carbon energy future. In the recently released IPCC's Sixth Assessment Report^[140], global net zero energy pathways to contain global warming to below 1.5°C envisage a significant role for solar PV where the solution space in 2050 could range between 4-42 TWp total installed capacity (Figure 3.1a). While encouraging, these scenarios fail to capture how the dynamics will develop within this solution space between UTSPV and decentralised rooftop solar PV (DCSPV), the latter encompassing non-residential rooftop solar PV (commercial/industrial) and residential rooftop solar PV. Globally, solar PV installation crossed the 100 GWp installed capacity mark in 2012 with DCSPV covering 70% of the total installed capacity. In 2020, with a total installed capacity of 310 GWp, DCSPV occupied 42% of installed solar PV capacity with non-residential rooftop solar PV and residential rooftop solar PV recording 208 and 102 GWp installed capacity respectively. Amongst the 310 GWp installed capacity, Western Europe contributed 91 GWp while China contributed 76 GWp

of DCSPV capacity^[137]. Globally, DCSPV as a percentage of total solar PV installed capacity ranges from 17% (South Asia) to 64% (Europe), (Figure 3.1b)

Accurately capturing the role of DCSPV in global energy systems is crucial as it currently accounts for 42% of the global total installed solar PV capacity in 2020, deployed both in developed and emerging economies (Figure 3.1b). Additionally, the nuanced investment dynamics of DCSPV where the decision-making lies with end users or prosumers is different from those of UTSPV. Moreover, DCSPV operates on distribution grid infrastructure with majority of the installations residing behind the meter as opposed to centralised transmission grid utilisation in UTSPV. The discussion around the interplay between DCSPV and UTSPV becomes more complex with steep regional convergence of investment costs (Figure 3.1c) and separate policy approach to their deployment. DCSPV has the potential to democratise renewable electricity generation which can lead to consumer-driven breakthrough in tackling climate change, reducing local air pollution, and providing sustainable energy access in areas lacking electrification^[141]. This can be complemented by socio-economic benefits, including job creation coupled with localised market for batteries, inverters, and equipment maintenance. In addition, the energy versus food-land-use competition can be mitigated by using previously developed and underutilised real-estate (rooftops)^[142] promoting sustainable life on land (SDG 15). Considering energy fuel's price volatility and its impact on energy security coupled with the COP26 declaration of "One Sun, One World, and One Grid"^[143] the role of DCSPV becomes ever important for energy access.

This raises concerns regarding the absence of robust DCSPV modelling within current Integrated Assessment Modelling (IAMs) and energy system models (ESM) which aid in analysing future low carbon energy pathways. The primary reason for this gap in research can be attributed to the lack of accurate assessment of how

DCSPV potentials will grow in the future corresponding to the anticipated increased growth in spatially explicit rooftop area^[60]. This assessment has traditionally been a highly complex and computationally intensive task as the assessment unit is individual building rooftop^[61]. This complexity is compounded by the fact that building stock archetypes change between geographies and are dependent on the socio-economic and cultural factors prevalent in the region of interest (ROI). Another reason is the underestimation of the steep learning rate, leading to a rapid decadal decline in investment costs which fell by 88% between years 2010-2020 coupled with emerging active global prosumer base^[46, 144-146].

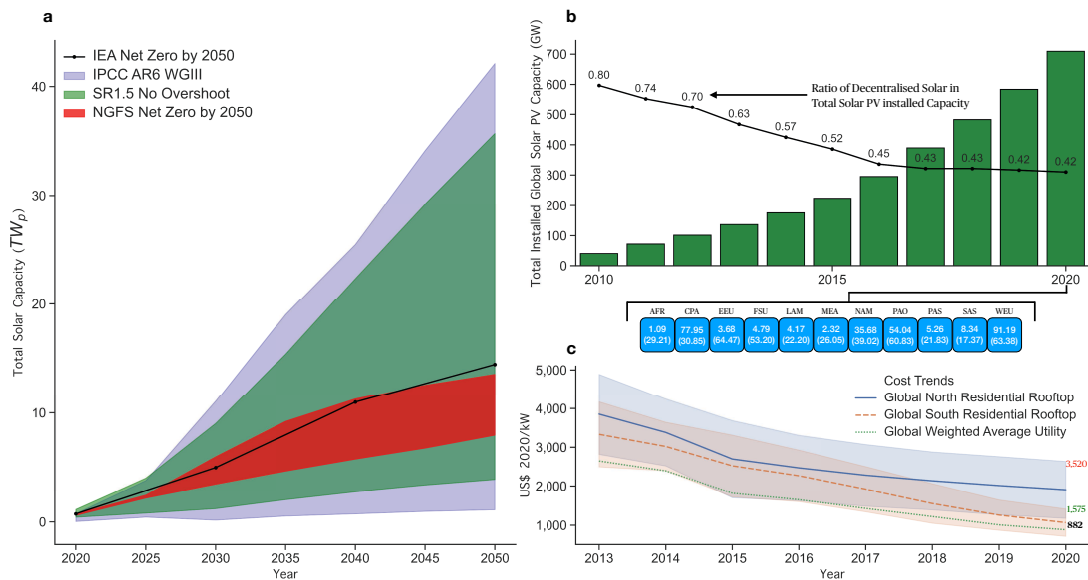


Figure 3.1 | Solar PV's historical capacity and cost trends along with future capacity solution space for 1.5° global warming.

a, Global growth in total installed solar PV capacity by 2050 for different Net Zero 1.5 degree scenarios with no overshoot^[147-150]. **b**, Global yearly annual solar PV capacity from 2010 till 2020. The black line represents the proportion of DCSPV in total yearly solar PV installed capacity. The blue boxes represent the regional total installed DCSPV capacity in 2020 in GWp with regional percentage of DCSPV in 2020 total solar PV installed capacity documented inside brackets. Regional definitions can be found in Supplementary Table B.6. **c**, Trends in solar PV costs for residential and utility solar PV. The number in black represent utility solar costs, numbers in red represent global north residential solar PV installation costs and the numbers in green represent global north residential solar PV installation costs.

In this analysis, we address this key research gap and advance the discussions regarding the role of DCSPV in global energy transitions. Here we execute a big data and machine learning (ML) based high-resolution spatiotemporal framework to estimate the global growth in spatially explicit rooftop area and the corresponding growth in monthly electricity generation potentials for different possible worlds envisioned under the Shared Socioeconomic Pathways (SSP) narratives^[151]. We further utilise these assessed potentials for SSP2 (middle of the road narrative) along with harmonised historical calibration, updated investment costs and a new electricity system sub-structure in a global IAM – MESSAGEix-GLOBIOM^[152] to reveal the potential medium-term role of DCSPV in achieving a low carbon energy future along with its co-benefits for sustainable development.

3.3 Results

The assessment framework uses SSP derived spatially explicit global growth in GDP, Population, and built-up area as drivers to estimate spatially explicit growth in global rooftop area. For this we train our ML assessment framework on >800 million global building footprints covering countries in various stages of socioeconomic development. The entire framework works at a spatial resolution of 1/8 degree global tiles arranged as fishnet grids (FN). The framework was designed in two cascading stages where the first stage extracts global building footprint training samples from open street maps (OSM) which we used in conjunction with our big dataset derived building footprints for training the second stage. The second stage was then used to estimate spatially explicit decadal growth in global rooftop area for SSP narratives, (Figure 3.2a). The first stage is an important methodological advancement in our analysis whereby we used learning from big dataset derived samples in North America, Australia, and Africa to extract accurate building samples from OSM derived regions to provide more variation in training data for our second stage of the framework (Figure 3.2b).

For details on framework development, training procedure and validation please see Methods section and Supplementary Item B.3.

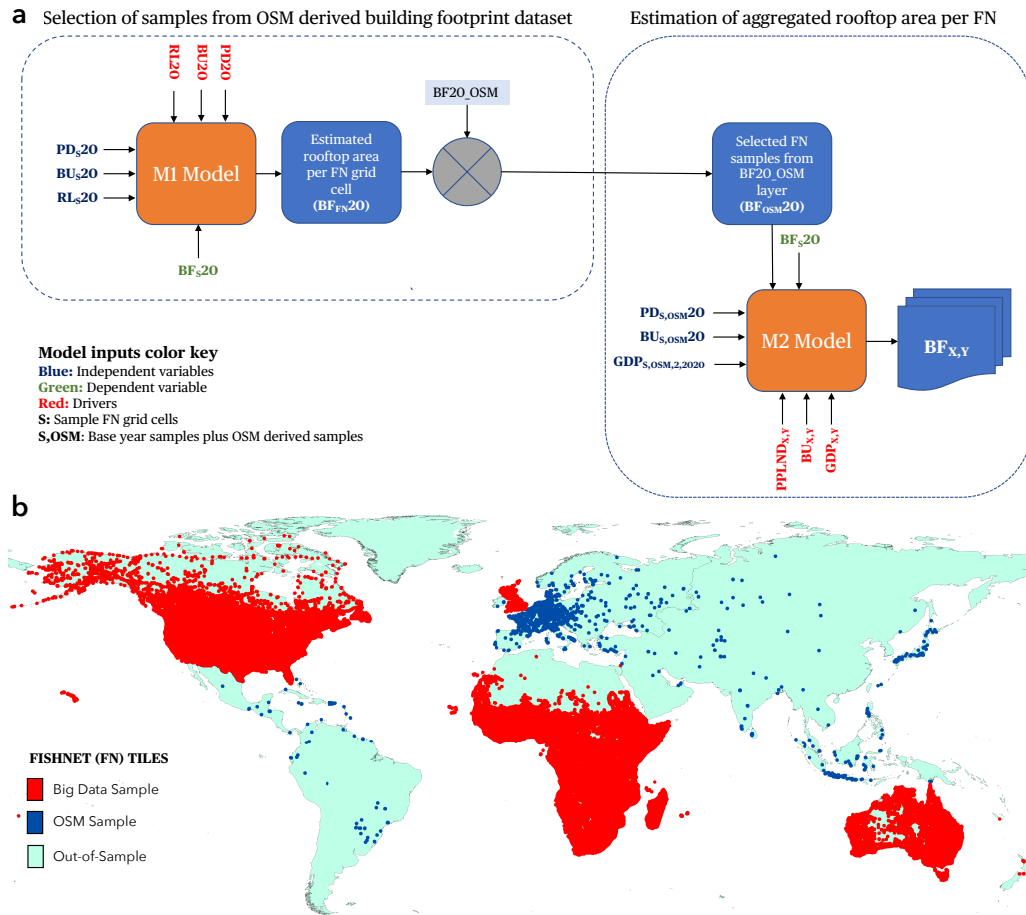


Figure 3.2 | Overview of ML framework

a, The ML framework is divided into two stacked XGBoost models. The first model “M1” aids in selection of samples from global OSM building footprint dataset (BF_{OSM20}). The second model “M2” combines the samples from first model with BF_{S20} samples and uses the SSP derived drivers to estimate the aggregated rooftop area per FN grid cell. The first stage of the framework named “Model M1” accepts global built-up area (BU_{20}), global road length (RL_{20}) and global population density (PD_{20}) as drivers to estimate global rooftop area per FN grid cell (BF_{FN20}) for the year 2020. The second stage of the framework named “Model M2” accepts SSP derived global built-up area ($BU_{X,Y}$), global downscaled GDP ($GDP_{X,Y}$) and global population density ($PPLND_{X,Y}$) to estimate global rooftop area per FN grid cell ($BF_{X,Y}$) where X is the SSP narrative and Y is the estimation year. Overall, the framework records an absolute error of $\pm 0.25 \text{ km}^2$ per 1/8-degree FN tile when predicting the dataset used to train the model. **b**, the spatial spread of sample FN tiles used in our analysis amounting to 148,441 FNs for big data derived samples and 2,654 FNs for OSM derived samples. More details in Supplementary Tables B.1, B.2, and B.3.

3.3.1 Spatially explicit assessment of growth in DCSPV and USPV potentials

From the assessment framework, the global aggregated rooftop area for year 2020 is estimated to be 0.25 million km² for a global aggregated built-up area of 1.46 million km². Amongst the 0.25 million km² of assessed global rooftop area, 0.12 million km² is in Asia and 0.047 million km² is in Europe. The Africa occupies 0.02 million km² of aggregated rooftop area in 2020 with North America occupying 0.039 million km² of aggregated rooftop area. For future growth in gross rooftop area, we observe that from a base value of 0.25 million km², the spread of global aggregated gross rooftop area in 2050 will lie in the range of 0.31-0.38 million km² for worlds envisioned under SSPs which represents a percentage increase of between 20-52% compared to 2020 values (Figure 3.3a).

At a global scale the highest growth rate of aggregated gross rooftop is observed for Africa across all the SSP narratives with doubling of aggregated rooftop area between 2020-2050. For all five possible SSP global growth scenarios, Africa will contribute to ~12% of global gross rooftop area by 2050 up from ~9% in 2020 (Supplementary Table B.4). Driven by the growth in population and GDP (Supplementary Figure B.3), the highest growth in aggregated gross rooftop area across the continents is observed for SSP5 narrative, with lowest growth being observed for SSP3 narrative. For Africa, Asia, and South America the SSP1 narrative (sustainable growth) registers the lowest growth in rooftop area between 2020-2050 (Figure 3.3b, Supplementary Table B.5). For Europe and North America, the SSP3 narrative (regional rivalry) registers the lowest growth in rooftop area between 2020-2050. In general, a growth in gross rooftop area of 7- 200% can be observed for different continents between SSP narratives, with emerging economies registering highest percentage growth in gross rooftop area across all SSPs between 2020-2050 (Figure 3.3b). Thus, it can be concluded that emerging economies will experience significant increase in their building stock between 2020-2050 for all possible growth trajectories narrated by the SSPs and the

developed economies will only observe significant growth in their building stock for growth driven by fossil fuelled development (SSP5).

The assessed technical potential of DCSPV at a global yearly aggregated level for the year 2020 is observed at 21 PWh/yr assuming 30% net rooftop availability and 20% panel efficiency. In line with the growth in gross rooftop area across the SSPs, the technical potential for DCSPV also scales up. The largest technical potential in the year 2050 is observed for SSP5 narrative with a value of 33 PWh/yr and the lowest technical potential in the year 2050 is observed for SSP1 narrative with a value of 26 PWh/yr. As a result, in the year 2050 the technical potential of global DCSPV is estimated to be between 26-33 PWh/yr representing an increase of between 24-57% relative to 2020 values. The effects of relative growth in regional gross rooftop area and the effects of inter-annual climatic cycles can be observed in future potentials where developed countries registering a significant increase in their potentials for SSP5 and emerging countries registering a significant increase in their potentials across all SSPs (Figure 3.3c).

Although high growth rates in future gross rooftop area are observed for emerging economies like China, an inverse relationship was observed between the major cities and areas with high grade solar capacity factors emphasising the geographical causation of city growth where mild climate areas are the preferred growth centres (Figure 3.3d-f). This highlights the complimentary global spatial dynamics between DCSPV-UTSPV potentials where location for UTSPV plant siting and for installation of DCSPV can be mutually exclusive.

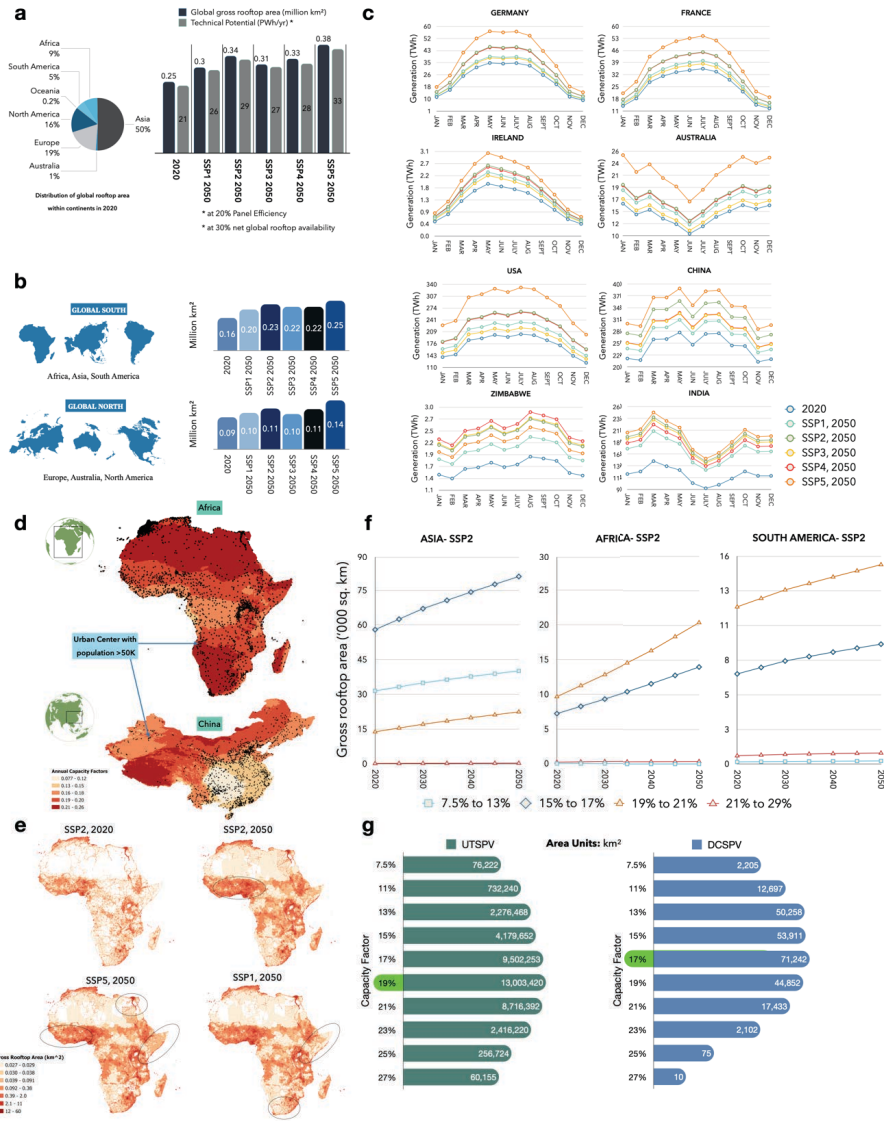


Figure 3.3 | Growth in rooftop area, technical potentials for SSPs and spatial growth dynamics of DCSPV

a, distribution of global gross rooftop area in 2020 between continents, growth in global gross rooftop area and technical potentials for 2050 for different SSPs. **b**, regional growth differences in gross rooftop area between Global South and Global North. **c**, intra annual variation in technical potentials for select countries. Effects of monsoon and location along with differential growth in rooftop area between SSPs can be observed. India and Zimbabwe show high growth in absolute potential for all SSPs. France and Australia show high growth in absolute potential for SSP5. **d**, mismatch between high grade solar capacity factor areas and urban centres. **e**, spatially explicit growth in rooftop area per FN for Africa can be observed in medium grade solar capacity factor areas. The black circles highlight selected regions where growth dynamics can be observed across selected SSPs. **f**, capacity factor wise growth in gross rooftop area for Asia, Africa, and South America for SSP2 narrative. Large growth in gross rooftop area can be observed for capacity factors between 13-19%. **g**, relationship between capacity factors and estimated global gross available land for UTSPV and global gross available rooftop area in km². The green regions highlight the highest capacity factor bin – area relationship for respective technologies. For UTSPV larger global available land is present beyond 17% annual capacity factor bin and for DCSPV more gross rooftop area is present below 17% annual capacity factor.

To expand on this, we conducted a separate assessment of global UTSPV potentials (see Methods) from which we concluded that UTSPV suitable land is spatially more prevalent in high grade solar capacity factor regions and DCSPV suitable rooftop area is more prevalent in medium grade solar capacity factor regions- highlighting the importance of separate representation of DCSPV in energy system analysis (Figure 3.3g) where it is often represented as aggregated solar PV supply technology. Thus, from a purely technology specific point of view, DCSPV's future electricity generation potential is limited by the spatial growth of conurbations in medium grade solar capacity factor areas as opposed to UTSPV whose growth is favoured by high grade solar capacity factor areas.

3.3.2 Role of DCSPV in future global energy transitions

To reveal the global energy system dynamics of utility and decentralised solar PV, we used the MESSAGEix-GLOBIOM IAM. Here we ran the base 11-region model for scenarios representing utility only and utility plus decentralised solar PV configurations to optimise for current policy and mitigation scenarios incorporating 'middle of the road' growth trajectory, (Table 3.1). The base model is configured to inform the energy infrastructure planning by providing a least cost partial equilibrium solution for modelling years 2020-2100. For this analysis we updated the base model which historically represented solar PV technology and cost parameters in aggregated form with a new energy sub-system (Figure 3.4a) that captures UTSPV and DCSPV individually. We also updated the regional model calibrations for historical topology-wise (UTSPV or DCSPV) installed capacity along with differentiated costs (Supplementary Figure B.4) to fully capture the real-world deployment characteristics (more details in Methods section).

Table 3.1 | Scenario description for 11 Region MESSAGEix-GLOBIOM IAM for SSP2 [150, 153]

Policy	Scenario	Technical Specifications	Policy Specifications
Current (CP)	CP _{UT}	Model with only UTSPV supplying electricity to the high-voltage grid. Updated investment costs to reflect regional costs for 2020. Historical capacity and generation calibration for years 2010, 2015, and 2020. UTSPV ground coverage ratio of 0.5 [95].	Incorporates middle of the road socio-economic conditions throughout the century, based on the second marker baseline scenario from the Shared Socioeconomic Pathways (SSP2). It also assumes that climate, energy, and land use policies that are currently ratified are implemented (cut-off date 1 July 2019). Both unconditional and conditional NDC actions as submitted by April 2020 are implemented by 2030. After 2030, the scenario reflects continuation of effort.
	CP _{UTDC}	Model with UTSPV supplying electricity to the high voltage grid and DCSPV supplying electricity directly to consumers with arrangements for self-consumption and grid supply. Updated investment costs to reflect regional costs for 2020. Historical capacity and generation calibration for years 2010, 2015, and 2020.	
Climate (M) [92]	M _{UT}	Same as CP _{UT} scenario	Same as CP with additional total global cumulative carbon budget of 500 GTCO ₂ eq. between 2018-2100 along with zero-carbon in 2050. Accelerated renewable deployment in first half of the 21st century. 1.5-degree global warming constraint with low temperature overshoot across the modelling years, from openly available scenarios of the ENGAGE project.
	M _{UTDC}	Same as CP _{UTDC} scenario	

From our analysis we find that inclusion of DCSPV in a CP scenario (CP_{UTDC}) can lead to minor increase (3%) in overall solar PV generation by 2050 over CP_{UT} scenario. This increase in uptake of solar PV comes at 9% reduction in UTSPV generation (Figure 3.4b). Overall, we observe that DCSPV generation share falls in total global solar PV from 42% in 2020 to 12% in 2050 (Figure 3.4c). This drop in the share can be attributed to reduced incentives for the model to invest in costlier technology compared to UTSPV even after including transmission and distribution costs and energy losses.

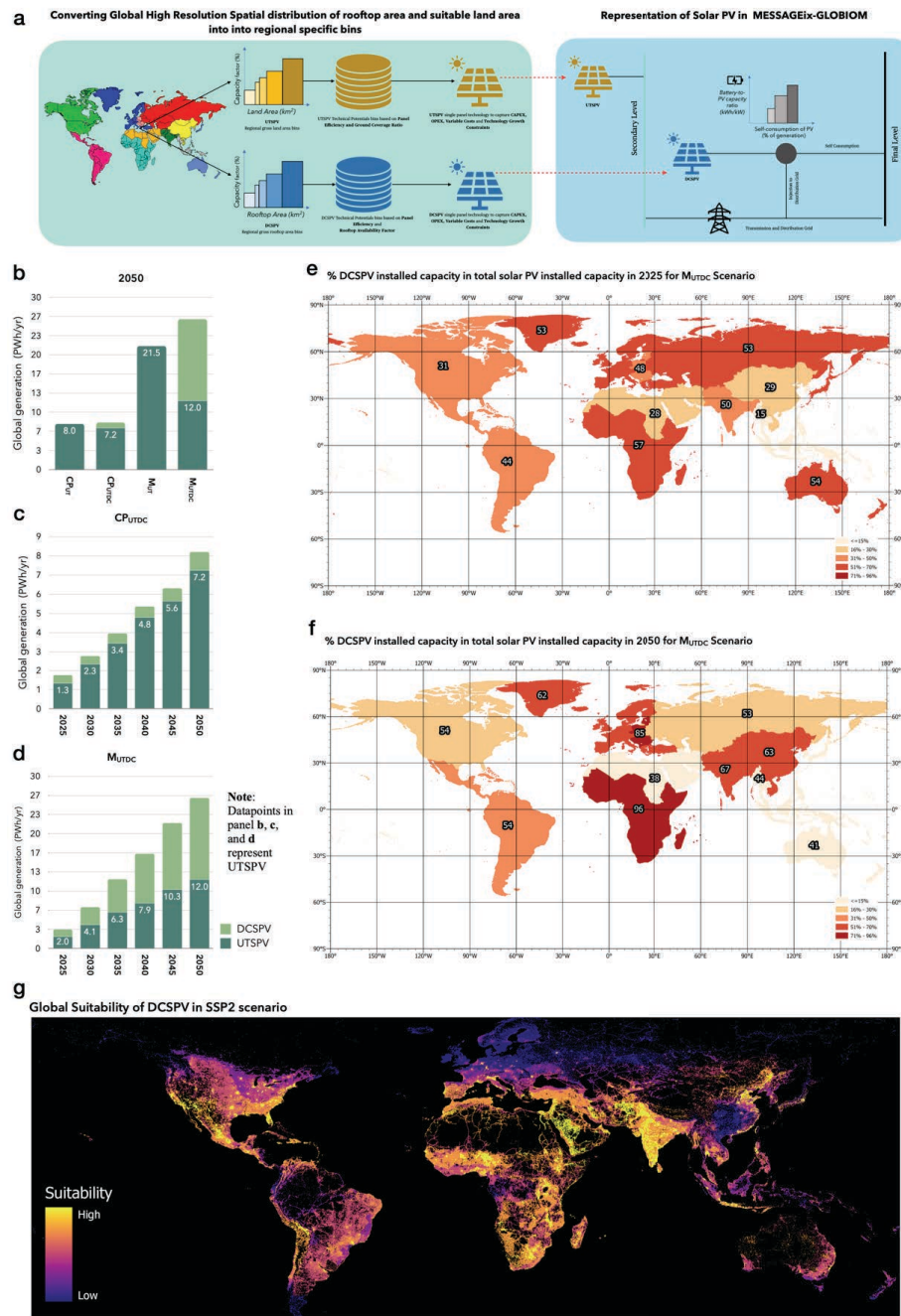


Figure 3.4 | Electricity sub-system flowchart and scenario inputs-outputs

a, the left section represents the steps in conversion of high-resolution spatial assessment into capacity factor binned potentials. The right section represents the updated electricity sub-system in MESSAGEix-GLOBIOM framework. **b**, global total solar PV generation split by topologies for current policy and climate policy scenarios in 2050. **c**, solar PV generation growth in current policy scenario for representation containing both UTSPV and DCSPV. **d**, solar PV generation growth in climate scenario for representation containing both UTSPV and DCSPV. **e**, percentage of DCSPV installed capacity in total installed solar PV capacity for the year 2025 for the 11 global regions. **f**, percentage of DCSPV installed capacity in total installed solar PV capacity for the year 2050 for the 11 global regions. **g**, global suitability of DCSPV considering growth in gross rooftop area between 2020-2050 for SSP2 narrative and solar yearly capacity factors. The regions with high suitability project high growth in rooftop area coupled with high grade solar capacity factors making these regions objectively better suited to deploy DCSPV. Extended details of capacity and generation for CP_{UTC} and M_{UTC} scenarios in Supplementary Figure B.6.

On the other hand, to achieve a more carbon neutral energy system by 2050 (MUTDC), it is more cost optimal to install DCSPV at consumption source. This can be observed whereby DCSPV generation share increases in total global solar PV from 42% in 2020 to 54% in 2050 for MUTDC scenario (Figure 3.4d) leading to an increase of 21% in overall solar PV generation by 2050 over MUT scenario. At a regional level, the biggest uptake of DCSPV in MUTDC scenario was observed for Asia, Africa and South America followed by Western Europe where share of DCSPV can go beyond 50% of total installed solar PV in 2050 (Figure 3.4e,f). Although high penetration of DCSPV can be observed in climate policy scenario, limited conclusions pertaining to intra-region spatial suitability of DCSPV can be drawn from the 11-region aggregated representation of global energy systems. To better understand the intra-regional spatial suitability of DCSPV w.r.t capacity factors, we conducted a multi criterion analysis for global spatial growth in gross rooftop area between 2020-2050 in SSP2 narrative (more in methods). Globally the best regions for rollout of DCSPV can be found in western and southern India, Western Africa, Eastern China, and Western USA along with few pockets in Southern Europe and Latin America (Figure 3.4g)

The effects of increase uptake of DCSPV in MUTDC scenario has significant impacts on other electricity generation sources also. The fossil fuelled, nuclear and wind powered electricity generation decrease by 7%, 12% and 14% in 2050 respectively compared to the MUT scenario, thereby shifting grid management focus from transmission side to distribution side. This also leads to a 10.5% reduction in energy losses in transmission grid and storage that otherwise must work when transmitting and storing electricity from centralised generation to end users (Figure 3.5a,b). When looking at the critical non-cost factors for uptake of DCSPV in MUTDC scenario and incorporating a real-world rooftop availability factor of 30% and panel efficiency of 15%, we observe that rooftop availability factor has a larger role to play than panel efficiency (Figure 3.5c,d). The threshold

of rooftop availability factor at 15% panel efficiency is 50% after which marginal increase in uptake of DCSPV can be achieved i.e., using up to 50% of the gross rooftop area will lead to sizeable uptake of DCSPV beyond which small gains DCSPV uptake can be achieved. Similarly, a panel efficiency of 19% is the threshold after which marginal increase in uptake of DCSPV can be achieved. Thus, in future sustainable building stocks larger gains in uptake of DCSPV can thereby be achieved by first prioritising increase in availability of rooftop for installing solar panels followed by increasing their efficiency.

In addition to providing low carbon electricity deployment, DCSPV can also provide co-benefits for sustainable development. Displacement of UTSPV by DCSPV in MUTDC scenario leads to avoided land-energy competition by 33,000 km² (Figure 3.5e). This avoided land becomes available because of solar PV derived generation shifting from land based UTSPV generation to prosumer rooftops. In addition to land avoidance co-benefit, DCSPV deployment will lead to new jobs in construction, manufacturing, and Operation & Maintenance of DCSPV with a peak of 30 million active jobs globally being made available in 2045 (Figure 3.5f).

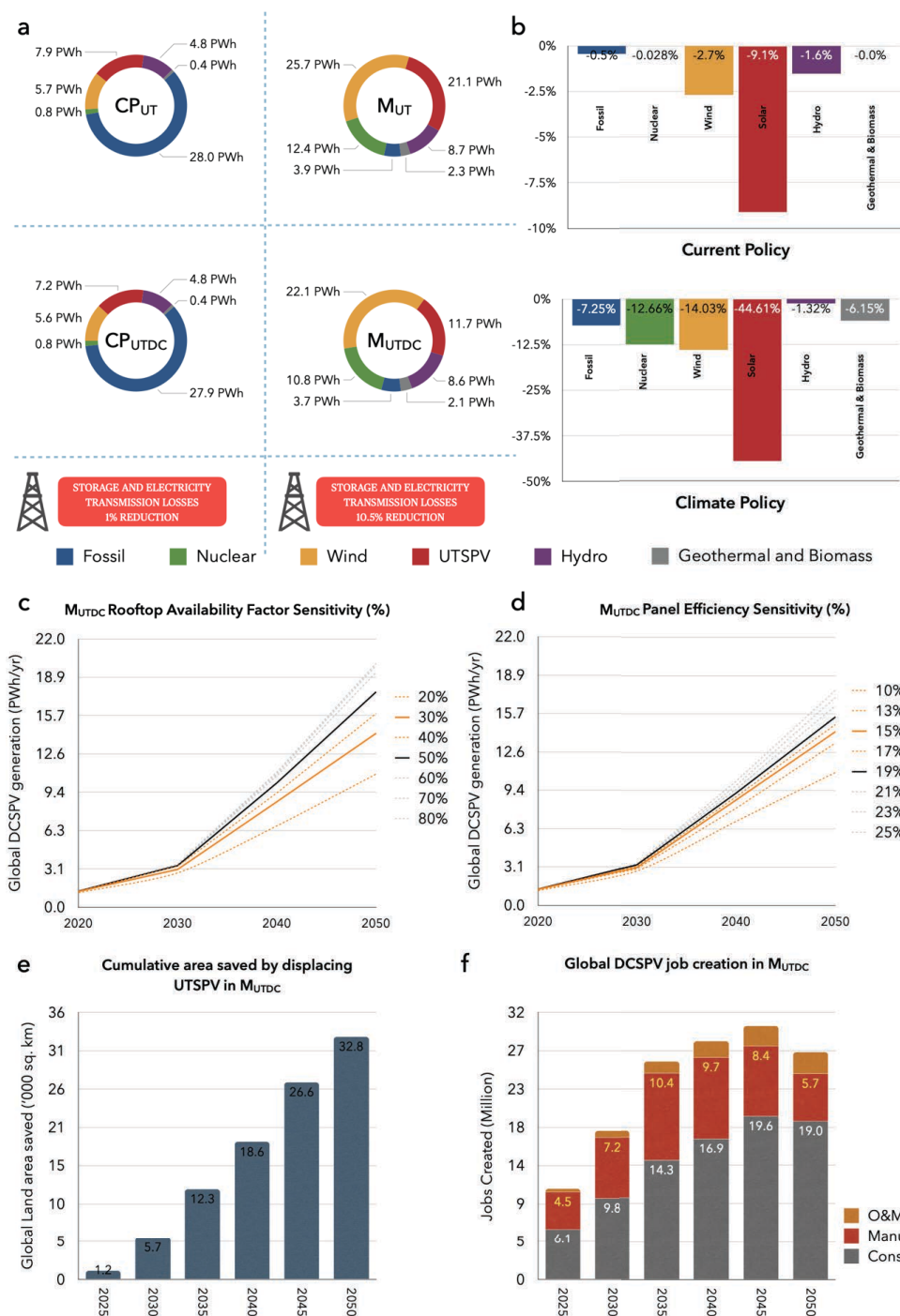


Figure 3.5 | Electricity generation mix for Current policy and Climate policy scenarios with sensitivity analysis

a, Electricity generation mix for CP and M scenarios in 2050. **b**, percentage change in generation mix for current policy and climate policy scenarios between UTSPV only and UTSPV+DCSPV representations for 2050. **c**, change in DCSPV generation in MUTDC scenario with constant panel efficiency of 15% and variable rooftop availability factor. A rooftop availability factor of 0.3 or 30% is the base result around which sensitivity is shown. **d**, change in DCSPV generation in MUTDC scenario with constant rooftop availability factor of 30% and variable panel efficiency. A panel efficiency of 0.15 or 15% is the base result around which sensitivity is shown. **e**, land area saved in MUTDC scenario due to displacement of UTSPV. **f**, global job creation in MUTDC scenario for DCSPV categorised by stages of implementation of DCSPV.

3.4 Discussion

Paris agreement calls for a just and sustainable energy transition including mitigation of climate change. The future energy systems to limit global warming to 1.5°C entails important role for solar PV. The evidence shows that the low carbon energy transitions have mutual synergies for advancing the SDGs^[154]. Pursuant to this the ESMs provide the understanding of how future energy systems shall evolve and the IAMs shall advance by incorporating non-energy dimensions like land and water used to capture the complex interactions of energy system with natural systems. Further, the outputs of the IAMs inform on the implications of energy transitions on sustainable development. Due to the limited information on how the growth in future global rooftop area will transpire, limited analysis has been done to assess the role of DCSPV in low carbon energy system, identification of policy entry points related to distributed energy systems and its sustainability dimensions. In this regard, this analysis draws important conclusions that elucidate the significant role of prosumer driven DCSPV in future low carbon energy systems along with complimentary benefits for sustainable development and energy security.

We find that for the different socioeconomic growth envisioned in SSP narratives, the global rooftop area will grow by 20-54% between 2020-2050. At the same time the electricity generation potential for DCSPV will grow by 24-57%, assuming no change in building archetypes or panel efficiencies. The largest growth in gross rooftop area will happen in the emerging economies spearheaded by Africa and Asia. This highlights the untapped potential for DCSPV as a decentralised renewable electricity generation source for countries undergoing socioeconomic transitions.

This is important as the biggest benefit^[155, 156] of clean energy and prosumer driven climate change mitigation are found in these regions. Additionally,

complementarity is provided by presence of manufacturing hubs of solar panels, high grade solar potential, cost effective labour, a large prosumer base and an active entrepreneurial spirit, providing a sustainable growth option to bring prosperity to growing population.

We show that presence of large DCSPV electricity generation potential does not automatically translate into large power generation levels by analysing the example of Africa and China where there is a misalignment between high grade solar resource and rooftop area growth hotspots. Further, this mismatch between solar capacity factors and regions with high growth in rooftop area lends itself to creation of favourable hotspots for DCSPV deployment. These regions exist in Asia and Africa primarily in Eastern China, Western India, and Western sub-Saharan Africa. Our analysis shows that high-resolution sub-national assessment of renewable resources especially DCSPV can help in identifying favourable hotspots for renewable technology deployment that can better inform policy makers while designing energy policies in developing nations. Additionally, for renewable resources that have fixed spatial attributions e.g., DCSPV whose deployment locations are fixed and cannot be spatially substituted like that of wind turbine driven energy generation, the importance of assessment of spatial distribution of the resource is evident as it can help with prioritising the locations of technology deployment.

Globally 757 million people were without access to electricity in 2021^[157] majority of whom are in Sub-Saharan African and Indian sub-continent region. Being analysed as one of the hotspots for deployment of DCSPV, these areas can rapidly benefit from rollout of DCSPV which have relatively quick deployment time leading to sustainable energy access. We test this hypothesis in a global energy system by implementing scenario analysis representing UTSPV and DCSPV separately in MESSAGEix-GLOBIOM IAM. From our scenario analysis to achieve

net zero carbon energy system by 2050, we conclude that implementation of DCSPV with UTSPV will increase the uptake of solar PV by 21% compared to the scenario where only UTSPV is considered. The share of total installed DCSPV global generation will go beyond 50% by 2050 with Africa and Asia exhibiting more than 60% of solar PV installed capacity in 2050 coming from DCSPV. Additionally, this increase in share of DCSPV will lead to displacement of centralised fossil fuelled and renewable generation to a more distributed electricity generation profile, requiring strengthening of distribution grid infrastructure. In contrast to this, current policy scenario only reveals minor role for DCSPV. This finding is very important as it points to a need for an equal focus on stable distributed grid infrastructure as for the centralised grid infrastructure. The increased distributed generation profile will benefit from micro-generation and will lead to energy security in developing economies.

Our analysis show that DCSPV can invaluablely aid in delivering on SDG11 (sustainable cities and communities) and SDG15 (life on land) by conserving land used for electricity generation infrastructure while providing energy access to underserved markets^[158]. In a future net zero carbon energy system, the transformation from centralised electricity delivery structure to a more decentralised electricity delivery structure will avoid 30,000 km² of land that will otherwise be used for energy related infrastructure. All this can be achieved by utilising a vacant real-estate (rooftops) without modifying the usable land as is required in the case of UTSPV where the majority of global installed capacity lies in croplands^[159]. This is especially important as urban landcover is already modifying around 10,000 km² of global land area per year^[160]. Increased uptake of DCSPV will also lead to reducing local air pollution and support local biodiversity owing to no moving parts or noise when generating electricity using solar PV technology. We also find that along with preserving land use, increased uptake of DCSPV will

lead to generation of 141 million jobs by 2050 which will in turn form a sizeable part of national growth narratives in developing economies.

Our analysis also reveals that principles of sustainability can also be beneficial for low carbon energy systems rather than other way around. For optimal uptake of DCSPV in medium term, rooftop availability will need to increase from a global average of 30% to 50% which would require rapid adaptation of nearly zero energy buildings (nZEB) principles in contemporary sustainable building stock. It can thus be observed from our analysis that sustainability and low carbon energy systems forms a synergistic relationship that will aid in mitigation of climate change. Hence, it is imperative that future energy policy should recognise the socioeconomic benefits that can be accrued by deploying renewable energy technologies. Separate delineation of DCSPV can capture the distinct dynamics of solar PV's role in global future energy transitions, energy storage^[161], new market mechanisms^[130] like utility owned rooftop^[124], and sustainable development.

3.5 Methods

A global assessment of DCSPV technology potential is a complex task as it requires accurate spatial mapping of building stocks and estimation of rooftop area from it. In the past, bottom-up modelling approaches^[80, 81, 84, 85, 89] were used to assess the roof area at sub-national and national scales. Here, the studies focussed on extrapolation of relationships between socioeconomic drivers and rooftop area from a small sample region to a larger ROI. Although these methods are useful for rapid estimation of rooftop area, they often report lower accuracies than the highly spatially resolved methods that utilise large scale surveying of building stocks^[90]. On the other hand, highly spatially resolved top-down^[75, 87, 92, 113, 162] techniques like LiDAR based rooftop mapping which use drone mounted laser to map landscape in 3D, and ML based object detection have shown promising results for ROI covering continental scale. However, extending this to a

global implementation is yet to be achieved due to complexities around capturing accurate geographically diverse samples to train the ML models and the prohibitive cost to map the globe using LiDAR. Moreover, the application of top-down method has been restricted to a single year estimation of rooftop area and only limited studies have researched into advancing the bottom-up methods to future high-resolution estimation of growth in global rooftop area^[60]. This understanding of future growth in rooftop area is an important factor for accurate representation of DCSPV technology in energy system models as the growth is dynamic and organic in nature in contrast to land estimation for UTSPV which is overall static in nature.

To mitigate these bottlenecks, with an assumption that deployment of DCSPV is exclusively reserved for rooftop mounting grid connected solution, for this analysis we combined the bottom-up and top-down approaches to develop a hybrid ML^[76] based framework built on our previous learnings from a single year global estimation of rooftop solar PV^[163]. The framework learns the spatial relationship between downscaled GDP^[164], Population^[91, 104], built-up area extent^[165], and sample building footprints to estimate rooftop area in out-of-sample regions. This way we combine the spatial attributes (built-up area) of top-down modelling with statistical modelling (socioeconomic parameters) of bottom-up methods. Further, by using SSP specific spatially explicit growth in GDP, population density^[166], and built-up area^[167] as drivers to the framework we estimated the growth in global rooftop area. For training the framework, we harmonised our base year data for 2020 and divided the datasets based on a fishnet grid (FN) measuring 1/8 degree (~14 km²) at equator, (Figure 3.6). We then used open-source vector datasets for building footprints^[106] (~700 million buildings covering >84k km² of gross rooftop area for regions across North America, Europe, Asia, Australia, and Africa), and >34 million km of global road network^[168]. For GDP, population density and built-

up extent metrics we used raster datasets upscaled to 1/8-degree resolution to align with our FN grid.

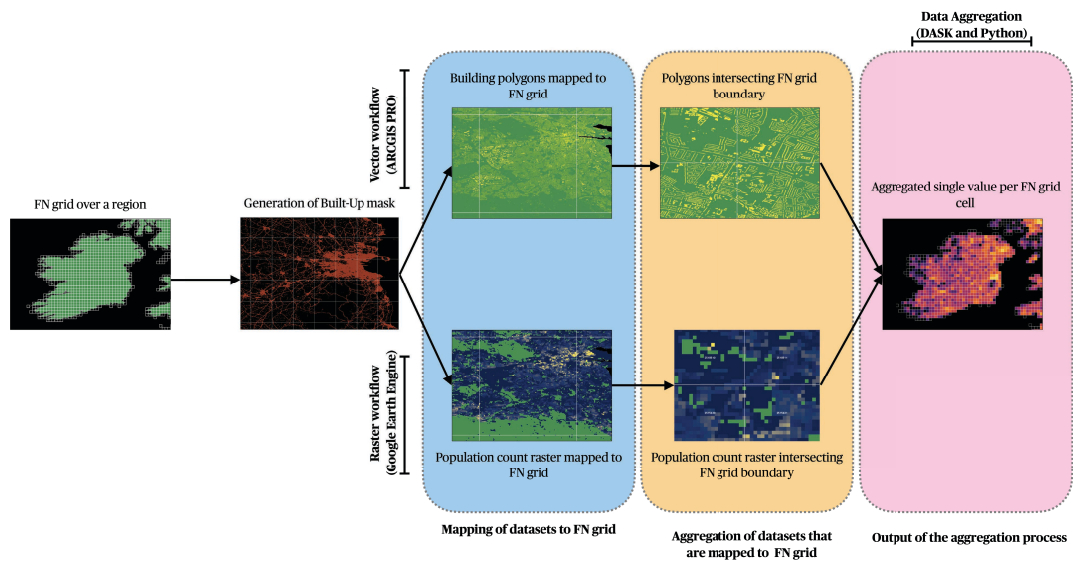


Figure 3.6 | Process flow of data aggregation for FN grid

The countries visualised here are Republic of Ireland and part of the UK. The process starts with creation of a FN grid of 1/8 degree resolution over global land mass. Next, built-up extent layer is used as a masking layer to delineate areas where built-up structures are present in year 2020. The masking layer along with the FN grid are then used to map vector and raster datasets to FN grid that underlie the masking layer. Finally, the vector and raster dataset values are aggregated for each fishnet to generate single value per FN grid cell. Here the vector datasets intersecting FN boundary are split at the boundary and aggregated to the respective FN grid cells while the raster datasets are aggregated by the means of weighted sum.

3.5.1 Data collection

A global fishnet (FN) grid at a spatial resolution of 1/8 degree was generated to define common resolution for all the matrices used in this analysis. This grid cell has an approximate resolution of 14 km² at the equator and the size of the grid cell is dynamic based on the latitude it lies in. This spatial resolution of the grid was chosen to match the FN resolution of SSP derived population and built-up extent datasets. A 14 km² FN also provides us with a large enough extent to capture city limits and a small enough extent to not cover the entire conurbations within itself. Next, we chose 2020 as our base year with 2030, 2040, and 2050 as our medium-term time horizon projection years. Primary datasets collected during this study can be categorised into either a vector dataset -big data derived building

footprint polygons (BF20), OSM derived building footprint (BF20_OSM) and geo-mapped roads (RL20) or raster datasets - base year population (PPLN20), base year built-up extent (BU20), future SSP derived griddled population ($PPLN_{X,Y}$), future SSP derived griddled built-up extent ($BU_{X,Y}$), and future country wise SSP derived GDP ($GDP_{X,Y}$), where X is the SSP narrative and Y is the year. The attributes of the different base year datasets and their sources are documented in Supplementary Table B.1 and Supplementary Figure B.1.

From the collected data from big data sources, we observed that full country coverage of base year building polygon data is available for USA, UK, Australia, and Canada. Full continental coverage is available for Africa except the North Africa covering countries north of the Sahara Desert. For the rest of the world, building polygon data is available in OSM, but the coverage is sporadic with adequate spatial coverage available for the European continent. The base year population count data covers the entire global landmass hence no further filtering or sampling of the dataset was required. The base year global built-up extent dataset has global coverage for the year 2019. We assumed that the coverage at the end of 2019 will be equivalent to the year 2020 built-up extents. The built-up layer captures the extent of human made modifications on the earth. Using a suite of remote sensing techniques, these structures can be isolated from the natural landscape and the area occupied by these structures can be converted into a raster grid where each grid cell can represent either the built-up area contained within it or the percentage of area that is built-up. Naturally, built-up extent will capture roads, tennis courts, carparks, airport runways etc. that do not form part of the building footprint and can sometime cover 2-3 times more area than a building footprint in a built-up raster cell. To account for this, we created a ML model to downscale the built-up extent to estimated rooftop area.

The next step in our study after collection of base datasets for the year 2020 is to collect SSP derived datasets for the years 2020, 2030, 2040 and 2050. In total, we collected SSP derived data for gridded population, built-up extent and GDP per country data for the years 2020-2050. The gridded population count dataset and built-up extent dataset are available as raster dataset at 1/8-degree resolution, with GDP per country dataset mapped to respective country boundaries using administrative boundary dataset from GADM project V3.6 (<https://gadm.org/data.html>). The attributes of the different SSP derived datasets are documented in Supplementary Table B.2 with visual depiction of change in metrics between year 2020 and 2050 depicted in Supplementary Figure B.2.

3.5.2 Base year calibration and spatial harmonisation

After collection and verification of base year datasets and SSP derived datasets we conducted a harmonisation of base years across the datasets. We assumed that the 2019 built-up extent of our BU20 layer will represent the 2020 datapoints. Additionally, the BF20 layer polygon was assumed to represent building footprints for 2020 year. These assumptions add-in a component of uncertainty in the harmonisation, but at a global scale these assumptions will have minimal effect on the final output of the study due to the design of our ML framework.

After temporally harmonising the datasets to a common base year, we aligned the datasets on a common spatial resolution. For this we first started mapping the base year datasets to the FN grid. We overlayed the FN grid on top of the BF20, PPLN20, BU20 and RL20 datasets and used a cookie cutter approach to cut and aggregate the datasets within each unique FN grid cells. Next, the BU20 layer boundary inside each FN was chosen as the region of interest and any datapoint outside this BU20 boundary but inside the FN boundary was not considered. This provided us with the first stage of spatial harmonisation where only datapoints inside the BU20 layer extents were considered. To achieve this, we used area

outside the BU20 layer as a masking layer to select datapoints that are not masked.

The base year vector datasets representing non-masked BF20 and RL20 layers were processed on the ARCGIS PRO V2.8 platform, where we used the inbuilt multicore enhancements to process the clipping and aggregation of vector datasets. After the cutting step, each building polygon and road polyline feature inside each unique FN grid cell was aggregated to represent a single value per FN grid cell. It should be noted that a polygon falling on the FN grid cell boundary was intersected at the boundary and only the area of the polygon inside of the respective FN was attributed to that FN. The base year raster datasets representing non-masked PPLN20 and BU20 datasets were processed on the Google Earth Engine platform^[132]. Both the datasets were clipped at the boundary of the overlapping FN and the pixels completely inside the FN were aggregated as is, with pixels falling on the boundary being aggregated using weighted summation. Here, the value attribution of the pixel in consideration was calculated based on the area of the pixel inside the FN. It should be noted that while PPLN20 dataset represents simple population count at 100m resolution, the BU20 layer pixel represents the percentage of built-up area inside each 100m pixel. Hence, the aggregation of BU20 pixel was undertaken by multiplying the pixel area by pixel value to represent true built-up area represented by each 100m resolution pixel.

The SSP derived population $PPLN_{X,Y}$ and $BU_{X,Y}$ for Y equal to 2020 were spatially harmonised to FN grid by mapping the values from spatially harmonised PPLN20 and BU20 datasets derived in the previous steps. This aids in first providing a common base year value for estimation of future aggregated rooftop areas per FN grid cell and second removes any mismatch of datapoints and data values between the base datasets and SSP derived datasets. The mismatch between the

datapoints occur due to $PPLN_{X,2020}$ and $BU_{X,2020}$ using exogenous methodologies and frameworks to estimate the values in their respective datasets. As an example the $BU_{X,2020}$ dataset points depicting presence of built-up area is derived from a model that uses GHSL^[111] layer from JRC for the year 2015 thereby not incorporating some newly developed areas in east China (Supplementary Figure B.5). Additionally, mismatch between data values can occur when for a FN grid cell $BU_{X,2020}$ layer either under- or over-represents the value depicted by BU20 dataset. As a result of these mismatches, for a BU20 layer's global aggregated built-up area of 1.46 million km², $BU_{X,2020}$ layer only represents 0.98 million km² of global aggregated built-up area. This highlights the importance of harmonising the datasets both at a common temporal and spatial scale.

After harmonising the $PPLN_{X,2020}$ and $BU_{X,2020}$ datasets for each of the SSP scenarios, the future datapoint and data values per FN grid cell of the respective datasets were recalculated using the following:

$$PPLN_{X,Y} = (PPLN_{X,Y} - PPLN_{X,2020}) + PPLN_{20} \quad (3.1)$$

$$BU_{X,Y} = (BU_{X,Y} - BU_{X,2020}) + BU_{20} \quad (3.2)$$

where, for each unique FN grid cell, X is the SSP scenario, Y is the year for which datapoint and value is calculated, $PPLN_{20}$ is the base year population count and BU_{20} is the base year built-up area. This effectively captures the absolute growth in the metrics per FN grid cell over the harmonised base datasets. For GDP value per FN grid cell, we devised population weighted down mapping of country level GDP value using the following:

$$GDP_{X,Y} = \frac{GDP_{C,X,Y}}{PPLN_{C,X,Y}} * PPLN_{X,Y} \quad (3.3)$$

where, for each unique FN grid cell, X is the SSP scenario, Y is the year for which datapoint and value is calculated, C is the country for which aggregated metrics are calculated at country level. This GDP downscaling methodology creates a new feature layer representing GDP weighted population count per FN grid cell for training our ML model discussed in next section. Finally, we create the population density layers for both base year datasets and SSP derived datasets using the following

$$PD20 = \frac{PPLN20}{FN_{Area}} \quad (3.4)$$

$$PPLND_{X,Y} = \frac{PPLN_{X,Y}}{FN_{Area}} \quad (3.5)$$

where, for each unique FN grid cell, X is the SSP scenario, Y is the year for which the datapoint and data value is calculated and FN_{Area} is the geodesic area occupied by the FN grid cell.

3.5.3 Machine Learning model

We designed a ML based framework based on XGBoost ML model^[135] to estimate aggregated rooftop area per FN grid cell. The ML framework accomplishes the task of *first* extracting FN grid cell from BF20_OSM layer derived from OSM global building footprint dataset that have complete building footprint polygon mapping and *second* to estimate the aggregated rooftop area per sample FN grid cells.

We start the development of the ML framework by extracting sample FN grid cells from the base year datasets. The FN grid cells that have complete coverage for PD20, BU20, RL20 and BF20 datasets are selected as sample FN grid cells and the

extracted sample layers are named here as PD_{S20} , BU_{S20} , RL_{S20} and BF_{S20} respectively. The PD_{S20} , BU_{S20} , RL_{S20} sample FN grid cells then act as independent variables with BF_{S20} acting as the dependent variable for the M1 model. The M1 model is then trained by using 10-fold cross validation strategy and 1000 hyper tuning iterations. The 10-fold cross validation strategy enables the use of complete input dataset for training purposes and aids in reducing the problem of overfitting in conjunction with 1000 rounds of hyper tuning iterations. The trained M1 model then accepts PD_{20} , BU_{20} , RL_{20} layers as drivers to estimate the aggregated gross rooftop area for all the global FN grid cells, BF_{FN20} layer.

At this stage, we have a global estimate of rooftop area for the year 2020 which we then use to extract samples from BF_{20_OSM} layer. For this, we compare at FN level the values of BF_{FN20} and BF_{20_OSM} layer. For the FN grid cells where the ratio between BF_{20_OSM} and BF_{FN20} is in between 1.1 and 0.9 i.e., where BF_{20_OSM} values show 90-110% of BF_{FN20} values, those FN grid cells are selected for their completeness of building footprint mapping and extracted as BF_{OSM20} sample layer.

After tuning, training, and inferencing of BF_{OSM20} layer from M1 model, we develop the M2 Model which will enable the estimation of global gross aggregated rooftop area per FN grid cell for SSP narratives. For this, we combined the BF_{S20} samples from base year dataset with BF_{OSM20} samples. We also resampled PD_{20} , BU_{20} and $GDP_{X,Y}$ layers to collect samples based on FN grid cells covering our combined building footprint samples to generate $PD_{S,OSM20}$, $BU_{S,OSM20}$ and $GDP_{S,OSM,2,2020}$ layers. The $GDP_{S,OSM,2,2020}$ layer here represent population based downscaled GDP per sample FN grid cell for samples covering base year and OSM derived Building footprint FN grid cells for SSP2 narrative and

2020 year. The $PD_{S,OSM20}$, $BU_{S,OSM20}$, $GDP_{S,OSM,2,2020}$ sample FN grid cells then act as independent variables with BF_{S20} and BF_{OSM20} acting as the dependent variable for the M2 model.

The M2 model is trained by using 10-fold cross validation strategy and 1000 hyper tuning iterations. At the conclusion of this step, we have our final M2 model which then accepts $PPLND_{X,Y}$, $BU_{X,Y}$ and $GDP_{X,Y}$ layers as drivers to estimate a global $BF_{X,Y}$ layer for five SSP narratives and years ranging from 2020-2050. The final $BF_{X,Y}$ layer is stored as individual geopackage files having 1/8 degree FN grid cell resolution with the value representing the aggregated gross rooftop area inside the FN grid cell.

Although the trained M1 model in conjunction with SSP derived drivers can aid in generation of final $BF_{X,Y}$ layer, we could not implement this as RL20 layer data is only available for base year of 2020 and multivariate regression would be required to estimate its value beyond 2020 which would add an extra layer of uncertainty in our results. Additionally, selection of $BU_{S,OSM20}$ and merger of this layer with BF_{20} layer provided us with additional global data points to retrain a new model M2 which would be more compliant with global trends rather than just the countries/region covered by BF_{20} dataset. Extended details of the attributes of the input building footprint datasets are documented in Supplementary Table B.3.

3.5.4 Technical potential assessment

For converting the estimated rooftop area to electricity generation potential per month, we utilised the PVOOUT factor from World Bank's PV potential dataset for locations between 60°N and 45°S, covering over 99% of the world's population. This dataset is provided as a gridded raster dataset representing kWh produced

by each kWp installed capacity per month. The locations outside the latitudes were assigned a constant PVOOUT value of 3.5 kWh/kWp/day (peak).

The PVOOUT dataset was available at 1km raster cell resolution which we upscaled to 1/8 degree resolution by taking the mean of the underlying raster cell values and converting each FN grid cell to represent monthly capacity factors which we then scale to yearly capacity factors. Next, we assume that for each FN grid cell the gross estimated rooftop area is the total available rooftop area for rooftop solar panel installation. To account for loss in gross estimated rooftop area we utilise the Rooftop Availability Factor which accounts for losses in gross rooftop area due to slope, orientation, and roof superstructures. In wider literature^[163], a rooftop availability factor of 0.3 is used to convert gross rooftop area to net rooftop area. Conversion from estimated rooftop area to technical potential is achieved using following equation:

$$POT_{X,Y} = BF_{X,Y} * CF_{FN} * PE * RAF \quad (3.6)$$

Where,

$POT_{X,Y}$ is the monthly potential in GWa per FN for SSP narrative X and year Y

$BF_{X,Y}$ is the aggregated gross rooftop area (km²) per FN for SSP narrative X and year Y

CF_{FN} is the mean yearly Capacity Factor per FN for SSP narrative X and year Y

PE is the panel efficiency (%)

RAF is the Rooftop Availability Factor (%)

3.5.5 Implementation of decentralised solar PV in MESSAGEix-GLOBIOM

MESSAGEix-GLOBIOM^[169] is a current state of the art global integrated assessment (IAM) model developed by IIASA. The solar PV panel technology is represented as a single technology that represent both UTSPV and DCSPV scale. The model comprises of 11 regions covering 195 countries. The regions are created by grouping countries that are linked by common trade mechanisms and

geographic affinity. The global model can represent future energy and emission pathways by optimising the supply and demand streams within the energy system along with constraints on emission and land use change. The model is technology rich and represents renewable technologies in the form of step-wise curve of generation potential based on capacity factor bins. Additionally, investment costs, operational costs and historical technology capacity can be implemented for each capacity factor bin. We calibrated solar PV in the base global MESSAGEix-GLOBIOM model by updating 1) technology potentials and capacity factor bins, 2) investment cost 3) historical installed capacity. These tasks were performed for both DCSPV technology and UTSPV for all the 11 world regions.

The first step in model calibration is to reassess the UTSPV potentials for all the countries covered by 11 world regions. For this, we utilised a global landcover mask that demarcates global areas that are suitable for installing UTSPV from World Bank. This mask accounts for suitable distance from urban areas, terrain topology, croplands, and protected areas where UTSPV deployment is not preferred either due to international conservation treaties or due to unsuitable land use. Next, we mapped the L2 mask to our FN grid cells that we used for DCSPV assessment. This mapping provides the advantage of having both UTSPV and DCSPV technology assessments on a common spatial resolution. Here it is important to highlight that unlike DCSPV potentials which change year on year based on drivers, UTSPV have been kept constant across the years. The second step in model calibration is to combine the monthly assessed potentials for DCSPV and UTSPV into a yearly value. This is done to align the potentials with the annual time resolution of the current global MESSAGEix-GLOBIOM model. The yearly aggregated potential values were then further grouped by yearly average capacity factor bins for 11 world regions. This step enables the representation of two separate technologies i.e., DCSPV and UTSPV in a structure that is compliant with the current global MESSAGEix-GLOBIOM model.

The capital cost and operational expenditure attribution of installing the DCSPV and UTSPV was derived from the cost of renewable generation 2020 report of IRENA. For each of the 11 regions inside the MESSAGEix-GLOBIOM model, we chose representative country(s) from IRENA report and took the mean of the values. This was repeated for historical installed capacity and generation per region using the historical net-capacity addition data from IEA's renewables 2020 report and IRENA's capacity statistics^[170]. The updated potentials, costs and historical capacity were then added to the base MESSAGEix-GLOBIOM model using custom python scripts that divide potentials into capacity factor bins and ingests the data into the global model. Finally, MESSAGEix-GLOBIOM can model the upper limit to installation growth rate for different regions and different technologies by using the parameter "growth_new_capacity_up". Here we can specify the highest annual growth rate the model can utilise to install a specific technology when finding an optimal solution. In our case we have fixed this to a conservative 5% annual growth rate for all regions except SAS and WEU where we have set 7.5% and 7% respectively in contrast to IEA Renewable 2021's^[171] 7.8% average annual growth rate estimate for its modelling.

The electricity subsystem was created to ensure DCSPV and UTSPV potentials are utilised separately and they feed into the transmission and distribution grid at different energy levels i.e. final and secondary respectively. The DCSPV potentials are directly connected to the final energy level for all the 11 world regions. Provisions were made to split the DCSPV generation into self-consumption and export to the distribution grid to mimic the real-world dynamics of roof mounted DCSPV. The self-consumption part is further divided into 4 steps to capture different levels of self-consumption with battery and without battery storage. The decision to split the DCPSV generation between self-consumption and grid-fed is made during the model run to reflect least cost optimising with perfect foresight. Additional provisions are provided for DCSPV to contribute towards grid stability

and grid management costs, which scales with amount of self-consumption being backed with onsite battery energy storage. This simulates a state where the PV-battery owners provision a portion of their generation or capacity for grid-level services. Finally, a proportional variable is added into the model to allocate additional grid infrastructure as contingency for self-consumption, to account for the fact that the grid needs to be maintained and expanded even if the prosumers would import electricity in fewer hours or days per year, see Supplementary Item B.4.

3.5.6 Land area, job creation and multi criterion analysis

Land area calculations were conducted by calculating five year time step difference in the UTSPV installed capacity between M_{UT} and M_{UTDC} scenarios. The differences in the UTSPV capacity were then converted to land area by back calculating the land required by MESSAGEix-GLOBIOM modelling runs using a ground coverage ratio of 0.5 for UTSPV. The category-wise job creation for global DCSPV installed capacity in M_{UTDC} scenario was calculated by using new installed capacity for rooftop solar PV to new job creation factors from A. Malik et al^[172]. To calculate new installed capacity for DCSPV, we used the installed capacity every 5 year from scenario runs. Multi Criterion Analysis was performed by first converting the FN derived yearly Capacity Factors in equally spaced 10 bins, reclassified from 1-10 where 1 is the lowest capacity factor bin and 10 the highest. Similarly FN derived growth in rooftop area for SSP2 narrative was converted into 10 equally spaced bins reclassified from 1-10. The reclassified binned Capacity Factor and rooftop area growth raster layers were summed to create a suitability value from 0-20 where 20 represent the highest suitability and 0 the lowest (missing or Null values).

Chapter 4: A nature inspired deep learning framework to improve transport energy service demand estimates for future shared socioeconomic pathways

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4.1 Abstract

Meeting current global passenger and freight transport energy service demands accounts for 20% of annual anthropogenic CO₂ emissions, and mitigating these emissions remains a considerable challenge for climate policy. Pursuant to this, energy service demands play a critical role in the energy systems and integrated assessment models but fail to get the attention they warrant. This study introduces a novel custom deep learning neural network architecture (called TrebuNet) that mimics the physical process of firing a trebuchet to model the nuanced dynamics inherent in energy service demand estimation. Here we show, how TrebuNet is designed, trained, and used to estimate transport energy service demand. We find that the TrebuNet architecture shows superior performance compared with traditional multivariate linear regression and state of the art methods like densely connected neural network, Recurrent Neural Network, and Gradient Boosted machine learning algorithms when evaluated for regional demand projection for all modes of transport demands at short, decadal, and medium-term time horizons. Finally, TrebuNet introduces a framework to project energy service demand for regions having multiple countries spanning different socio-economic development pathways which can be replicated for wider regression-based task for time series having non-uniform variance.

4.2 Introduction

Global efforts to contain atmospheric warming within 2°C compared to pre-industrial era form the backbone of our response to mitigate the detrimental effects of climate change. Amongst the energy sectors, the transport sector accounted for 29% of the total global final energy consumption in 2018^[173] and contributed to circa 20% of the total global anthropogenic CO₂ emissions^[174]. This makes accurate analysis of transport sector energy demands considerable with respect to the aim of climate change mitigation, while negotiating one of the basic needs of humanity – the need for mobility^[175]. The United Nations estimates that the global population could grow from 7.7 billion people worldwide in 2019 to around 9.7 billion in 2050. The additional population and economic growth will likely lead to increased demand for transport services.

To enable formulation, evaluation and refining of global and national energy policies, accurate representation of historical and future energy demands in the transport sector is important. Additionally, projecting future energy demands in the transport sector is important for various applications ranging from energy system models that inform future energy scenarios for policy formulation, to infrastructure planning projects that requires future demand estimates to determine the scale of additional infrastructure requirements, to energy companies that use demand estimates to project energy commodities futures prices. In this context, increasing the accuracy of the transport sector's energy demand projections become pertinent.

Projection of energy demand in the transport sector is a nuanced exercise, with infrastructure availability, behavioural aspects and geography of the countries making the prospect of creating a generalised projection method convoluted. In the context of energy systems modelling that inform the global and national climate mitigation efforts, the integrated assessment modelling (IAM)^[176] and

energy system modelling (ESM) communities represent energy demand for the transport sector typically as a physical energy service demand metric in the form of passenger kilometres (PKM) and tonne kilometres (TKM). The PKM metric is the product of the total number of passengers travelling and the total distance travelled by the vehicles for a specific mode of transport. Analogous to PKM, TKM is the product of total tonnes transported by a transport mode and the total distance travelled by the vehicles for that mode.

Projection of energy service demands (henceforth named as demands) requires three main components – historical demands, drivers of the demand and finally mathematical relationships between the demand and its drivers. The drivers are the metrics that have historical coupling with the historical demands and have a sound methodology for their future projected values. Naturally, improving the projection accuracies of future transport demands will require improvement in all the three components. This was resonated in a paper by Yeh et al.^[68] where a renewed call to improve the future transport demands was documented. The paper also called for incorporation of the transport sector related big data to improve the insights presented by the energy system modelling exercise. While big data can provide synergies for the development of transport sector in an IAMs and ESMs, equally important are the methods that model the relationships between demands and drivers.

To model the relationship between drivers and demands, various methods are used ranging from regression to simulation-based approaches. Regression based methods are the most common form of relationship analysis done by the energy system modelling teams to project transport demands^[177]. In regression-based methods the energy demand (including transport demand) is modelled as dependent variable and drivers like Gross Domestic Product (GDP), population, fuel prices etc. are modelled as independent variables^[178-181]. The relationship

between demand and drivers is calculated by mathematically modelling the historical demand-driver trends, which is then used to project future demand values. Simulation based approaches are used to simulate demands for a specific set of demand-driver assumptions and future growth narratives^[182-187]. Here the demand projection is dependent on base year calibrations, elasticity of demands for different drivers, assumptions around how the drivers will evolve over the projection time horizon etc. The simulation of demands is also contingent on the demand dependence of one sector on another sector e.g., relationship between growth in electricity charging infrastructure to growth in electric vehicle ownership. In some studies, simulation-based demand projection is done by assuming the growth in drivers for the projection time horizon. These assumptions are often dependent on the narratives of a specific policy. In any case, Business as Usual (BAU) projections are done using a regression-based approach followed by simulation of demands for different scenarios^[188]. Even outside the sphere of energy system modelling e.g., in the economic analysis of a project, infrastructure planning, etc. transport demand projections tasks are handled by a combination of regression and simulation based methodologies.

Recently, machine learning based approaches that use artificial neural network (ANN) architectures^[189-194] to project transport demand at country level have shown sizeable gain in accuracy over traditional regression-based methods. The machine learning based methods have also shown advantages over nuanced transport demand forecasting methods like discrete choice^[195] and commuter mode choice modelling approaches^[196]. Projecting transport demand is a time-series forecasting exercise and deep-learning architectures have shown promising results in this field^[44, 197-200].

While the contemporary methods work well for projecting transport demands for a single country, projection of these demands for a region as a whole is complex

due to non-uniform variance of the historical demand i.e., the demand cannot be accurately represented by a single regression line. This is because different countries in a region have different demand growth trajectories as they are in different stages of socioeconomic development. One solution to mitigate this issue is to generate demand projection models for each country in a region and then aggregate projected demands for the region. To this further complexity in demand projection is added by different modes of transportation e.g., Air, Rail, Road and Marine and different classes like passenger or freight. It can be observed that generation of multiple individual country's model is not the ideal solution as a region may have more than 30 countries e.g., African continent. At the same time, it is also important to analyse a region as a whole to account for interdependencies of demands between countries.

Acknowledging the complications in the projection of future regional transport demands it can be concluded that any method developed to mitigate this research gap would need to automatically group countries based on their demand trajectories in relation to the drivers and choose an accurate pathway for their demand projection. Additionally, the model should account for different modes and classes of transportation. This task cannot be accomplished by the contemporary artificial neural network methods as these methods learn from the historical demand and driver data, aggregating countries into a single regional time series and providing projections that are biased towards the mean of the aggregated datasets. Effectively, the issues highlighted in the introduction remains the same for both traditional and contemporary methods.

Here, to mitigate the complexities around regional transport demand projection we introduce a novel machine learning architecture – TrebuNet (Figure 4.1), that draws its design inspiration from firing of a trebuchet. The architecture can project the future transport demands of individual countries in a region by training on

historical transport demand and driver relationships and further by automatically selecting accurate demand projection quantile for each country. We further evaluate this architecture on its 1) ability to learn from historical demand and driver data, 2) short term projection capabilities, and 3) decadal projection accuracy on recorded data. The architecture is then applied to generate 1) medium-term transport demand projection for Organisation for Economic Co-operation and Development (OECD) countries for both passenger and freight class of transportation and 2) medium-term global maritime freight transport demand projection. The medium-term transport demand projections are finally compared for their accuracies and fidelity. The machine learning based model architectures are often referred to as a 'Black box', where the internal working of the architecture is not exposed to the end user. We attempt to demystify the 'Black Box' perception by introducing relationship surfaces to aid in visualising the internal workings of the TrebuNet.

4.3 Methods

In this study we explored and analysed the application of TrebuNet by projecting transport demands for OECD countries. We designed transport demand projection models for Air, Road, and Rail mode of transport for passenger and freight classes. Further we applied TrebuNet to global maritime freight transport demand projection. TrebuNet architecture was evaluated for its accuracy with multivariate linear regression, ANN model, Recurrent Neural Networks (RNN), Gradient Boosted machine learning methods.

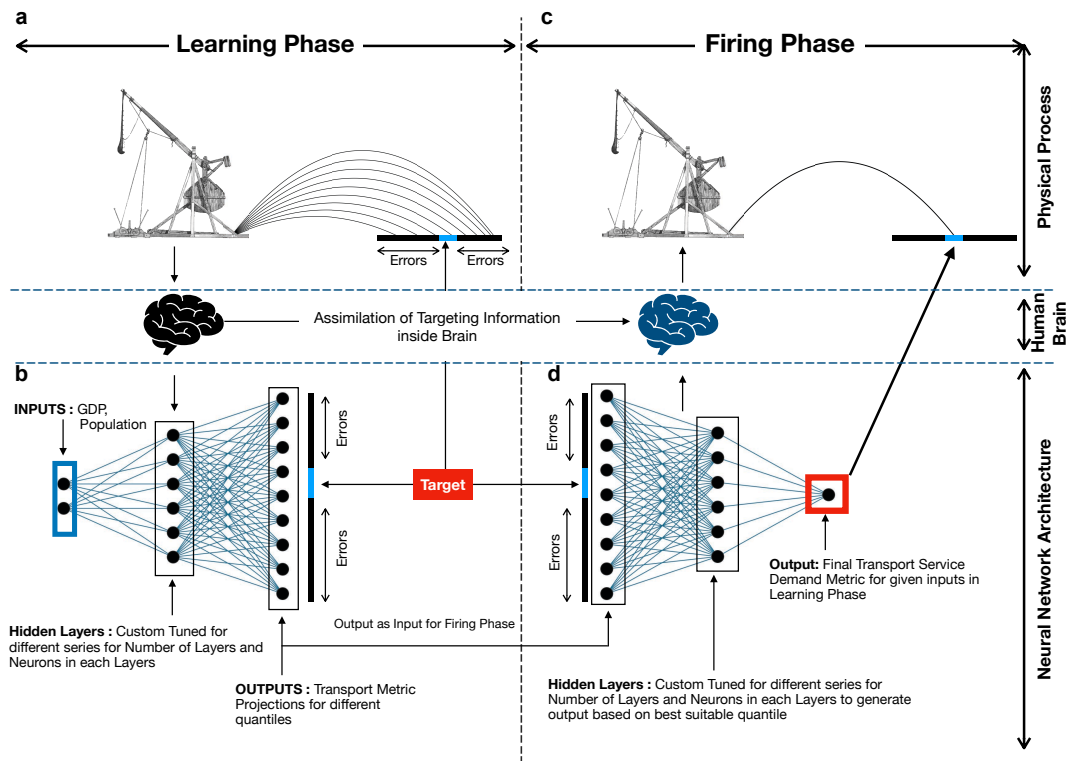


Figure 4.1 | TrebuNet Concept.

a represents the physical process of learning during launch of a projectile, **b** represents the Learning Phase of TrebuNet where different projections for different quantiles are generated. **c** represents the physical process of firing the projectile accurately after learning, **d** represents the Firing Phase of TrebuNet where different quantiles are combined into one accurate projection based on errors in different quantile projections.

4.3.1 Demand and driver relationship

We developed individual TrebuNet models for a combination of transport modes and classes to mitigate the complexity around representing different transport configurations in a single projection architecture. The historical transport demand data for OECD countries was collected for six data series: Aviation- Passenger (AP) and Freight/Goods (AG), Road-Passenger (RoP) and Freight/Goods (RoG), and Rail-Passenger (RaP) and Freight/Goods (RaG). The historical transport demand data for global countries was collected for Maritime Goods data-series (MI), Table 4.1. Spread of the collected data is shown in Figure 4.2, Supplementary Figures C.1-3.

Table 4.1 | Description of data-series and their sources

Data series	Short Name	Transport Metric	Years Covered	URL
Aviation Passenger	AP	PKM	2000-2017	https://unstats.un.org/unsd/mbs/app/DataSearchTable.aspx
Aviation Goods	AG	TKM	1980-2017	https://data.worldbank.org/indicator/IS.AIR.GOOD.MT.K1
Rail Passenger	RaP	PKM	1980-2017	https://doi.org/10.1787/3272dc99-en
Rail Goods	RaG	TKM	1980-2017	https://doi.org/10.1787/b16cb4da-en
Road Passenger	RoP	PKM	1980-2017	https://doi.org/10.1787/3272dc99-en
Road Goods	RoG	TKM	1980-2017	https://doi.org/10.1787/b16cb4da-en
Maritime Goods	MI	TKM	2000-2017	https://unctad.org/system/files/official-document/rmt2018_en.pdf
Gross Domestic Product	GDP	N.A.	1980-2017	https://www.imf.org/en/Publications/WEO/weo-database/2019/October
Population	PPLN	N.A.	1980-2017	https://population.un.org/wpp/Download/Archive/Standard/
Shared Socioeconomic Pathways	SSP	N.A.	2015-2050	https://tntcat.iiasa.ac.at/SspDb/dsd?Action=htmlpage&page=about

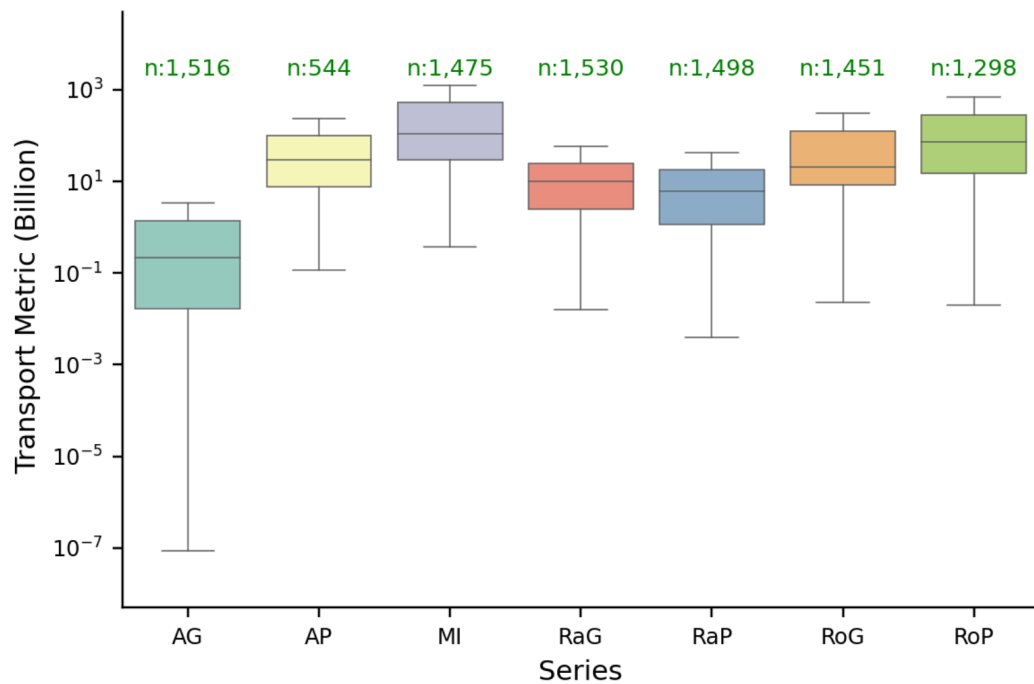


Figure 4.2 | Boxplots showing the spread of the collected transport demands .

Boxplot shows the minimum, maximum, mean and interquartile range for the transport demand data collected for different data-series. The units on x-axis are either PKM or TKM in billions depending on the data-series. The number of observations per data-series is shown on top of the respective box-plot.

The historical demand data was collected from the United Nations and International Transport Outlook'2018 reports. For drivers we used historical socioeconomic matrices in the form of Population^[201] and GDP^[202] (Purchasing Power Parity (PPP), 2005\$). We chose these drivers as they have sound methodology for their future estimation and have shown high correlation with historical transport demand^[203-206]. The relationship between historical transport demand and drivers was established using TrebuNet architecture. A visualisation of trends between transport demand, GDP and Population is shown in Supplementary Figures C.1-3. Statistical description of collected datasets is shown in Supplementary Tables C.1, C.2.

Future projections of transport demands were based on the Shared Socioeconomic Pathway (SSP) database^[151, 207, 208]. The SSPs^[209-211] were created by an international team of climate researchers, economists, and energy systems modellers to generate internally consistent pathways for future worlds across the physical sciences, impacts and mitigation research fields. SSPs are a framework to quantify and represent via socio-economic metrics the different worlds that are possible into the future. The framework for SSPs starts with a narrative defining five different worlds based on challenges to adaptation and mitigation. SSP1 is the sustainable world, SSP2 is the middle ground, SSP3 is the world under regional rivalry having highest challenges to mitigation and adaptation, SSP4 is the world of inequality with highest challenge to adaptation, and SSP5 is the fossil fuelled world with highest challenge to mitigation. The SSP narratives are quantified into different socioeconomic driver metrics, of which we use GDP and population metrics which are proxy for economic and social development respectively to project transport demands using the TrebuNet architecture. SSP pathways were also used to generate scenarios for IPCC 6th Assessment Report (AR6) reports^[212].

4.3.2 TrebuNet Deep Learning Architecture

The Trebuchet Network deep learning architecture or TrebuNet was designed to deliver on two main goals 1) to construct a model that was capable of learning from a pool of transport demand and driver data for a set of countries and 2) the trained model should be capable of accurately projecting transport demand for each country based on its drivers. While achieving the aims, the TrebuNet architecture was designed to work on sparse datasets that have incomplete temporal datapoints.

The inspiration for TrebuNet architecture was drawn from the physical process of hitting a target using a trebuchet. In a trebuchet, the human operator initially learns by trial and error the different projectile pathways to hit a target and then

chooses an optimal pathway to hit the target. To simplify, the physical process of firing a trebuchet can be divided into learning phase where the operator learns different projectile firing pathways and firing phase where the operator uses the learned knowledge to choose best pathway for the target. Correspondingly, the TrebuNet architecture was constructed in two cascading phases - Learning and Firing, (Figure 4.3).

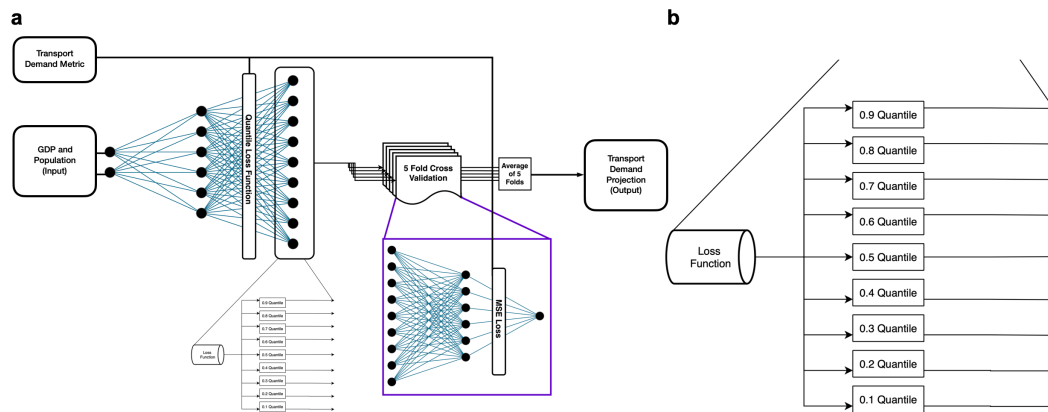


Figure 4.3 | TrebuNet Framework.

a process flow diagram depicting the configuration of the TrebuNet architecture along with flow of independent and dependent variables. **b** presents the zoomed in view of the configuration of custom quantile loss function.

The Learning phase of the TrebuNet comprised of densely connected ANN layers, custom built for each data-series e.g. Aviation Passenger (AP) and Aviation Freight (AG). The densely connected layers had historical socioeconomic driver metrics as inputs (independent variables) and nine outputs (dependent variable) representing transport demands in quantiles from 0.1 - 0.9. The independent variables in this phase were GDP and Population metrics and the corresponding dependent variable were the transport demand metric. The Learning phase had either five or six densely connected input layers, each having neurons ranging from 100-3000. Each layer used uniform activation with 'ReLU'^[213] transfer function for tracking non-linearities. In between each densely connect layer, BatchNormalisation^[214] layers were added to increase learning rates and provide

basic generalising tendencies. The output layer had 9 nodes corresponding to quantiles ranging from 0.1-0.9. The learning phase was trained on historical driver and demand data to reduce a custom quantile loss function. The custom loss (E_t) for the Learning phase is defined as

$$E_\tau = \frac{1}{N} \sum_{t=1}^N \rho_\tau(y(t) - \hat{y}_\tau(t)) \quad (4.1)$$

Where,

$$\rho_\tau(u) = \begin{cases} \tau u & \text{if } u \geq 0 \\ (\tau - 1)u & \text{if } u < 0 \end{cases}$$

$\hat{y}_\tau(t)$ is the predicted value for the datapoint,

τ is the quantile

The Firing phase of the TrebuNet was constructed as a five-fold cross-validated architecture that takes the output of the learning phase as its input. The output was the projected transport demand. Here, the structure comprised of four densely connected layers with neurons ranging from 100-3000. Between each densely connected layer ReLU activation was used. The densely connected layers in this phase were devoid of BatchNormalisation layers due to processing overhead and relative uniformity and likeness of data points. The application of five-fold cross validation methodology helps in reducing overfitting and subsequently in selecting the best model for projection. A combined learning and firing phases were optimised in a single step to realise the best possible model with lowest average Mean Squared Error (MSE) across five folds of the firing phase. Thus, each data-series had two models saved i.e. Learning and Firing arranged virtually as stacked model. A flowchart of the combined stacked TrebuNet model is shown in Figure 4.4, and Supplementary Figures C.4, C.5.

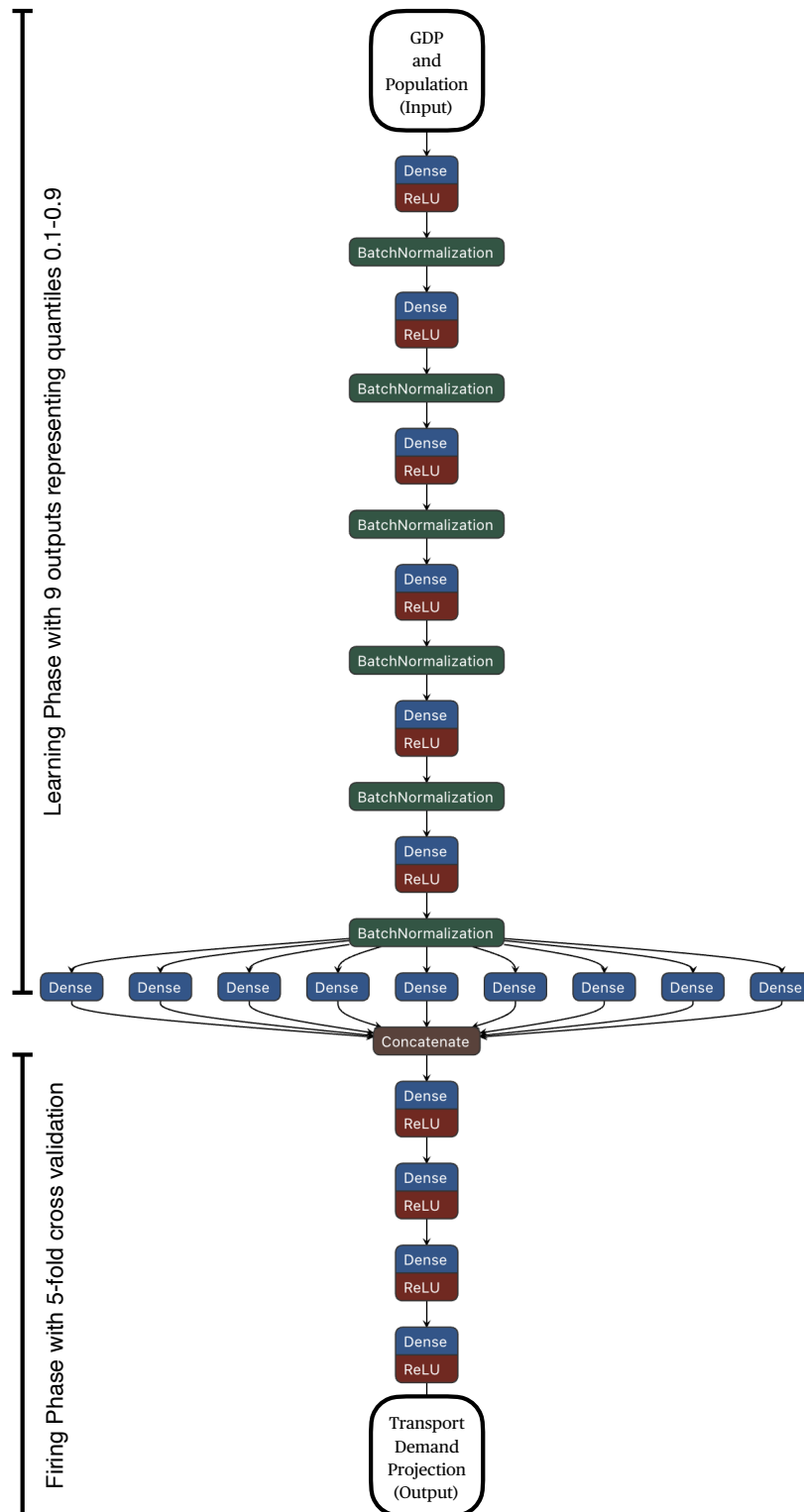


Figure 4.4 | TrebuNet Model flowchart.

Learning and Firing phase of TrebuNet is connected in a stacked architecture. Each densely connected layer in both the phases have ReLU transfer function. BatchNormalisation is implemented between densely connected layers of Learning phase. The inputs to Learning phase are GDP and Population with output being constructed as nine nodes representing quantiles from 0.1-0.9. The Firing phase has nine inputs, and the output is represented by a single node which is the transport demand projection. See also Supplementary Figures C.4,5.

TrebuNet was implemented using python programming language with Pandas^[215], Keras^[216] and Scipy^[217] modules. Keras module was used to implement the densely connected layers and Pandas was used to store, pre-process, and normalise the input driver and transport demand data. The physical process of firing a trebuchet was represented programmatically in the TrebuNet using a feed-forward and back-propagating architecture^[218-220]. This method of learning customised the internal weights and bias of the TrebuNet architecture for countries in different quantiles of global demand growth trajectory and helps in overcoming the problem of mean projections observed when learning to reduce the global Mean Squared Error (MSE) metric^[221]. This method also aided in mitigating the problems caused by non-uniform variance in data across the time series and increases the dimensionality of features.

4.3.3 Hyperparameter optimisation and model selection

The model optimisation and selection were performed by iteratively testing the hyperparameters and selecting the hyperparameters that showed the lowest MSE at the output of the firing phase. The entire TrebuNet architecture was optimised as a single entity and the hyperparameters were selected to obtain the best model with the least amount of average Mean Square Error from the five folds of the firing phase using the Hyperopt module^[222] of python. In total the combined stacked architecture was optimised for 1) Two losses - custom loss in learning phase and MSE in firing phase 2) number of layers in learning phase 3) number of neurons in learning and firing phase 4) number of epochs for both learning and firing phase. The Hyperopt module was run for 500 iterations for each data-series using dual GPU running in parallel comprising of Nvidia 2080Ti and Nvidia 1060Ti (See Supplementary Item). The firing phase of the TrebuNet was designed for five-fold cross validation with the average MSE loss of the five-folds acting as the metric to be reduced by the Hyperopt module. The dual GPU configuration aided in memory sharing between GPU which enabled the parallel five-fold cross

validation in the firing phase. As the firing phase loss was internally connected to the learning phase via virtual back propagation, the custom loss of learning phase was also optimised with the optimisation of MSE. Details of the hyperparameters of the models are documented in Supplementary Tables C.3, C.4, C.5 and C.6.

4.3.4 TrebuNet model generation and evaluation

We generated six different models based on TrebuNet framework for AP, AG, RoP, RoG, RaP, RoG data series using respective historical transport demand and historical driver datasets for OECD countries. Additionally, a global maritime freight model (MI) was also created. Except for aviation and marine freight data-series (see Application in Global marine freight projections) which have 15 years (2000-2015) worth of historical data, all other data-series had 35 years (1980-2015) of historical data to learn from. Each of the data-series generate custom TrebuNet models after choosing the best models during the training and hyperparameter optimisation steps of the TrebuNet architecture. At this stage all the models had learned the historical relationship between their respective transport demand and driver data and stored it inside the architecture as custom weights and bias. The trained models were then further evaluated for their short-term accuracy on unseen data for 2016 and 2017, followed by evaluation of their medium-term accuracy on unseen data from 2020-2050. To enable faster convergence to stability while training, both the historical drivers and transport demands were normalised between 0-1 for their respective data-series. Similar normalisation was done for the SSP derived future drivers using the upper and lower bounds from the historical drivers. During the evaluation process the projections from the models were rescaled based on their original demand data bounds, Figure 4.5.

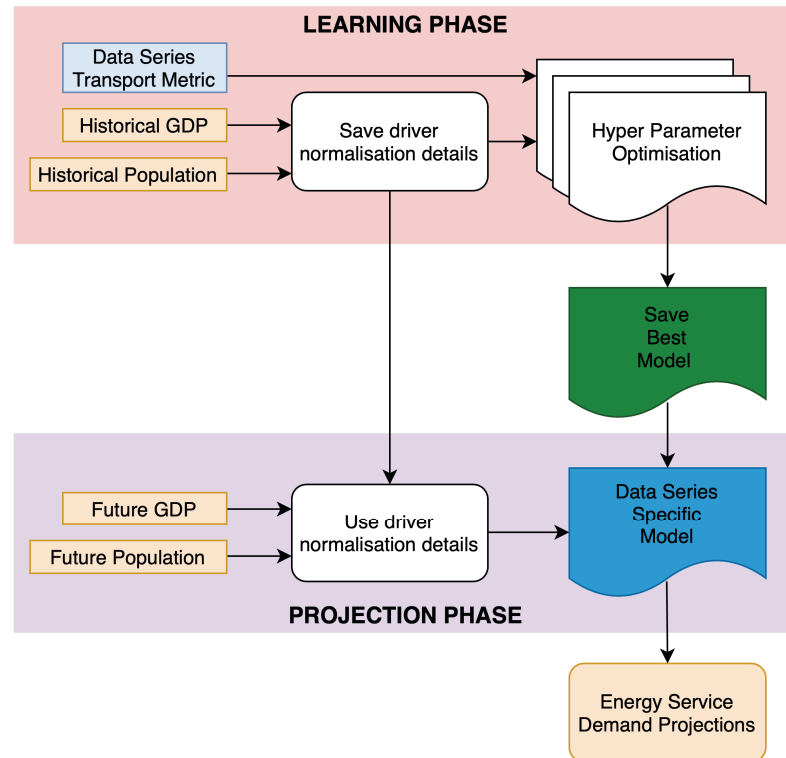


Figure 4.5 | Flow of data and hyperparameter optimisation.

Flowchart depicting the data pre-processing, normalisation, hyperparameter optimisation and prediction steps in a TrebuNet architecture. The training process starts with normalisation of historical drivers and demands. The normalisation information from historical data is saved and used for further normalising future driver values. Hyperparameter optimisation is performed to select the best performing architecture, which is saved as two models- one for the learning phase and other for firing phase. The saved models are then used to project transport demands using normalised future drivers.

Due care was taken to filter out countries from projections where the respective transport medium was not present e.g. land locked countries for marine freight transport projections. One caveat of this approach of projections is that some countries with limited historical data points during the learning phase will result in over or under projected results. One can circumvent this caveat by dropping the country from projection aggregations, but for this study, we kept the countries in the aggregation as it would have resulted in underestimation of regional transport metrics.

Maritime Freight model (MI) was a variant of TrebuNet where instead of OECD, global dataset was used for learning. Transport demand dataset for marine freight is not readily available and the geographical resolution is often limited to aggregated global level with yearly data points. International Energy Agency (IEA) ^[223] provides extended energy balances at regional and country level that has an energy metric that tracks total energy used in international marine freight transport. The data from IEA is available in Exa Joule (EJ) and kilo-tonne of oil equivalent (ktoe) variants. The historical global transport demand was mapped down to country level transport demands using global tonne nautical mile to global ktoe relationship, where tonne mile metric was provided by United Nations Conference on Trade and Development (UNCTAD) and ktoe metric by IEA. Gaps are present in IEA data wherein the aggregation after down mapping doesn't add-up to global tonne mile metric. This model assumes that the down mapped aggregations are the one that TrebuNet learns and projects from. The TrebuNet model for marine freight also follows the same data pre-processing and hyperparameter optimisation steps as the other six TrebuNet models used for short-term evaluations.

The transport demand projections generated by the TrebuNet architecture-based models were compared with the results of multivariate linear regression, a densely connected ANN, RNN networks like Long Short Term Memory (LSTM), Gated Recurrent Unit (GRU), BiDirectional LSTM (BiLSTM), BiDirectional GRU (BiGRU), and finally with gradient boosted method – XGBoost. Details of these models and their flowcharts are shown in Table 4.2, Supplementary Figure C.6.

Table 4.2 | Attributes of models used for evaluation

Model name	Model type	Independent variables (input)	Dependent variables (output)	Spatial Resolution
Reg	Multivariate Linear Regression	GDP, Population	Transport Metric	Individual Countries
ANN	Deep Learning Artificial Neural Network	GDP, Population	Transport Metric	Individual Countries
TrebuNet	Deep Learning Artificial Neural Network	GDP, Population	Transport Metric	Individual Countries
LSTM	Recurrent Neural Network	GDP, Population	Transport Metric	Region
BiLSTM	Recurrent Neural Network	GDP, Population	Transport Metric	Region
GRU	Recurrent Neural Network	GDP, Population	Transport Metric	Region
BiGRU	Recurrent Neural Network	GDP, Population	Transport Metric	Region
XGBoost	Gradient-boosted decision tree	GDP, Population	Transport Metric	Individual Countries

Table 4.2 | Attributes of models used for evaluation (continued)

Model name	Locked parameters**	Hyperparameters used	Training method
Reg	N.A.	N.A.	N.A.
ANN	<ul style="list-style-type: none"> BATCH SIZE OPTIMISER = RMSPROP ACTIVATION_FUNCTION=RELU KERNEL_INITIALIZER=NORMAL 	<ul style="list-style-type: none"> Layers Neurons in each layer Epoch 	Early stopping with MSE metric
TrebuNet	<ul style="list-style-type: none"> BATCH SIZE CV= 5 RANDOM CV SAMPLING PRECISION = 32 BIT OPTIMISER = RMSPROP ACTIVATION_FUNCTION=RELU KERNEL_INITIALIZER=NORMAL 	<ul style="list-style-type: none"> Layers Neurons in each layer Epoch 	5 Fold Cross Validation with custom loss function in Learning Phase and MSE in Firing Phase
LSTM	<ul style="list-style-type: none"> UNITS =32 DROPOUT = 0.2 BATCH SIZE = 32 OPTIMISER = ADAM PATIENCE =10 LOSS = MSE ACTIVATION_FUNCTION=TANH 	Epoch	Early stopping with MSE metric. Training data uses current and previous year driver value i.e. TimeStep=N,N-1
BiLSTM	<ul style="list-style-type: none"> UNITS =32 DROPOUT = 0.2 BATCH SIZE = 32 OPTIMISER = ADAM PATIENCE =10 LOSS = MSE ACTIVATION_FUNCTION=TANH 	Epoch	Early stopping with MSE metric. Training data uses current and previous year driver value i.e. TimeStep=N,N-1
GRU	<ul style="list-style-type: none"> UNITS =32 DROPOUT = 0.2 BATCH SIZE = 32 OPTIMISER = ADAM PATIENCE =10 LOSS = MSE ACTIVATION_FUNCTION=TANH 	Epoch	Early stopping with MSE metric. Training data uses current and previous year driver value i.e. TimeStep=N,N-1
BiGRU	<ul style="list-style-type: none"> UNITS =32 DROPOUT = 0.2 BATCH SIZE = 32 OPTIMISER = ADAM PATIENCE =10 LOSS = MSE ACTIVATION_FUNCTION=TANH 	Epoch	Early stopping with MSE metric. Training data uses current and previous year driver value i.e. TimeStep=N,N-1
XGBoost	<ul style="list-style-type: none"> N_ESTIMATORS=10 CLASS = XGBREGRESSOR 	Number of gradient boosted trees	N.A.

** Unless otherwise stated, all the other parameters to build the model use the "default value". XGBoost v1.6.2, Keras v2.10.0, scikit-learn v1.1.1

These comparisons were performed for *first*- the ability of the models to learn from historical data and project historical transport demand, thereby objectively evaluating the training potentials of models. *Second*- short term projection for unseen future drivers for 2016 and 2017. For comparison of historical learning accuracies between results from different methods, we used R2, Mean Absolute Error (MAE), Root Mean Squared Error (RMSE) metrics. For short term projection comparisons, we used Absolute Error (AE) between recorded and projected transport demands, Absolute Percentage Error (APE) between recorded and projected transport demands, and MAE. These evaluation metrics are defined as follows:

$$AE = \sum_{i=1}^n abs(y_i - \lambda(x_i)) \quad (4.2)$$

$$MAE = \frac{\sum_{i=1}^n abs(y_i - \lambda(x_i))}{n} \quad (4.3)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i - \lambda(x_i))^2}{n}} \quad (4.4)$$

$$APE = \frac{abs(\sum_{i=1}^n \lambda(x_i) - \sum_{i=1}^n y_i)}{\sum_{i=1}^n y_i} \quad (4.5)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \lambda(x_i))^2}{\sum_{i=1}^n (y_i - \frac{1}{n} \sum_{i=1}^n y_i)^2} \quad (4.6)$$

where y_i is the actual transport demand for test instance x_i ,
 $\lambda(x_i)$ is the projected transport demand for test instance x_i ,
 n is the number of test instances.

Comparison of TrebuNet based models with RNN based models is an involved task. The way RNN models are designed and trained allows for projection of only a single country's transport demand. Additionally, RNN based models require the training data and future drivers in a uniform time step e.g., when training data has yearly temporal resolution, the future predictions of transport demands can only be made at a per year basis. This would effectively mean that if the future drivers are available at a five-year timestep (which is the default case for SSPs) then RNN based models cannot be used.

Nonetheless, RNN are currently the state of the art in time-series projection and to enable a comparison between TrebuNet and RNN based models we aggregated the country-wise transport demand and driver data into a single regional time series. This single region time series was then used to train the RNN models. Thus, when comparing results with RNN, the transport demand projections from all the other models had to be aggregated on a per year basis. For regression-based models we used Ordinary Least Square multivariate linear regression model from SKLearn⁷¹ module. For RNN and ANN models we used Keras module, with XGBoost being implemented via XGBoost library for Python.

In addition to the previously created models. TrebuNet architecture was also used to construct three different models for AP, RoP, and RaP data series to evaluate the decadal projection accuracy. Here, historical drivers and energy service demand till 2005 instead of 2015 was used to train and tune the three models. The three TrebuNet models also followed the same data pre-processing and hyperparameter optimisation steps as the other six TrebuNet models generated for short-term projection evaluation. Projections of transport demand for one decade (2006-2015) were done using unseen recorded GDP and Population drivers for the decade. The projections and actual data were then compared to evaluate the performance of the models. A second set of projections were also

generated for the decade which included all the OECD countries for the entire decade with all the transport modes aggregated to compare the results with the IAM models. A summary of the models generated in this study and their evaluation paradigm is shown in Table 4.3.

Table 4.3 | Models and their evaluation paradigm

EVALUATION STEP	METHOD	MODEL	TRAINING YEARS	TESTING YEARS	SPATIAL RESOLUTION
HISTORICAL	TrebuNet	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Country level*
	ANN	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Country level*
	Regression	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Country level*
	XGBoost	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Country level
	LSTM	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Regional level
	GRU	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Regional level
	BiLSTM	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Regional level
	BiGRU	AP, AG, RaP, RaG, RoP, RoG	<=2015	<=2015	Regional level
SHORT TERM	TrebuNet	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Country level*
	ANN	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Country level*
	Regression	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Country level*
	XGBoost	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Country level
	LSTM	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Regional level
	GRU	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Regional level
	BiLSTM	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Regional level
	BiGRU	AP, AG, RaP, RaG, RoP, RoG	<=2015	2016, 2017	Regional level
DECADAL	TrebuNet	AP, RaP, RoP	<=2005	2006-2015	Country level

* When comparing with RNN methods, the country level projections are aggregated to regional level

4.3.5 Relationship Surface

The concept of a Relationship Surface was formulated to visually represent the inner working of the TrebuNet architecture. The idea behind this visualisation was to highlight the learnings and historical demand trends inside the saved models over the real historical data. The relationship surface was generated using historical GDP, population driver data and predictions from a trained model for transport demand based on historical drivers. We generated a new series of input driver data points that covered the entire historical GDP and population metrics by taking the minimum of each driver metric and incrementing it by one unit to reach the maximum of the driver metric. We then ran these driver data points through the trained model and generated the 3D surface called a relationship surface. The three axes of the relationship comprised of GDP, Population, and projected transport demand metrics. Historical transport demands from countries in different stages of economic development inside the OECD region were projected on to the relationship surface for visualisation. These visualisations can help in understanding the approximation and smoothening being done while learning from historical trends and to compare the model against trends expected from other modelling frameworks. This visualisation also aids in circumventing the “black box” notion of deep learning algorithms by closely monitoring trends with respect to each of the input driver metrics.

4.3.6 Uncertainties

Due to the computationally exhaustive nature of machine learning training process, some randomness can always be attributed to the trained models. To minimise the uncertainties in the TrebuNet architecture, all the coding steps involving generation of random numbers both implicit and explicit were seeded with a constant value of 17 during the model saving part of the algorithm. Even with setting of random number seeds inside the code, variance was observed with each subsequent run of the model. To speed up the cross-validation part of the firing phase, each cross-validation fold was designed to run as a parallel

framework of original architecture to be analysed rather than the standard sequential framework. This method also included some randomness into the model as all the five neural networks representing each fold in the cross validation were processed in parallel with simultaneous back propagation. During model retraining after hyperparameter optimisation rounds, multiple runs were performed and the best model with highest R2 value was chosen as the representative model. Due to the nature of transport demands, this randomness provides us with an opportunity to understand a spread of future values which was more practical rather than a set value which tends towards determinism. All other forms of uncertainties e.g. due to parallelisation in workload, limited precision GPU based multiplication, and random weights initiation have been kept out of the scope of this research and can form base for future research work.

4.4 Results

4.4.1 Historical learning potential

Once the models were prepared based on the TrebuNet architecture, they were evaluated on their potential to project the historical transport demand data that was used for training. This exercise was important to compare the different demand projection methods namely regression, ANN, RNN, XGBoost and TrebuNet based. Two separate tests were conducted to analyse the historical learning potentials. The first test was at a regional level where country level historical projections from TrebuNet, ANN and Regression models were aggregated to the regional level and compared with historical projections from RNN model. Second test was at a country level where historical projections from ANN, Regression models and XGBoost models were compared with historical projections from TrebuNet models. For all the test metrics, the projected historical transport demand was compared with the actual recorded transport demand. Here, it is important to note that the best models should not only provide accurate

trends, but also improve on under and over projection tendencies usually associated with time series projection tasks.

From the Regional level tests, it was observed that TrebuNet based models showed a better R^2 , MAE and RMSE values than other three projection methods for AP, AG, and RoG data-series. For RoP, RaP, RaG, and BiGRU based approaches showed better R^2 , MAE and RMSE values. From this we conclude that TrebuNet based models performed better in half of the data-series. For rest of the three data-series, TrebuNet was a close second contender. From the country level tests, it was observed that TrebuNet based models showed a better R^2 , MAE and RMSE values than the other three projection methods for AP, AG, RaG, and RoG data-series. For RoP, RaP XGBoost based approaches showed better R^2 , MAE and RMSE values. For RoP and RaP data-series TrebuNet based models were a close second.

Overall, from the historical learning tests both at regional and country level it was concluded that TrebuNet provides sizeable increase in demand projection accuracies compared to other traditional and contemporary methods, see Table 4.4 with Supplementary Tables C.7 and C.8. This meant that TrebuNet was capable of accurately capturing the historical relationship between transport demand and its drivers both for a country level disaggregation and regional aggregations. Additionally better R^2 , MAE and RMSE compared to other methods meant that the TrebuNet based models were not only improving the absolute accuracy in projecting demand, but they were also tracking the demands in a way that reduced the under or over projection tendencies. The primary reason for better performance of TrebuNet based models was the implementation of quantile-based disaggregation within the framework. It was observed during the initial runs of the data exploratory exercise using ordinary linear regression, that different countries produce better results in different quantiles e.g. USA performed best in

circa 0.9 quantile of input data and Iceland in 0.1 quantile approximation. Other methods provided learnings and projections for only the median quantile i.e. 0.5, which presented an opportunity to develop TrebuNet architecture. As such the ANN and RNN based approach performed much better than a linear regression model in approximating historical data but implementing TrebuNet provided sizeable gains.

4.4.2 Short-Term projection evaluation

Short term or a year look ahead transport demand projection is an important use case for development of novel demand forecasting models. While the historical learning capability of the models aids in selection of the best model, short term demand projection accuracy delineates the generalisation capability of the trained models over unseen data. Using the same test methodology as the historical learning comparisons, we tested the short-term demand projection capabilities of all the methods at regional and country level. The short-term demand projection evaluations were performed for 2016 and 2017 using unseen socioeconomic drivers that were not exposed to the training steps. Here we used Absolute Error (AE), Absolute Percentage Error (APE) and MAE as the evaluation metrics which were calculated by comparing the projected transport demand with recorded transport demand for 2016 and 2017.

For the regional level tests, it was observed that TrebuNet based models performed better for AP, RaP, and RoG data-series compared to other methods, see Table 4.4 with Supplementary Tables C.7 and C.8. For country level tests, TrebuNet performed better for all the data-series except RoG where XGBoost based model performed better. The model suitability when evaluating historical trends also manifested in their suitability for short-term projections. Of importance was to note that ANN and regression-based models showed the least favourable results both in historical and short-term evaluations. For some data-series like RaP

and RoP both in regional and country wise short term evaluations, TrebuNet based models showed better results compared to their historical evaluation performance. In terms of APE for different data-series, TrebuNet based models showed objectively better performance than ANN and regression-based methods and equal performance to RNN and XGBoost based methods especially in regional RaP and RoG data-series, Figure 4.6. Large errors observed in case of RaG and RoG data-series can be attributed to function of transport demand being dependent on movement of goods, where even small GDP countries can record high volume of goods movement and dependence of some countries on predominantly road or rail as means of goods transfer.

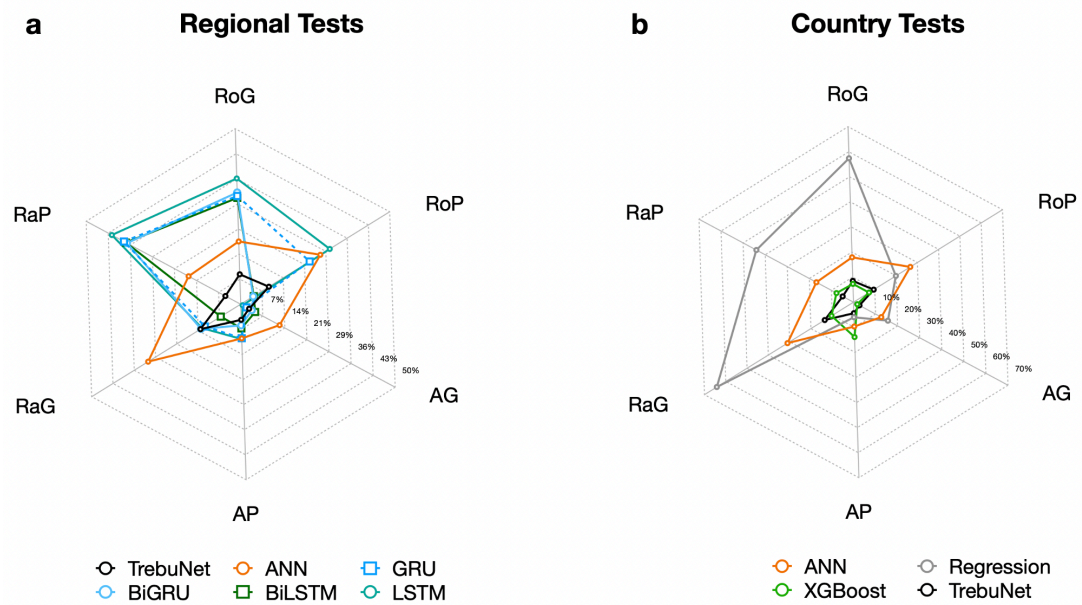


Figure 4.6 | Absolute Percentage Error in short-term transport demand projection

a absolute percentage error in predicting respective data-series using trained model over recorded 2016 and 2017 data-points for regional level assessments. **b** absolute percentage error in predicting respective data-series using trained model over recorded 2016 and 2017 data-points for country level assessments.

Table 4.4 | Historical and Short-term model ranking based on MAE.

	Regional Level		Country Wise	
Series	Historical	Short Term	Historical	Short Term
AP	TrebuNet (57,982)	TrebuNet (166,271)	TrebuNet (9,443)	TrebuNet (23,960)
AP	LSTM (187,057)	BiGRU (226,042)	XGBoost (12,089)	ANN (30,164)
AP	BiGRU (187,078)	BiLSTM (257,712)	ANN (17,060)	XGBoost (35,667)
AP	BiLSTM (188,377)	GRU (362,542)	Regression (29,243)	Regression (41,356)
AP	GRU (207,135)	ANN (364,822)		
AP	ANN (242,429)	LSTM (371,620)		
RoP	BiGRU (240,146)	BiGRU (301,518)	XGBoost (18,988)	TrebuNet (45,762)
RoP	BiLSTM (257,977)	BiLSTM (304,709)	TrebuNet (23,736)	XGBoost (50,820)
RoP	TrebuNet (518,592)	TrebuNet (644,432)	ANN (43,475)	Regression (71,940)
RoP	GRU (525,919)	GRU (1,641,243)	Regression (58,412)	ANN (82,096)
RoP	LSTM (578,491)	ANN (1,819,154)		
RoP	ANN (691,897)	LSTM (2,033,868)		
RaP	BiGRU (36,366)	TrebuNet (32,110)	XGBoost (2,446)	TrebuNet (4,525)
RaP	BiLSTM (41,414)	ANN (109,535)	TrebuNet (2,584)	ANN (5,491)
RaP	TrebuNet (41,501)	BiGRU (260,572)	ANN (4,333)	XGBoost (6,362)
RaP	GRU (57,160)	BiLSTM (268,421)	Regression (22,556)	Regression (19,014)
RaP	LSTM (59,210)	GRU (272,149)		
RaP	ANN (105,547)	LSTM (278,898)		

Note: The green coloured cell represent TrebuNet models and Red coloured cells represents top performing model. MAE values are in bracket and have units in billion TKM or PKM based on the data-series.

Table 4.4 | Historical and Short-term model ranking based on MAE. (Continued)

	Regional Level		Country Wise	
Series	Historical	Short Term	Historical	Short Term
AG	TrebuNet (2,064)	LSTM (1,921)	TrebuNet (225)	TrebuNet (636)
AG	BiGRU (3,122)	GRU (2,794)	XGBoost (343)	XGBoost (683)
AG	BiLSTM (3,287)	BiGRU (3,484)	ANN (541)	ANN (865)
AG	ANN (4,815)	TrebuNet (4,473)	Regression (741)	Regression (998)
AG	LSTM (9,213)	BiLSTM (4,556)		
AG	GRU (9,883)	ANN (12,250)		
RaG	BiGRU (80,086)	GRU (372,453)	TrebuNet (6,320)	TrebuNet (19,953)
RaG	TrebuNet (118,654)	BiLSTM (386,091)	XGBoost (6,496)	XGBoost (24,027)
RaG	ANN (153,763)	LSTM (400,862)	ANN (13,134)	ANN (36,703)
RaG	BiLSTM (268,386)	BiGRU (412,652)	Regression (70,604)	Regression (88,569)
RaG	LSTM (289,437)	TrebuNet (417,824)		
RaG	GRU (324,291)	ANN (962,240)		
RoG	TrebuNet (166,025)	TrebuNet (321,730)	TrebuNet (10,695)	XGBoost (24,591)
RoG	ANN (389,483)	ANN (674,452)	XGBoost (10,885)	TrebuNet (43,422)
RoG	BiGRU (417,701)	BiLSTM (1,142,575)	ANN (24,952)	ANN (47,162)
RoG	BiLSTM (485,643)	GRU (1,163,011)	Regression (89,682)	Regression (126,012)
RoG	LSTM (517,323)	BiGRU (1,200,845)		
RoG	GRU (526,371)	LSTM (1,35,1167)		

Note: The green coloured cell represent TrebuNet models and Red coloured cells represents top performing model. MAE values are in bracket and have units in billion TKM or PKM based on the data-series.

4.4.3 Decadal projection evaluation

To evaluate the performance of the TrebuNet architecture for multi-year projection tasks, we compared the decadal transport demand projection capabilities of the TrebuNet architecture with the actual transport demand and further with benchmark SSP marker model IAM model results. We chose passenger mode of transportation for this comparison as this mode of transportation has relatively more complex transport demand and driver dynamics compared to freight class due to the dynamics of passenger movement. Historical demand and driver data until the year 2005 for AP (year 2000-2005), RaP (year 1980-2005), and RoP (year 1980-2005) were used to generate three models based on TrebuNet architecture, Supplementary Table C.5, C.6. The trained models were then used to project the country wise demands for the years 2005-2015 based on the driver data.

All three models recorded an $R^2 > 0.97$ when comparing decadal projected and actual transport demand, (Figure 4.7a-c). These results demonstrated the accuracy of the architecture and highlighted its long-term projection capabilities. Further, we aggregated the projected transport demands for Air, Road, and Rail mode of transport to generate a single aggregated transport demand projection with yearly time step. This aggregated decadal transport demand projection enabled harmonised comparison with the results of the IAM modelling runs. Here, the results compared well with the projections generated by the global IAM teams utilising different statistical modelling approaches (Figure 4.7d). It was also worth noting that a future unseen event i.e., dips in demand due to the great recession induced drop in GDP for the year 2009 (Figure 4.7e) was successfully captured by the TrebuNet architecture.

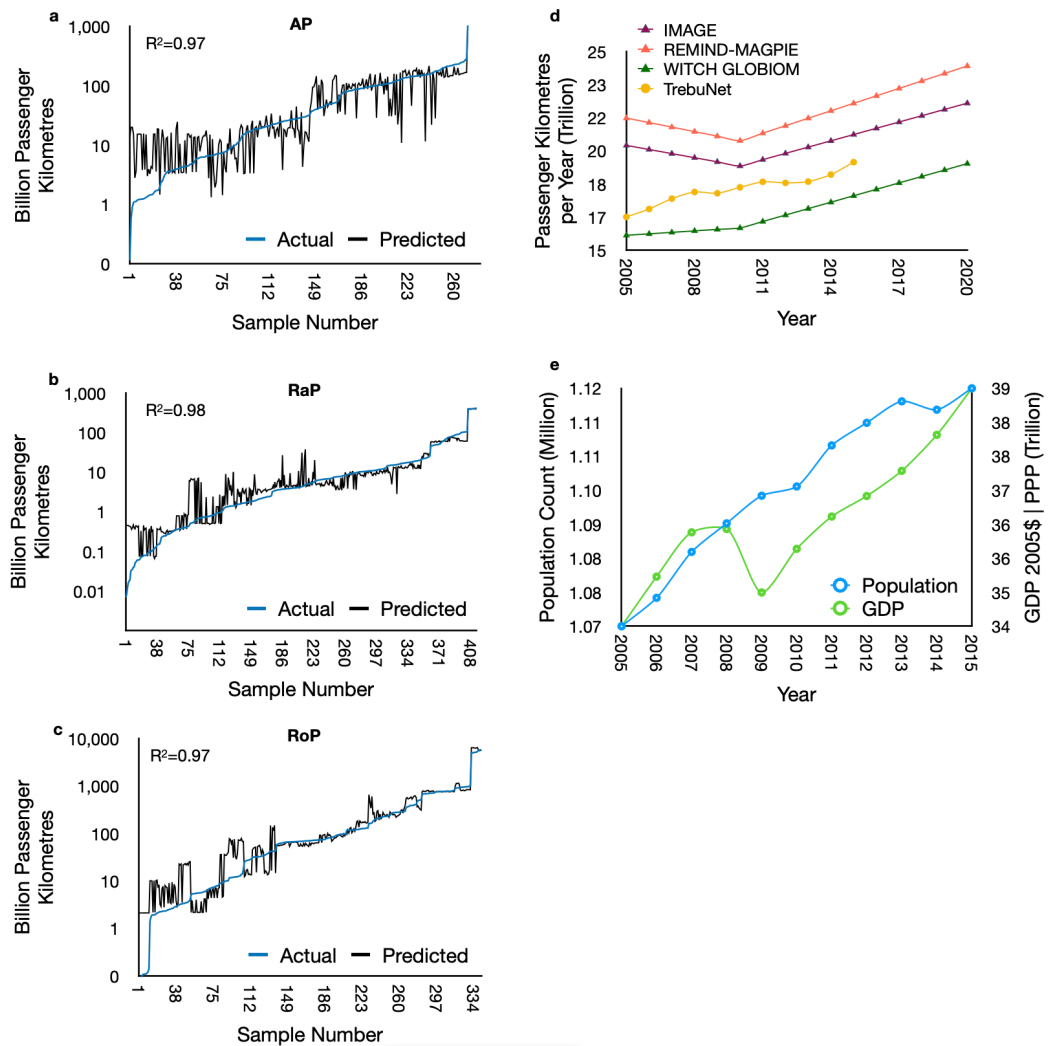


Figure 4.7 | Decadal projection evaluation

a-c, figures showing the trend between actual recorded historical decadal demand and predicted historical decadal demand from the TrebuNet models. Three different models were used to generate predicted historical demand for RaP, RoP, AP data-series. The data series have data points for OECD countries. **d**, total aggregated decadal demand projections for three different sub-categories of passenger mode and comparison with IAM models. **e**, trends in GDP and Population metrics between 2005-2015. Here Population is on the primary Y-axis and GDP on secondary Y-axis.

4.4.4 Medium-Term projection application

Medium-term projections were generated for years 2020-2050 for all six data-series based on learning from historical transport demand and driver data until 2015. Here SSP derived future driver datasets were used to generate future transport demand projections. The training historical demand and driver data was provided at country level at yearly time step. The transport demand projections were generated at country level with five-year time steps. Here the flexibility of the TrebuNet model over state of the art RNN methods was apparent where yearly time step training data can generate the model which can be used for five yearly time step projections. From the projected transport demands, passenger and freight data-series were aggregated under respective modes i.e., Air, Road, and Rail to compare with the projections from IAM modelling runs. Further, saturation characteristic of the total transport demands with respect to GDP per capita were generated. These saturation curves are indicative of natural phenomenon in transport sector where a saturating trend in demand is observed with increasing GDP per capita. Here, SSP1 (Supplementary Figure C.7), and SSP2 (Figure 4.8) narratives-based scenarios are highlighted to show demand trajectories. From the results we observed that the medium-term projections of transport demands generated by TrebuNet based models were within the range of values projected by global IAM teams^[224]. Similar results were observed for saturation curves for both passenger and freight series highlighting that the TrebuNet architecture was capable of accurately recording the natural historic saturation trends in the transport demands.

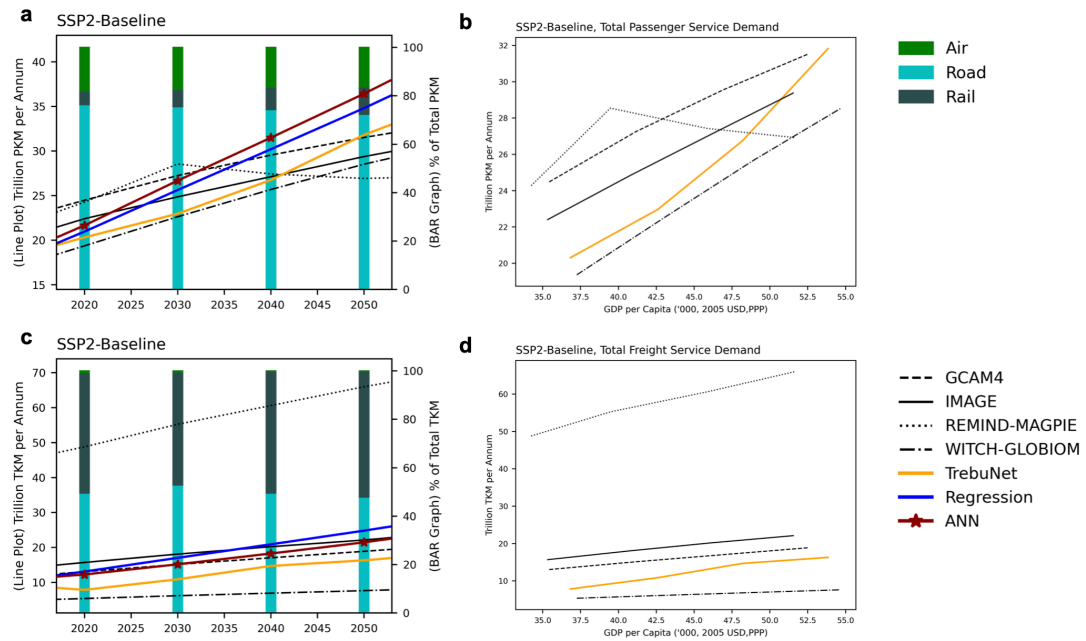


Figure 4.8 | Medium-term projection evaluations

SSP2 narrative based transport demand projections in Trillion Passenger Kilometres units **(a)** and saturation curves **(b)** for passenger mode of transport for OECD countries with TrebuNet model and IAM comparisons. SSP2 narrative based transport demand projections in Trillion Tonnes Kilometres units **(c)** and saturation curves **(d)** for freight mode of transport for OECD countries with TrebuNet model and IAM comparisons. Bar graph in panels **a**, **c** represent the percentage contribution of each transport mode in total demand. Additional comparison with other methods used in this study are also depicted along with established global IAMs

4.4.5 Application in global marine freight projections

To evaluate the application of TrebuNet architecture, a seventh data-series was generated for the global marine freight transport which was not included in the medium-term transport freight projections. The marine freight demand projection is lacking in current energy literature due to the lack of historical country specific maritime freight transport demand data-series. However, the IEA does generate country-wise disaggregated total energy consumption for marine freight which provided a rudimentary method to increase the resolution of the transport demand data from global to regional and country levels.

A custom TrebuNet model was generated for marine freight at the global level instead of OECD level as was the case with the rest of the models. Generation of marine freight demand at the global level helps in comparing global medium-term projections with established reports from the international organisations^[225-227]. The model generated an R^2 of 0.86 for 2000-2015 years' worth of historical learning. The projections of maritime freight demand until 2050 are shown for all five SSP scenarios with comparison points depicting various international organisations (Figure 4.9). Here it is pertinent to highlight that the model performed commensurate with other global reports based on just two input driver metrics i.e., GDP and population. As this sector contributed to 80% of global freight transport demand in 2016^[228], applying TrebuNet architecture to this problem filled data gaps, improved data aggregation methods, and finally provided a new toolset to validate transport demands in other IAM models.

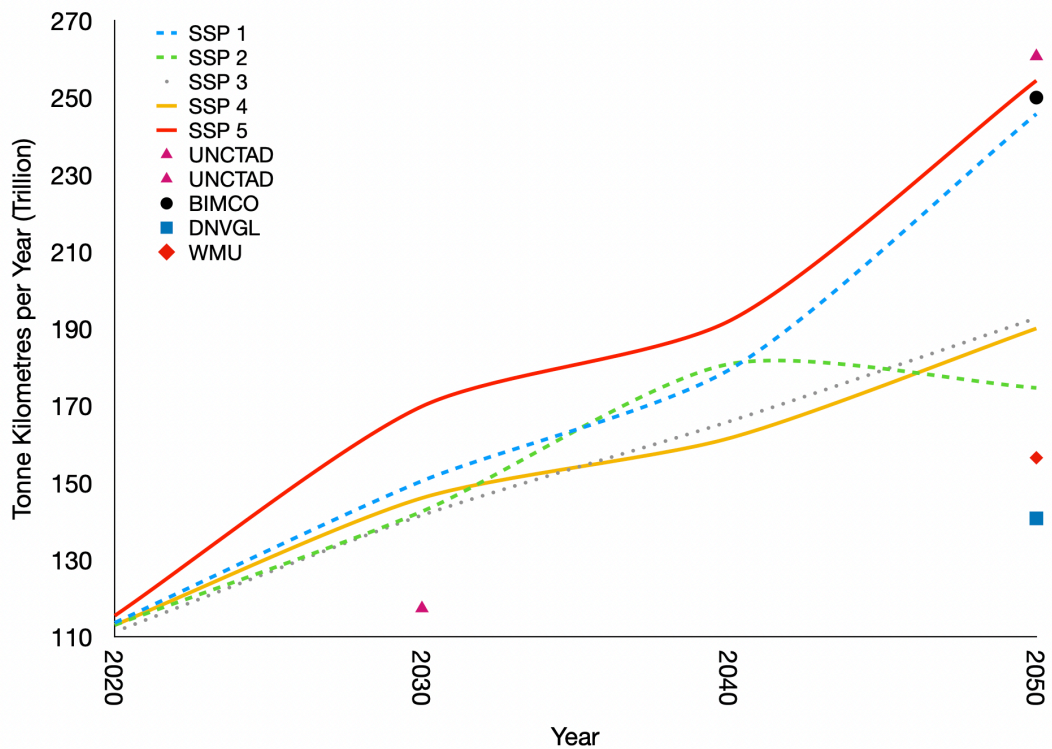


Figure 4.9 | Global Maritime Freight projections

Global maritime freight projections using TrebuNet architecture and its comparison with various world organisation's demand projections using fundamentally different modelling techniques.

4.4.6 Relationship Surface

A Deep Learning architecture such as TrebuNet is often dismissed due to it being perceived as a 'Black Box', where the internal working of the architecture is not exposed to the end user. The internal workings of a model are important to aid in validating the trends that the architecture has learned and hence to check the compliance of the model with the established knowledge base. When doing the demand projection, it becomes pertinent to check if the socio-economic drivers and demands are following proper historical relationships. Often this is represented in the form of polynomial relationship equations between driver and demand. We circumvented this "Black Box" perception by generating relationship surfaces between historical values of drivers and model projected historical demands and plotting how this relationship surface mimics the historical trends. Figure 4.10 showcases aviation cargo (Goods), Road Passenger and Road Freight

relationship surfaces with a zoomed in view of Germany and France. Here it was observed that the TrebuNet has accurately subsumed the country wise trends into its learnings. Any projection within the driver and demand input ranges will fall on the relationship surface which is fixed for every model.

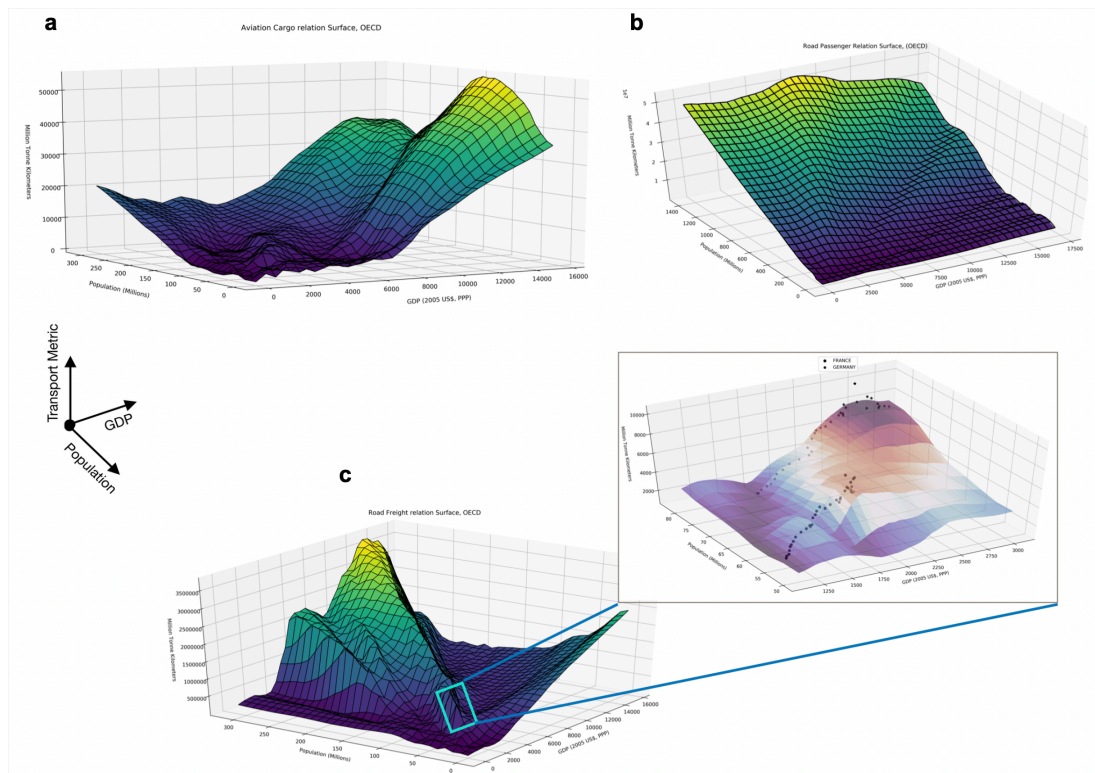


Figure 4.10 | Depiction of relationship surfaces inside Trebunet

a, Aviation Freight Relationship surface between GDP, Population, and Transport demand. **b**, Road Passenger Relationship surface between GDP, Population, and Transport demand. **c**, Road Freight relationship surface inside TrebuNet with zoomed in figure representing Germany and France trend curves.

4.5 Discussion

Accurate projection of transport demands can lead to improved accuracies in designing global energy system models which in turn inform the current climate change mitigation efforts. Not only are the accurate transport demand projections important for energy system models, but they also act as a backbone for global energy markets. Energy planners, infrastructure developers, energy technology companies require accurate demand projections for conducting scenario feasibility and economic analysis. Until now, transport demand projection tasks were handled by simulating demands or by using regression-based analysis. Due to the exponential increase in computational power, machine learning based methods have started augmenting the traditional methods. They provide improved accuracies, work with noisy data, and eventually aid in discovering hidden trends and relationships between variables.

Along with improvements in accuracy for projection of transport demands, machine learning methods can aid in simplifying the process of generating transport demand projection models for regions comprising of countries in different socioeconomic stages of development. The state of the art in machine learning based demand projection methods like ANN and RNN requires individual models for each country in a region. This limitation manifests in longer transport demand prototyping time and precludes training of a pool of countries together to capture their mutual effects on transport demand.

The presented work has built upon the fundamentals of machine learning, to propose a methodology and an architecture that draws its inspiration from firing of a trebuchet. The method has shown through the analysis that it is highly suitable for demand estimation, surpassing performance of traditional methods like regression and simulation based transport demand projection. The models developed via TrebuNet architecture have shown superior performance and

flexibility of prototyping over state of the art machine learning methods like ANN, RNN and gradient boosted when comparing accuracy in learning from historical trends, projection of short term and decadal transport demand. The training of the TrebuNet models, their benchmarking and demand projection have used two drivers, which in turn reduces the assumptions that goes into demand estimation tasks. The results have also shown that the architecture can perform equally well for small datasets which have breaks in the time series. Using quantile-based segregation inside the architecture, we have mitigated the issues related to projection being biased toward the mean. Since each country follows a different quantile in their growth, using a mean error metric will continually underestimate or overestimate that country's demand projection. From the evaluations of models generated by TrebuNet, we have concluded that the framework developed in this study works equally well both for a country level disaggregation and regional aggregations in data-series. We have also shown that the applicability of the demand projection methods can be accurately scaled from regional level to global level.

Finally, medium term projections using the trained models and marine freight series projection revealed promising results when compared with other established IAMs and more complex modelling done by international organisations. These use cases have highlighted the utility of the TrebuNet architecture for fast prototyping of demand projections, without understanding and coding complex relationships - as is traditionally the case with the established IAM frameworks. With just two socio-economic input features, TrebuNet architecture was able to match the results of more complex models. Increasing the input training features (in our case drivers) and using higher resolution data with more data points will no doubt increase the accuracy of the results as the models will be exposed to more trends and missing data. Further work is being done to

expand the algorithm by incorporating more drivers and to generate residential and industrial demands.

We have highlighted through this research, how a physical process can be mimicked on an established deep learning architecture and applied to a complex problem with a high degree of success. This work illustrates the utility of TrebuNet architecture in not only the present use case but also for other general regression tasks like residential, industrial, commercial etc. demand forecasting. Moreover, the fundamentals of the TrebuNet framework can be applied to other disciplines where time series forecasting for a non-uniform variance dataset is required. TrebuNet models can also provide modularity to the demand projection tasks by using different models containing groups of countries in different socio-economic stages of development, to project for different time horizons. This way, learnings from different groups can be used to emulate changes in demand due to the economic progression of a country. Projecting future demands is an uncertain exercise where convergence towards certainty is aided by ensemble of different modelling techniques. Demand estimation has historically been the lesser focused albeit very important area of the energy systems. The architecture no doubt provides a new set of tools for the IAM community to experiment with and enrich the energy service demands for accurate energy systems model development.

Chapter 5: Conclusions

5.1 Introduction

Since the introduction of the Paris Agreement in 2015, global nation-states have reiterated their commitment to containing global warming below 2°C compared to pre-industrial levels^[229]. Precipitating from this renewed commitment, national government, citizens and industrial lobby have acknowledged that the future of energy systems will include a sizeable portion of renewable energy and a sustained transition from fossil-fuelled energy is required. Since 2015, from the electricity supply side wind and solar have presented themselves as the prime candidates to spearhead this transition, out of which solar has proven to be the cheapest, most robust and fastest growing^[230]. From the demand side, automobile manufacturers have committed to transitioning their new stock to electric vehicles, with some manufacturers planning to cease manufacturing fossil fuelled inventories in the next decade^[231].

Along with perceptible changes in the supply side of an energy system, demand for energy services is also expected to see a radical shift to a smarter consumption pattern. Recently Apple Inc. has introduced software changes to provide users with an option to charge their smartphones when the grid is “green”^[232]. The next decade for energy systems will see a fundamental shift in their operation as humans seek to mitigate the perils of climate change. In the Introduction chapter, the author discussed how ESMs and IAMs are important for narrating the future energy systems for policy formulation. With an overall aim to improve the accuracy of the ESMs and IAMs, this thesis explores the application of big data and

machine learning to answer the research questions introduced in section 1.2. In this chapter, based on the case studies researched in chapters 2, 3, and 4, the author will synthesise the conclusions to the research questions, which are as follows

RQ-1. What are the benefits and limitations of machine learning based approaches in supply and demand side modelling of energy system models?

RQ-2. How can machine learning based frameworks aid in the high-resolution spatiotemporal assessment of current and future growth in global rooftop solar PV's renewable electricity generation potentials?

RQ-3. How do the advancements in energy resource potential estimations elicited by the machine learning, GIS and big data based frameworks improve the representation of decentralised solar PV in global Integrated Assessment Models?

RQ-4. How do machine learning based approaches improve the accuracy of short, decadal, and medium-term transport energy service demand estimations?

In addition to the detailed discussion section in the respective chapters, the following sections summarise the overall conclusions that were synthesised when answering the research questions stated in section 1.3. In the following, RQ 2 and 3 are grouped in the first section to conclude the outcome of the assessment and IAM representation of decentralised solar PV. The second section provides the conclusion to RQ 4. Important conclusions for RQ 1 are documented in the last section with insights drawn from Chapters 2, 3, and 4. This chapter ends with recommendations for future work.

5.2 Conclusions on supply side application (RQ 2,3)

Decadal reductions in capital costs and fast deployment characteristics have pitted Solar PV technology as a prime contender for renewable electricity generation at a global scale^[170]. Amongst Solar PV, decentralised rooftop solar PV has the potential to disrupt how consumers generate and consume energy. Decentralised solar PV provides twin benefits of energy independence and climate change mitigation at a prosumer level. Chapters 2 and 3 highlighted that due to the complexity of the assessment of where and how much rooftop area is available at a global scale, generalisations and simplifications were incorporated in ESMs and IAMs to represent this technology^[46, 59, 60]. Specifically, the chapters highlighted that in ESM and IAM Solar PV is often represented as a single technology covering both utility-scale and decentralised technologies. It was also argued that their separate representation is required due to the unique techno-economic characteristics of each Solar PV sub-technologies. Moreover, targeted policy evaluation for a single technology is not possible when solar PV is represented as a single technology.

These limitations culminated in ESMs and IAMs underestimating the role of Solar PV in global energy systems. Some ESMs and IAMs have started representing utility Solar PV and decentralised Solar PV as a separate technology^[233, 234]. But even in these implementations, simplifying generalisations and assumptions are used to represent decentralised Solar PV. From Chapter 2, we can deduce that these generalisations are incorporated in the form of transferring the spatial characteristics of rooftop area e.g. rooftop area per capita, rooftop area per household, average rooftop size per building archetype etc. from the regions that have adequate cadastral survey data to the other regions. Such examples have used generalised building attribute data from the European and American continents to assess rooftop area in different continents^[60, 84, 89, 90, 235]. Chapter 3 moved beyond the issue of assessment of rooftop area in a single time slice to

future growth. Here, it was highlighted that very limited studies have researched where and by how much the global rooftop area will grow in the future^[60, 89, 235].

Considering how energy system optimisation works in ESMs and IAMs, a detailed assessment of its current and future technical potential is required for an accurate representation of decentralised Solar PV. It can be argued that the biggest bottleneck in realising this technology representation thus far has been a lack of a global database demarcating the geospatial rooftop area^[60, 163]. In Chapter 2, it was stated that the reason for this lack of a global rooftop area dataset is due to the computational complexity and cost of analysing high-resolution remote sensed imagery *first* to demarcate human-made structures, *second* to extract building out of the human-made structures and *finally* to calculate the rooftop space in each building.

With the advancements in computational hardware and resolution of remotely sensed imagery over the last decade^[19, 91, 111, 119, 168, 236], we now have a vast amount of data pertaining to building footprints, road networks, population count etc. Pursuant to this, Chapters 2 and 3 have successfully demonstrated how we can utilise machine learning to conduct a harmonised assessment of rooftop area at a global scale using these big datasets. To answer the RQ-2, machine learning and big data have enabled an accurate high-resolution assessment of current rooftop area and future growth in rooftop area at a global scale.

Chapter 2 introduced a novel assessment framework that utilises GIS-based geospatial metrics like building footprints, road length and population counts within sample Fishnet Tiles to estimate the rooftop area in non-sample Fishnet Tiles. This approach provided the flexibility of selecting the size of the Fishnet to increase or decrease the resolution of the assessment. It can be said that the approach used in Chapter 2 is agnostic to the size of the Fishnet and can be retrained for dynamic spatial resolution. This dynamic spatial resolution methodology, combined with machine learning models, provided the required

flexibility in the assessment framework. This is an important innovation that can be attributed to the application of big data and machine learning as dynamic spatial resolution aids in analysing the energy system from a sub-national level to a continental level. Specifically, the application of machine learning methods aided in finding patterns in big data and generalising the prediction capability of the assessment framework. Chapter 2 further highlighted that machine learning methods provided superior accuracy compared to the state of the art linear regression and random forest methods.

In Chapter 3, the assessment framework introduced in Chapter 2 was revisited and rebuilt from scratch to incorporate a higher number of independent variables, sample countries and datasets. This rebuilt framework was then trained to predict future growth in the rooftop area at a global level. Chapter 3 also demonstrated how a purpose-built framework has the capacity to retrain itself for different tasks, e.g. interpolation for Chapter 2 and extrapolation for Chapter 3. Additionally, the dynamic spatial resolution innovation was implemented in Chapter 3, where the Fishnet grid was modified from a constant area 10 km grid of Chapter 2 to a constant 1/8 degree grid.

In conclusion, as stated previously, the prime challenge in assessing the technical potential of decentralised solar PV was the need for a harmonised global rooftop area dataset. This thesis specifically targeted this bottleneck by generating the required dataset by utilising open-source big data and machine learning methods. In doing so, Chapters 2 and 3 have showcased a novel framework for converting geospatial metrics into numerical metrics for machine learning training which is computationally simple and within reach of affordable desktop hardware. The RQ-2 was drafted with an aim to advance the accuracy of the assessment of decentralised solar PV, but it has culminated in providing a new framework, datasets and quantitative analysis that is capable of moving the frontier in the energy system modelling space by enabling policy research from sub-national to

continental levels. Further work is ongoing to incorporate other global metrics like night-time lights and building height data to refine the assessment further^[236, 237].

The ultimate role of assessment of renewable technology's technical potential in this thesis was to accurately represent the technology in an ESM and IAM in a way that enables competition between different technologies when finding the least cost-optimal solution. Here the thesis demonstrates how the technical potential of a single decentralised renewable technology can be assessed and its economic potential is evaluated for mitigation of climate change.

One of the ways to achieve this goal is to convert the assessed potential into 'bins' of technical potentials that can provide a 'merit order' to the technology. This is done by creating technology technical potential bins based on LCOE, Capacity Factors etc. Naturally, binning process summarises the continuous geospatial metric of technical potential into averaged bins. The advancements in assessment elicited by the methods discussed in Chapters 2 and 3 can thereby aid in defining these bins with higher accuracies. The datasets generated by the assessment framework are mapped to a spatial land grid that can be dynamically modified before the framework construction and further upscaled to cover cities/states/countries/regions. It can thus be concluded that based on the modelling question's geographical scope (Global or Country), the flexibility afforded by advancements in GIS, big data and machine learning can aid in different ways. For the global modelling question, the upscaling of the grid to a country/regional level can aid in defining custom technical potential bins, where the number of bins can be defined based on the if the study requires rooftop area based quantiles or capacity factor based quantiles. The first approach provides equal sized rooftop area bins with non-uniform capacity factors and vice versa for the latter. It was expected that with the updated assessment and separate representation of decentralised rooftop Solar PV technology in a global IAM, new insights could be realised^[128, 238, 239]. These expected outcomes were realised in Chapter 3, where a

separate representation of decentralised Solar PV into the global energy system of MESSAGEix-GLOBIOM IAM resulted in a significant uptake of overall Solar PV by 2050 in a climate mitigation scenario amongst which decentralised Solar PV contributed upwards of 50% to the electricity generated by Solar PV. It can be argued that updated capital cost assumptions could have also played a significant role in this outcome, but ultimately it was the increased flexibility afforded by the assessment that aided in the proper demarcation of utility vs decentralised rooftop solar PV technologies.

Additionally, on a qualitative front, the spatial resolution of the assessment provided important insights. First, based on current building stock African continent has lower rooftop solar PV technical potential than European and American Continents, but in the future African continent will show the highest growth in technical potential. Second, decentralised solar PV is concentrated below the 17% annual capacity factor due to its spatial characteristics, whereas utility solar PV is concentrated above that. Third, a significant mismatch exists between areas of high solar insolation and hotspots for decentralised solar PV deployment. For the first time, the assessment captured the combined potential of the industrial, commercial and residential sectors.

In conclusion, to answer RQ-3, the advancements afforded by GIS, big data and machine learning significantly improved the representation of decentralised rooftop solar PV technology in a global IAM. Moreover, the spatial flexibility in the assessment datasets would enable its usage from country-level studies to global studies with equal accuracy. Currently, further research is being conducted in tailoring the assessment framework introduced in Chapter 3 to generate an open-source toolkit for demarcating gaps in OSM building footprint datasets, which will be useful across broader disciplines. The Annex of this thesis documents a country-level analysis for rooftop solar PV that benefitted from the direct application of the datasets generated in Chapters 2 and 3.

5.3 Conclusions on demand side application (RQ 4)

Energy service demand estimation tasks are traditionally delegated to the ex-ante construction of an energy system model. Lately, some studies have started incorporating feedback between energy service demand estimation and energy systems models to track the effects of changing macroeconomic assumptions and shifts in demand profiles between the ESM model's optimisation iterations^[240, 241]. A review of the literature in Chapter 4 suggests that the transport energy service demand has historically relied on regression-based methodologies with some advanced studies integrating discrete choice modelling to track inter-modal transitions. Machine learning applications have shown superior performance to regression-based methodologies and in some cases also discrete choice modelling. Upon closer inspection, the literature suggests that the application of machine learning in transport energy service demand estimation has been limited to a country-level analysis^[190, 192-194]. While many considerations are incorporated when executing the energy service demand estimation, the foremost task of this exercise has been to learn from the past and follow the historical trends to estimate a future trajectory for energy service demands. It is here that machine learning can contribute the most, as has been empirically shown from cross-disciplinary studies that incorporate time series forecasting and trend analysis. While contemporary machine learning models are excellent for single-trend analysis, they offer reduced performance when dealing with datasets having non-uniform variance across historical time horizons. This is especially true when estimating energy service demands for a region comprising a group of dissimilar and socioeconomically unique countries.

Chapter 4 investigates the challenges of transport energy service demand from the perspective of improving the estimation accuracy in short, decadal and medium-term time horizons. This thesis did not analyse these methods for long-term estimation (2050-2100) due to the high uncertainty of how long-term energy service demands will look like. Especially with the ever-evolving policy landscape,

long-term predictions are bound to be dynamic^[242]. To incorporate the nuances of non-uniform variance in pool data of dissimilar countries, Chapter 4 introduces a novel machine learning method “TreuNet”. TreuNet has been evaluated for its accuracy in estimating the short (two-year look ahead), decadal (10-year look ahead) and medium-term (4-decade look ahead) time horizons. The comparisons were made with recorded data and energy service demand projections of a suite of global IAMs. Along with the projection accuracies, the TreuNet was also evaluated for its performance with traditional methods like multivariate linear regression, state of the art in machine learning based methods like LSTM and GRU and finally with the industry standard of XGBoost.

Application of TreuNet for the task of transport energy service demand resulted in both methodological and time consumption advantages. First, TreuNet enabled the modelling of energy service demands for a group of countries in a single execution step. Effectively, for a pool of N counties, we traditionally had to construct individual models for each country. With TreuNet, this task can be done in a single shot with projections available for multiple countries at the model's output. Second, if a group of countries form a region, then traditional methods can only provide the ‘averaged’ trajectory of the energy service demand for the region. With TreuNet, data points of the individual countries contribute to providing multiple quantiled trajectories that can be used to construct the regional energy service demands. Third, the sparse data availability, which can act as an Achilles heel for more data-intensive machine learning models, can be mitigated by TreuNet due to the automatic implementation of cross-validation inside the model.

In conclusion, to answer the RQ4, yes machine learning can provide methodological benefits to the task of transport energy service demands projection. The key area where machine learning can contribute is to improve the accuracy of the “business as usual” projection^[243]. Another area where machine

learning can contribute significantly is the ability to continuously train the model when new data becomes available. This technique, called “transfer learning”, enables iterative training of the model for course correction across the projection horizon. It can also be concluded from Chapter 4 that machine learning is adequate for both downscaling (region to country level) and upscaling (country level to regional) of energy service demands and matrices^[19, 244, 245]. Further research is being conducted to enable combining all modes of transport and additional independent variables into a single TrebuNet model to capture the inter-modal effects of transport energy service demands.

5.4 Implementation and revisiting the limitations (RQ 1)

In this thesis, arguments and case studies have been presented that conclude that machine learning, big data and GIS can provide a multitude of benefits to the designing of global energy systems. But these tools and methods also come with a set of limitations which preclude their faster adoption within the broader energy community. Although the limitations of the machine learning based approaches have been widely documented in the contemporary literature, a set of guiding principles for designing a coherent methodology for a specific application area is not well documented.

Currently, the process of designing a machine learning workflow is heavily dependent on a researcher's experience with various machine learning models which has led to the slow percolation of applications of machine learning methods in global ESMs and IAMs. Based on the learning from the case studies presented in this thesis, some challenges to the practical implementation of these methods and solutions are presented next.

The first challenge stems from the machine learning models' perceived “black box” approach^[246, 247]. This black box limitation is attributed to how machine learning models subsume the information they are trained on. For example, researchers can mathematically document the relationship between dependent

and independent variables for multivariate linear regression tasks. Applying machine learning models to the same study leads to better accuracies, but the researcher cannot diagnose or represent the relationships between dependent and independent variables. This limitation can be mitigated by observing the outputs of the machine learning models and evaluating the prediction errors over known data points. In Chapters 2 and 3 this limitation was encountered when evaluating the accuracy of the machine learning based models. In these case studies, mitigation strategies involved generating error bins and plotting predicted vs true data points. The former metric provided a quantitative basis to generalise the errors in prediction and the latter in visualising them. In Chapter 4, the concept of relationship surfaces was introduced to provide a visual aid of how the model performs over the known dataset.

The second challenge is the pre-processing of big data for training the machine learning model. While pre-processing of big datasets is a crucial step in any relationship modelling methodology, for machine learning based methods, this process is especially important. This is because a majority of machine learning methods utilise the concept of "gradient descent" which is extremely sensitive to the scale of the input training data. In the case studies, a normalisation and scaling approach was used to mould the training features. This is especially true for Artificial Neural Network based machine learning methods where training features should be scaled between 0-1 for faster model training convergence time.

In addition to the scaling/normalisation step, due care should be taken to eliminate the features that have a similar relationship with the target variable. In Chapters 2 and 3 this was done by selecting independent variables or features that provide new information to the model. If two or more features provide the same information to the model, then there is a high chance that the model is not learning anything new during training runs and hence there will be a tendency for the model to be biased towards similar features. As an example, if the case studies

for Chapters 2 and 3 included building footprint data for the same country from two different sources, then the model will not learn anything new, rather it is important to merge these building footprints to create a harmonised set of data for training.

The third limitation of the machine learning approaches is the time spent in pre-processing big data and further in training the models. Although it is well known that machine learning will naturally require a higher runtime to find a solution to the problem, the thesis concluded that this additional time is well worth the effort, considering 'inferencing' from the trained model can be performed relatively quickly. The question at the end is to balance the time required for training the model and the compromise in the perceived accuracy. During the development of the models for the case studies presented in this thesis, it was observed that the default machine learning model libraries are a good point to start machine learning framework prototyping, but the model hyperparameters should be finally tuned to the specific training feature/target dataset for more accurate performance. Here, users can limit the hyperparameter search space to reach the final model faster and also acknowledge that with each smaller increase in accuracy, the model would train for an increasingly longer time.

The fourth limitation of the machine learning models is the ease with which the model can specialise the learning from training data and consequently perform worse when used for inferencing tasks on unseen datasets. Since the objective of the iterating training steps in a machine learning model is to reduce error metrics, the over-enthusiastic approach of seeking minute improvements in accuracy can lead to the "overfitting" of the model. In the case studies presented in this thesis, this tendency for overfitting the model was mitigated by implementing cross-validation across all the machine learning models used^[248].

The fifth limitation of the machine learning models is the objective evaluation of the methods and the use case. While machine learning based methods have

shown better accuracies over traditional methods in regression and classification tasks, no set guidelines exist on how to choose the right machine learning method for a given use case. As an example, both Artificial Neural Network based and Gradient Boosted methods are used in the contemporary literature for regression and classification based tasks, yet the fundamental differentiator of one method over the other has been to observe the error metric. After successive hyperparameter tuning and longer training time, both methods have shown nearly equal performance. This can often lead to spending additional time diagnosing the right method for a given research question.

Inferring from the case studies presented in this thesis it is recommended that machine learning methods in global IAM/ESMs should focus on using Gradient Boosted methods for regression tasks in the numerical domain and Artificial Neural Network based methods for image classification and time-series projection tasks. In conclusion, machine learning is a double-edged sword. It can provide superior accuracies compared to other methods, but due care is required when training the model to reduce overfitting and finally to make the results of the models verifiable and explainable.

Another aspect of the application of machine learning method in this thesis is the processing and analysis of big data especially geospatial datasets in Chapters 2 and 3. The processing of geospatial big data can be divided into three steps - data collection, data transformation and data storage. Each step comes with its own sets of complexities and the next paragraphs document them and discuss how these limitations were mitigated in this thesis.

The first step in geospatial big data processing is the data collection stage. Geospatial datasets are available as raw data e.g. pixel level values of remote sensed images where each pixel can have multiple "band" information, polygons representing building footprints in a vector format, pre-processed remote sensed products that have results from image segmentation/classification etc. The

limitations encountered during this step are the completeness and validity of the big datasets. In this thesis, the completeness of the datasets and their validity were ascertained both by analysing the technical report documented along with the datasets and also using automated and visual inspections. While this strategy is time-consuming, the author recommends using a predefined validation protocol and also verifying the datasets from multiple studies. As an example, building footprint dataset completeness can be verified by taking a ratio of aggregated building footprint area to the extent of built-up area in a fishnet tile. Manual thresholds on the ratios can then be set to filter out sample fishnets.

The second step in geospatial big data processing is the data transformation stage which covers the usage of GIS tools like projection, clip, intersect etc. The complexity in this stage is to design a data transformation pipeline that transforms the raw data into case study-specific metrics. Depending on the size of the big datasets and the tools employed, this stage can take the largest amount of time in the experimental protocols which can often range from hours to days. Additional challenges are a result of error cropping in the middle of the data transformation pipeline due to corrupted data.

In this thesis, the data transformation protocol followed a strict pipeline that started with harmonising projected coordinate systems for all datasets with a strict focus on using projected coordinate systems that are equal in area and have units of measurement in meters. Choosing the right projected coordinate systems at the head of the data transformation pipeline is essential in getting the right results from the succeeding GIS tools. Additionally, careful attention should be provided to the projected coordinate system as for each use case and localised area of interest e.g. finding the area of a polygon, different projected coordinate systems might be required for different geographies.

The next step in the data transformation pipeline is to make sure that the geometries of the polygon dataset are valid and free from self-intersections, voids

etc. As an example, for polygon based big datasets, the validity of geometry should be checked for each polygon. This check can be performed by “check/repair” geometry tools in any mainstream GIS software. Invalid geometries have the notoriety to cause exceptions/crashes in the data transformation tools and can lead to loss of progress made in preceding steps.

Finally, in this thesis whenever a GIS tool was executed, a copy of the tool's output was stored in persistent memory to save the work at each stage. The choice and order of application of GIS tools were decided based on the performance of the tools on sample fishnet tiles. In this thesis, four geographically disparate fishnet sample tiles were used to check the order of GIS tool execution. These four sample tiles were located east, west, north and south extremities of the geospatial big datasets.

The last step in geospatial big data processing is data storage. The primary challenge here is to store processed GIS datasets in a format that is fast to access and provides interoperability with the analysis toolkits downstream. In this thesis, the processed geospatial datasets were stored as numerical datasets in compressed “.parquet” format which supports multithreaded read and write support within the python environment. The processed spatial datasets were stored in “geodatabase” format to enable faster read and write access with ARCGIS Pro. It is essential to highlight here that faster medium of storage and access like solid state drives are essential for GIS workflows and should be prioritised over larger system memory. In conclusion, due efforts are required to prototype big data analysis workflows using the strategy of prototyping workflows on a smaller sample dataset. The sampling strategy should incorporate all the obvious attributes present in the dataset. Time spent in testing prototype workflows on sample sets can save the time lost due to the eventual issues that can crop up when processing whole datasets.

5.5 Future work

This thesis researched the application of big data and machine learning in global energy systems. The applications in supply and demand side technologies were discussed in the form of the construction of methods and frameworks followed by a case study. During the course of the research and further, during the scientific dissemination of the results, it became evident that the methodological learnings of this thesis should be transferred to other aspects of energy systems modelling like demand downscaling, spatial analysis of energy systems etc. Based on the stakeholder feedback received during conferences and internships, the author recommends two directions in which further work should be targeted 1) refinement in machine learning model development and evaluation and 2) implementation of high-resolution spatiotemporal energy system model development.

Building on the findings from **RQ 1**, the first stream of advancement should be focussed on improving how we select, design, train and evaluate the machine learning models. A wide variety of machine learning models are currently available to a researcher^[249]. Some methods are exclusively reserved for CPU-based training, and others benefit massively from GPU-based training. Concluding from the case studies presented in this thesis, a majority of regression-based tasks can be successfully executed by using CPU-based machine learning models. This can also help in the rapid uptake of machine learning models as researchers have adequate access to modern multi-core CPUs. For tasks dealing with time series forecasting, GPU-based machine learning methods have shown the desired flexibility. Due to a lack of standardisation in the training procedure of machine learning models and the inherent uncertainties in training, the future focus should be on standardising the result reporting. As each machine learning-based application in energy systems analysis will invariably build upon a common set of based machine learning models, the energy research community should work together in demarcating the standard reporting metrics, especially the variables

and bounds used to normalise the inputs to a machine learning model. Inspiration can be drawn from the standardisation of IAM result reporting templates for the IPCC AR6 report^[250]. Here, the author also recommends exploring the model “ensemble” to reduce uncertainties in any application of machine learning^[242]. For model evaluation, this thesis has introduced a concept of relationship surface to visualise the relationship between dependent and independent variables.

Further work is required to provide tools for the researchers to mitigate the “black box” notion associated with machine learning methods. Deriving from the key results of Chapter 3, an open-source toolkit to detect global gaps in OSM’s building dataset is being finalised. This toolkit will be used to evaluate the assessment framework’s performance visually.

The second stream of advancement should focus on doing justice to the information provided by the high-resolution assessment datasets generated in this thesis and are part of the findings from **RQ 2** and **RQ 3**. Chapter 3 documents the assessment of the global technical potentials of RTSPV which was further extended to the calculation of the economic potential of RTSPV/DCSPV in 11 global regions. Further work is required to assess the realisable potential of RTSPV/DCSPV which would require designing and running the global ESMs/IAMs on a sub-annual time-slice especially capturing the diurnal and seasonal attributes of VRE technologies like solar PV/wind-based renewable electricity generation technologies. At the same time, the spatial resolution of the ESMs/IAMs should also increase to incorporate the spatial dynamics of the VRE technologies e.g. coastal regions vs inland regions for wind-based technologies.

One of the fundamental limitations of current ESMs and IAMs is the computational non-feasibility of running the optimisation models for a high-resolution spatiotemporal level at a global scale. Success has been reported in running country-level hourly resolution ESMs^[4, 251, 252]. Efforts to increase the spatiotemporal scale of the input datasets for ESMs and IAMs should be

complemented by advancements in the modelling of energy systems. State-of-the-art research has demonstrated the need and feasibility of a high-resolution spatiotemporal power system model - PLEXOS-World^[238]. Motivated by this, the author is conducting further research in designing the first fully open source ESM - GEO-TIMES. The core philosophy of GEO-TIMES is to provide an ESM with a spatial resolution of 32 world regions and a sub-annual time slice. The author recommends similar development in other IAMs.

In conclusion, the machine learning methods in themselves are fairly mature methodologically. This is due to the cross-domain efforts of data scientists that use these methods for different use cases. Vast literature and a robust peer community are currently present to aid in every step of machine learning, big data and GIS-based analysis. Standardisation of reporting and model evaluation guidelines specifically targeted towards energy system modelling, along with improvements in the spatiotemporal attributes of ESMs and IAMs will provide a synergistic boost to the application of machine learning, big data and GIS in energy system modelling.

Appendices

Appendix A: Supplementary Information for Chapter 2

A.1 Supplementary Tables

Table A.1 | Distribution of sample FNs

World Regions	Countries	Building Footprint (km ²)	Number of sample FNs
NORTH AMERICA	13	29,343	112,574
AFRICA	48	6,337	53,142
EUROPE	35	1,070	2,724
ASIA	39	333	696
AUSTRALIA	2	17	55
SOUTH AMERICA	10	15	79

Table A.2 | Input big datasets and links to validation studies

Datasets	Resolution	Usage	Validation
Building Footprints	Vector Dataset	Calculation of aggregated ground truth rooftop area	Heris, M.P., Foks, N.L., Bagstad, K.J. <i>et al.</i> A rasterized building footprint dataset for the United States. <i>Sci Data</i> 7 , 207 (2020). https://doi.org/10.1038/s41597-020-0542-3
Population	100 m ²	Proxy for building density	Lloyd, C., Sorichetta, A. & Tatem, A. High resolution global gridded data for use in population studies. <i>Sci Data</i> 4 , 170001 (2017). https://doi.org/10.1038/sdata.2017.1
Road	Vector dataset	Proxy for built-up area density	Barrington-Leigh, C., & Millard-Ball, A. (2017). The world's user-generated road map is more than 80% complete. <i>PloS one</i> , 12(8), e0180698. https://doi.org/10.1371/journal.pone.0180698
Conversion Factor	1 km ²	Conversion of rooftop area to electricity generation potential	ESMAP. 2019. Validation Report: Global Solar Atlas 2.0 Validation Report. Washington, DC: World Bank.
Land Cover	100 m ²	Built-up area extent	Tsendbazar, N.E., Tarko, A., Linlin, L., Herold, M., Lesiv, M., Fritz, S., Maus, V.; (2020): Copernicus Global Land Service: Land Cover 100m: Version 3 Globe 2015-2019: Validation Report; Zenodo, Geneva, Switzerland, September 2020; doi: 10.5281/zenodo.3938974

Table A.3 | Model Comparison

Model Name	Dependent Variable	Independent Variable	10 fold Cross validation			Predicted Rooftop Area for Select Countries (km ²)							
			MSE	RMSE	R ²	220 countries	IRL	FRA	DEU	ESP	UK	USA	IND
Linear Regression	BFE	BA, RL, PPLN	0.036	0.189	0.957	198,826	182	4,567	4,820	1,959	2,530	27,440	12,605
Random Forest	BFE	BA, RL, PPLN	0.026	0.161	0.984	194,798	209	4,036	4,224	1,847	2,321	27,553	11,468
XGBoost	BFE	BA, RL, PPLN	0.025	0.158	0.981	193,910	218	3,938	4,164	1,851	2,400	27,585	11,731

Note: BFE is estimated aggregated rooftop area per FN, BA is built-up area per FN, RL is aggregated road length per FN, PPLN is aggregated population count per FN.

Table A.4 | Assessed global RTSPV potential in TWh/Year

Rooftop Scaling (%)	Panel Efficiency										
	10%	11%	12%	13%	14%	15%	16%	17%	18%	19%	20%
100	27,512	30,263	33,014	35,766	38,517	41,268	44,019	46,770	49,522	52,273	55,024
90	24,761	27,237	29,713	32,189	34,665	37,141	39,617	42,093	44,569	47,046	49,522
80	22,010	24,211	26,412	28,612	30,813	33,014	35,215	37,416	39,617	41,818	44,019
70	19,258	21,184	23,110	25,036	26,962	28,888	30,813	32,739	34,665	36,591	38,517
60	16,507	18,158	19,809	21,459	23,110	24,761	26,412	28,062	29,713	31,364	33,014
50	13,756	15,132	16,507	17,883	19,258	20,634	22,010	23,385	24,761	26,136	27,512
40	11,005	12,105	13,206	14,306	15,407	16,507	17,608	18,708	19,809	20,909	22,010
30	8,254	9,079	9,904	10,730	11,555	12,380	13,206	14,031	14,856	15,682	16,507
20	5,502	6,053	6,603	7,153	7,703	8,254	8,804	9,354	9,904	10,455	11,005
10	2,751	3,026	3,301	3,577	3,852	4,127	4,402	4,677	4,952	5,227	5,502

^a Assuming 27,512 TWh per year global assessed RTSPV potential at 100% rooftop scaling factor scaling and 10% panel efficiency

Table A.5 | Change in Regional potentials with different combinations of panel efficiency and Rooftop Scaling Factor

32 Region	Potential ^a	Eff_12_ RS_80	Eff_12_ _RS_60	Eff_12_ RS_40	Eff_12_ _RS_20	Eff_14_ _RS_80	Eff_14_ RS_60	Eff_14_ RS_40
AFE (Africa East)	214	205	154	103	51	240	180	120
AFN (Africa North)	592	568	426	284	142	663	497	332
AFS (Africa South)	413	396	297	198	99	463	347	231
AFW (Africa West)	1,317	1,264	948	632	316	1,475	1,106	738
ANZ (Australia and NZ)	404	388	291	194	97	452	339	226
ARG	285	274	205	137	68	319	239	160
ASC (Asia Central)	748	718	539	359	180	838	628	419
ASE (Asia South East)	1,354	1,300	975	650	325	1,516	1,137	758
ASO (Asia Other)	304	292	219	146	73	340	255	170
ASR (Rest of Asia)	219	210	158	105	53	245	184	123
BRA	997	957	718	479	239	1,117	837	558
CAN	327	314	235	157	78	366	275	183
CHN	4,375	4,200	3,150	2,100	1,050	4,900	3,675	2,450
ENE (Non-EU East)	499	479	359	240	120	559	419	279
ENW (Non-EU West)	75	72	54	36	18	84	63	42
EUE (Europe East)	648	622	467	311	156	726	544	363
EUW (Europe West)	2,210	2,122	1,591	1,061	530	2,475	1,856	1,238
GBR	238	228	171	114	57	267	200	133
IDN	878	843	632	421	211	983	738	492
IND	1,815	1,742	1,307	871	436	2,033	1,525	1,016
IRN	341	327	246	164	82	382	286	191
JPN	1,044	1,002	752	501	251	1,169	877	585
KOR	201	193	145	96	48	225	169	113
LAM (Latin America)	805	773	580	386	193	902	676	451
MEA (Middle East)	462	444	333	222	111	517	388	259
MEX	720	691	518	346	173	806	605	403
ROW (Rest of the world)	35	34	25	17	8	39	29	20
RUS	941	903	678	452	226	1,054	790	527
SAU	169	162	122	81	41	189	142	95
TUR	265	254	191	127	64	297	223	148
USA	4,247	4,077	3,058	2,039	1,019	4,757	3,567	2,378
ZAF	374	359	269	180	90	419	314	209
Total	27,516	26,415	19,812	13,208	6,604	30,818	23,113	15,409

^a Assuming 27,512 TWh per year global assessed RTSPV potential at 100% rooftop scaling factor scaling and 10% panel efficiency.

Note: Eff_X_RS_Y, where "X" is the panel efficiency and "Y" is the Rooftop Scaling Factor. Colour coded cells are the aggregated regional potentials considering the average panel efficiency and rooftop scaling factor that are present in the wider literature.

Table A.5 Continued

Eff_14_ RS_20	Eff_16_ RS_80	Eff_16_ RS_60	Eff_16_ RS_40	Eff_16_ RS_20	Eff_18_ RS_80	Eff_18_ RS_60	Eff_18_ RS_40	Eff_18_RS_20
60	274	205	137	68	308	231	154	77
166	758	568	379	189	852	639	426	213
116	529	396	264	132	595	446	297	149
369	1,686	1,264	843	421	1,896	1,422	948	474
113	517	388	259	129	582	436	291	145
80	365	274	182	91	410	308	205	103
209	957	718	479	239	1,077	808	539	269
379	1,733	1,300	867	433	1,950	1,462	975	487
85	389	292	195	97	438	328	219	109
61	280	210	140	70	315	237	158	79
279	1,276	957	638	319	1,436	1,077	718	359
92	419	314	209	105	471	353	235	118
1,225	5,600	4,200	2,800	1,400	6,300	4,725	3,150	1,575
140	639	479	319	160	719	539	359	180
21	96	72	48	24	108	81	54	27
181	829	622	415	207	933	700	467	233
619	2,829	2,122	1,414	707	3,182	2,387	1,591	796
67	305	228	152	76	343	257	171	86
246	1,124	843	562	281	1,264	948	632	316
508	2,323	1,742	1,162	581	2,614	1,960	1,307	653
95	436	327	218	109	491	368	246	123
292	1,336	1,002	668	334	1,503	1,128	752	376
56	257	193	129	64	289	217	145	72
225	1,030	773	515	258	1,159	869	580	290
129	591	444	296	148	665	499	333	166
202	922	691	461	230	1,037	778	518	259
10	45	34	22	11	50	38	25	13
263	1,204	903	602	301	1,355	1,016	678	339
47	216	162	108	54	243	183	122	61
74	339	254	170	85	382	286	191	95
1,189	5,436	4,077	2,718	1,359	6,116	4,587	3,058	1,529
105	479	359	239	120	539	404	269	135
7,704	35,220	26,415	17,610	8,805	39,623	29,717	19,812	9,906

Table A.6 | XGBoost Parameters

Parameters	Values
Gamma	3
Learning Rate	0.0445008698564836
Max Depth	3
Min Child Weight	3
Estimators	540
Regulation Alpha	4
Booster	Gbtree
Objective	Reg:squarederror
Column Sample By Tree	1
Threads	12
Hypertuning Iterations	500
Cross Validation	10 Fold

Base Model Download : <https://xgboost.readthedocs.io/en/latest/>

Table A.7 | Result Validation

Reference	Meta Data		Comparison Study				Our Study			
	Study Area	Methodology	RoofTop Attributes	Incubation	RoofTop Area Calculation	RoofTop Area	RoofTop Area Potential (m ² /yr)	RoofTop Area Potential (m ² /yr)	RoofTop Area Potential (m ² /yr)	RoofTop Area Potential (m ² /yr)
GLOBAL/REGIONAL Level										
1	EU ^a	Top Down	Statistical Scaling	NO	NO	0.30	N.A.	N.A.	7,597	N.A.
2	Global ^b	Bottom Up	Compress Curve	NO	NO	0.32	14%	N.A.	12,300	RoofTop Area
3	Global ^c	Bottom Up	Statistical Scaling	NO	NO	0.30	13%	N.A.	19,385	Aggregated Potential
4	179 countries ^d	Bottom Up	Statistical Scaling	YES	YES	0.42	20.40%	N.A.	27,92	RoofTop Area
5	17 Regions ^e	Bottom Up	Statistical Scaling	NO	NO	0.11	14%	N.A.	8,428	RoofTop Area
COUNTRY Level										
Switzerland										
6	Switzerland	Top Down	Random Forest	YES	YES	0.94	13%	N.A.	640	RoofTop Area
7	Switzerland	Top Down	Random Forest	YES	YES	0.96	15%	N.A.	8,300	Aggregated Potential
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.28	20.40%	N.A.	19,385	RoofTop Area
Spain										
8	Spain	Top Down	Stratified Sampling	NO	NO	0.20	N.A.	N.A.	1,488	RoofTop Area
1	Spain	Top Down	Statistical Scaling	NO	NO	0.30	N.A.	N.A.	8,611	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.36	20.40%	N.A.	294	RoofTop Area
USA										
9	USA	Hybrid	Statistical Scaling	YES	YES	0.32	14%	N.A.	1,488	RoofTop Area
2	USA	Bottom Up	Compress Curve	NO	NO	0.32	14%	N.A.	2,637	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.36	20.40%	N.A.	10,778	RoofTop Area
Germany										
10	Germany	Bottom Up	Building Type	NO	NO	0.27-0.38	12.00%	N.A.	148	RoofTop Area
1	Germany	Top Down	Statistical Scaling	NO	NO	0.30	N.A.	N.A.	1,249	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.36	20.40%	N.A.	827	RoofTop Area
France										
11	France	Bottom Up	Statistical Scaling	NO	NO	0.40	12.70%	N.A.	3,938	RoofTop Area
1	France	Top Down	Statistical Scaling	NO	NO	0.30	N.A.	N.A.	1,346	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.29	20.40%	N.A.	943	RoofTop Area
UK										
11	UK	Bottom Up	Statistical Scaling	NO	NO	0.40	12.70%	N.A.	500	RoofTop Area
1	UK	Top Down	Statistical Scaling	NO	NO	0.30	N.A.	N.A.	770	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.29	20.40%	N.A.	488	RoofTop Area
Vietnam										
12	Vietnam	Bottom Up	Statistical Scaling	YES	NO	0.4-0.58	16.50%	N.A.	1,402	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.35	20.40%	N.A.	1,072	RoofTop Area
Tanzania										
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.71	20.40%	N.A.	810	RoofTop Area
Moroccanque										
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.36	20.40%	N.A.	428	RoofTop Area
Canada										
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.25	20.40%	N.A.	79	RoofTop Area
China										
2	China	Bottom Up	Compress Curve	NO	NO	0.32	14%	N.A.	2,890	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.35	20.40%	N.A.	11,983	RoofTop Area
Russia										
2	Russia	Bottom Up	Compress Curve	NO	NO	0.32	14%	N.A.	450	RoofTop Area
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.29	20.40%	N.A.	1,592	RoofTop Area
Brazil										
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.53	20.40%	N.A.	4,411	RoofTop Area
Angola										
4	179 countries	Bottom Up	Statistical Scaling	YES	YES	0.65	20.40%	N.A.	416	RoofTop Area
City/District Level										
13	Gangnam District, Seoul, South Korea	Top Down	Hillshade Analysis	NO	YES	0.66	15%	N.A.	1	RoofTop Area
14	Osaka	Top Down	Statistical Scaling	YES	YES	0.55-0.65	20%	N.A.	42.9	RoofTop Area

^a Study conducted for EU-27 countries including UK. We have used the same regional definition for our comparison

^b Only residential sector covered in the study. We have compared all sectors here

^c All sectors considered in the study

^d We are comparing our results for 220 countries with 179 countries in the study

^e Only global study to use GDP as a driver for rooftop area

^f Original values documented in our studies

^g Scaled values after incorporating assumptions of the comparison study

Table A.8 | 8 Global World Region Mapping

World Regions	Country Name
AFRICA	Angola, Burundi, Benin, Burkina Faso, Botswana, Central African Republic, Côte d'Ivoire, Cameroon, Democratic Republic of the Congo, Republic of Congo, Comoros, Cape Verde, Djibouti, Algeria, Egypt, Eritrea, Western Sahara, Ethiopia, Gabon, Ghana, Guinea, Gambia, Guinea-Bissau, Equatorial Guinea, Kenya, Liberia, Libya, Lesotho, Morocco, Madagascar, Mali, Mozambique, Mauritania, Mauritius, Malawi, Mayotte, Namibia, Niger, Nigeria, Reunion, Rwanda, Sudan, Senegal, Saint Helena, Sierra Leone, Somalia, South Sudan, São Tomé and Príncipe, Swaziland, Seychelles, Chad, Togo, Tunisia, Tanzania, Uganda, South Africa, Zambia, Zimbabwe
ASIA	Afghanistan, United Arab Emirates, Armenia, Azerbaijan, Bangladesh, Bahrain, Brunei, Bhutan, China, Cyprus, Georgia, Hong Kong, Indonesia, India, Iran, Iraq, Israel, Jordan, Japan, Kazakhstan, Kyrgyzstan, Cambodia, South Korea, Kuwait, Laos, Lebanon, Sri Lanka, Macao, Maldives, Myanmar, Mongolia, Malaysia, New Caledonia, Nepal, Oman, Pakistan, Philippines, Papua New Guinea, North Korea, Palestina, Qatar, Russia, Saudi Arabia, Singapore, Solomon Islands, Syria, Thailand, Tajikistan, Turkmenistan, Timor-Leste, Turkey, Taiwan, Uzbekistan, Vietnam, Vanuatu, Yemen
AUSTRALIA	Australia, New Zealand
EUROPE	Kosovo, Albania, Andorra, Austria, Belgium, Bulgaria, Bosnia and Herzegovina, Belarus, Switzerland, Czech Republic, Germany, Denmark, Spain, Estonia, Finland, France, Faroe Islands, United Kingdom, Gibraltar, Greece, Croatia, Hungary, Isle of Man, Ireland, Iceland, Italy, Liechtenstein, Lithuania, Luxembourg, Latvia, Monaco, Moldova, Macedonia, Malta, Montenegro, Netherlands, Norway, Poland, Portugal, Romania, San Marino, Serbia, Slovakia, Slovenia, Sweden, Ukraine, Vatican City
ISLAND NATIONS	American Samoa, Cook Islands, Fiji, Micronesia, Guam, Kiribati, Marshall Islands, Northern Mariana Islands, Niue, Nauru, Palau, French Polynesia, Tokelau, Tonga, Tuvalu, Wallis and Futuna, Samoa
NORTH AMERICA	Aruba, Antigua and Barbuda, Bonaire, Sint Eustatius and Saba, Bahamas, Belize, Bermuda, Barbados, Canada, Costa Rica, Cuba, Curaçao, Cayman Islands, Dominica, Dominican Republic, Guadeloupe, Grenada, Greenland, Guatemala, Honduras, Haiti, Jamaica, Saint Kitts and Nevis, Saint Lucia, Mexico, Montserrat, Martinique, Nicaragua, Panama, Puerto Rico, El Salvador, Saint Pierre and Miquelon, Turks and Caicos Islands, Trinidad and Tobago, United States, Saint Vincent and the Grenadines, British Virgin Islands, Virgin Islands, U.S.
ROW	Anguilla, Saint-Barthélemy, Saint-Martin, Sint Maarten
SOUTH AMERICA	Argentina, Bolivia, Brazil, Chile, Colombia, Ecuador, Falkland Islands, French Guiana, Guyana, Peru, Paraguay, Suriname, Uruguay, Venezuela

Table A.9 | CAPEX mapping

CAPEX Mappings	Country Name
AUS	Australia, New Caledonia, New Zealand, Palau, Solomon Islands, Tonga, Vanuatu
BRA	Argentina, Bahamas, Belize, Bolivia, Brazil, Chile, Colombia, Costa Rica, Cuba, Dominican Republic, Ecuador, Falkland Islands, Guatemala, French Guiana, Guyana, Honduras, Haiti, Jamaica, Mexico, Nicaragua, Panama, Peru, Puerto Rico, Paraguay, El Salvador, Suriname, Uruguay, Venezuela
CHE	Switzerland
CHN	China
DEU	Germany
ESP	Spain
FRA	France
GBR	United Kingdom
IND	India
ITA	Italy, San Marino, Vatican City
JPN	Japan
KOR	South Korea
MYS	Malaysia
THA	Thailand
USA	Canada, United States
ZAF	Lesotho, South Africa
EU_AVG	Kosovo, Albania, Andorra, Armenia, Austria, Azerbaijan, Belgium, Bulgaria, Bosnia and Herzegovina, Belarus, Cyprus, Czech Republic, Denmark, Estonia, Finland, Georgia, Greece, Croatia, Hungary, Isle of Man, Ireland, Iceland, Liechtenstein, Lithuania, Luxembourg, Latvia, Monaco, Moldova, Macedonia, Malta, Montenegro, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovakia, Slovenia, Sweden, Ukraine
ASIA_AVG	Afghanistan, United Arab Emirates, Bangladesh, Bahrain, Brunei, Bhutan, Hong Kong, Indonesia, Iran, Iraq, Israel, Jordan, Kazakhstan, Kyrgyzstan, Cambodia, Kuwait, Laos, Lebanon, Sri Lanka, Macao, Myanmar, Mongolia, Nepal, Oman, Pakistan, Philippines, Papua New Guinea, North Korea, Palestina, Qatar, Russia, Saudi Arabia, Singapore, Syria, Tajikistan, Turkmenistan, Timor-Leste, Turkey, Taiwan, Uzbekistan, Vietnam, Yemen
WLD_AVG	Aruba, Angola, Anguilla, American Samoa, Antigua and Barbuda, Burundi, Benin, Bonaire, Sint Eustatius and Saba, Burkina Faso, Saint-Barthélemy, Bermuda, Barbados, Botswana, Central African Republic, Côte d'Ivoire, Cameroon, Democratic Republic of the Congo, Republic of Congo, Cook Islands, Comoros, Cape Verde, Curaçao, Cayman Islands, Djibouti, Dominica, Algeria, Egypt, Eritrea, Western Sahara, Ethiopia, Fiji, Faroe Islands, Micronesia, Gabon, Ghana, Guinea, Guadeloupe, Gambia, Guinea-Bissau, Equatorial Guinea, Grenada, Greenland, Guam, Kenya, Kiribati, Saint Kitts and Nevis, Liberia, Libya, Saint Lucia, Saint-Martin, Morocco, Madagascar, Maldives, Marshall Islands, Mali, Northern Mariana Islands, Mozambique, Mauritania, Montserrat, Martinique, Mauritius, Malawi, Mayotte, Namibia, Niger, Nigeria, Niue, Nauru, French Polynesia, Reunion, Rwanda, Sudan, Senegal, Saint Helena, Sierra Leone, Somalia, Saint Pierre and Miquelon, South Sudan, São Tomé and Príncipe, Swaziland, Sint Maarten, Seychelles, Turks and Caicos Islands, Chad, Togo, Tokelau, Trinidad and Tobago, Tunisia, Tuvalu, Tanzania, Uganda, Saint Vincent and the Grenadines, British Virgin Islands, Virgin Islands, U.S., Wallis and Futuna, Samoa, Zambia, Zimbabwe

Table A.10 | 32 Global Region Mapping

Regions	Country Name
AFE	Eritrea, Ethiopia, Kenya, Mauritius, Sudan, South Sudan
AFN	Algeria, Egypt, Libya, Morocco, Tunisia
AFS	Angola, Botswana, Mozambique, Namibia, Tanzania, Zambia, Zimbabwe
AFW	Burundi, Benin, Burkina Faso, Central African Republic, Côte d'Ivoire, Cameroon, Democratic Republic of the Congo, Republic of Congo, Comoros, Cape Verde, Djibouti, Gabon, Ghana, Guinea, Gambia, Guinea-Bissau, Equatorial Guinea, Liberia, Lesotho, Madagascar, Mali, Mauritania, Malawi, Niger, Nigeria, Reunion, Rwanda, Senegal, Sierra Leone, Somalia, São Tomé and Príncipe, Swaziland, Seychelles, Chad, Togo, Uganda
ANZ	Australia, New Zealand
ARG	Argentina
ASC	Armenia, Azerbaijan, Georgia, Kazakhstan, Kyrgyzstan, Mongolia, Pakistan, Tajikistan, Turkmenistan, Uzbekistan
ASE	Brunei, Cambodia, Myanmar, Malaysia, Philippines, Singapore, Thailand, Vietnam
ASO	Bangladesh, Sri Lanka, Nepal
ASR	Afghanistan, Bhutan, Cook Islands, Fiji, Hong Kong, Kiribati, Laos, Macao, Maldives, New Caledonia, Palau, Papua New Guinea, North Korea, French Polynesia, Solomon Islands, Timor-Leste, Tonga, Taiwan, Vanuatu, Samoa
BRA	Brazil
CAN	Canada
CHN	China
ENE	Albania, Bosnia and Herzegovina, Belarus, Moldova, Macedonia, Montenegro, Serbia, Ukraine
ENW	Switzerland, Iceland, Norway
EUE	Bulgaria, Cyprus, Czech Republic, Estonia, Croatia, Hungary, Lithuania, Latvia, Malta, Poland, Romania, Slovakia, Slovenia
EUW	Austria, Belgium, Germany, Denmark, Spain, Finland, France, Greece, Ireland, Italy, Luxembourg, Netherlands, Portugal, Sweden
GBR	United Kingdom, Gibraltar
IDN	Indonesia
IND	India
IRN	Iran
JPN	Japan
KOR	South Korea
LAM	Aruba, Antigua and Barbuda, Bonaire, Sint Eustatius and Saba, Bahamas, Belize, Bermuda, Bolivia, Barbados, Chile, Colombia, Costa Rica, Cuba, Curaçao, Cayman Islands, Dominica, Dominican Republic, Ecuador, Falkland Islands, Guadeloupe, Grenada, Guatemala, French Guiana, Guyana, Honduras, Haiti, Jamaica, Saint Kitts and Nevis, Saint Lucia, Montserrat, Martinique, Nicaragua, Panama, Peru, Puerto Rico, Paraguay, El Salvador, Saint Pierre and Miquelon, Suriname, Sint Maarten, Turks and Caicos Islands, Trinidad and Tobago, Uruguay, Saint Vincent and the Grenadines, Venezuela, British Virgin Islands
MEA	United Arab Emirates, Bahrain, Iraq, Israel, Jordan, Kuwait, Lebanon, Oman, Qatar, Syria, Yemen
MEX	Mexico
ROW	Kosovo, Anguilla, Andorra, American Samoa, Saint-Barthélemy, Western Sahara, Faroe Islands, Micronesia, Greenland, Guam, Isle of Man, Liechtenstein, Saint-Martin, Monaco, Marshall Islands, Northern Mariana Islands, Mayotte, Niue, Nauru, Palestina, Saint Helena, San Marino, Tokelau, Tuvalu, Vatican City, Virgin Islands, U.S., Wallis and Futuna
RUS	Russia
SAU	Saudi Arabia
TUR	Turkey
USA	United States
ZAF	South Africa

A.2 Supplementary Figures

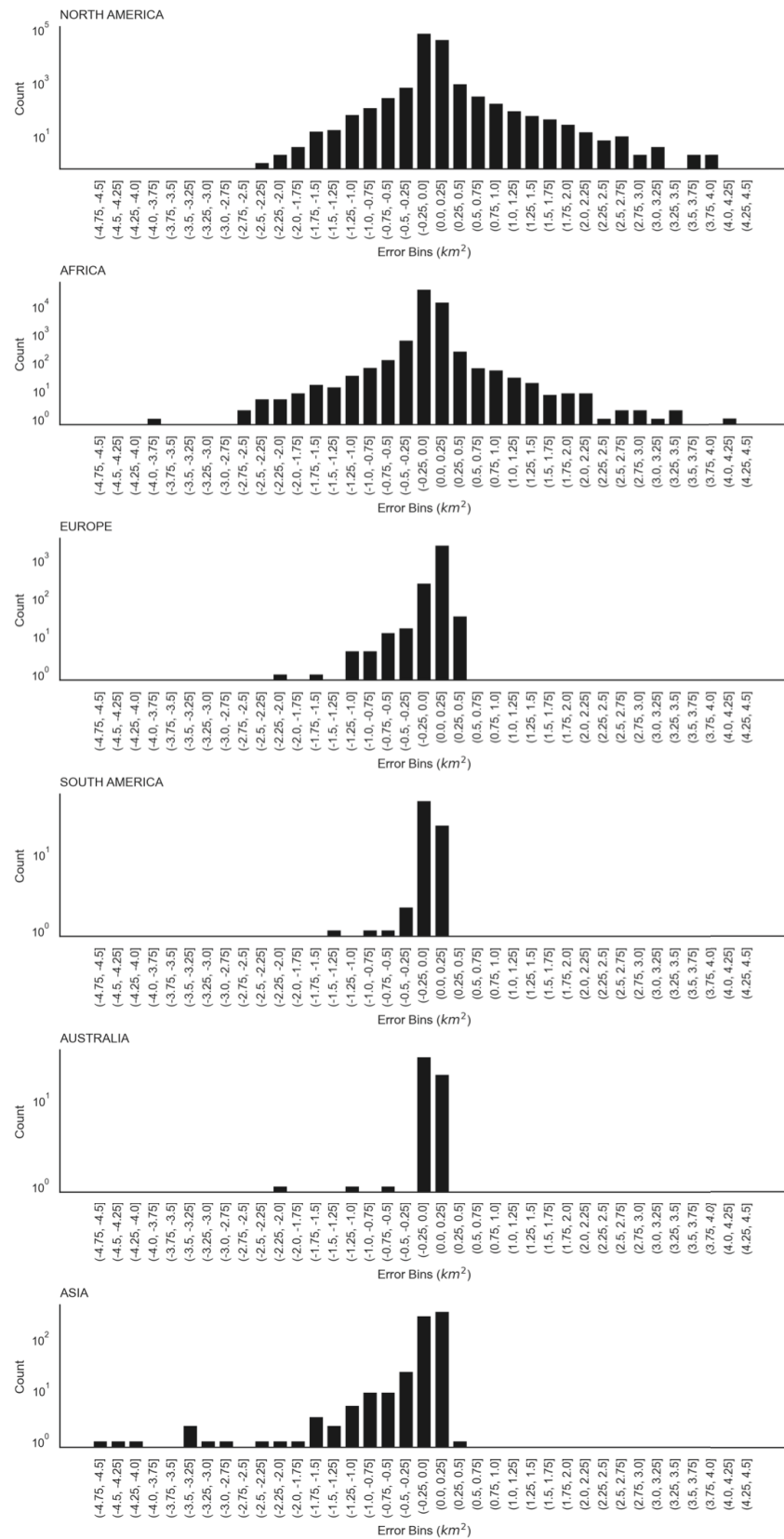


Figure A.1 | Distribution of error bins at a regional level

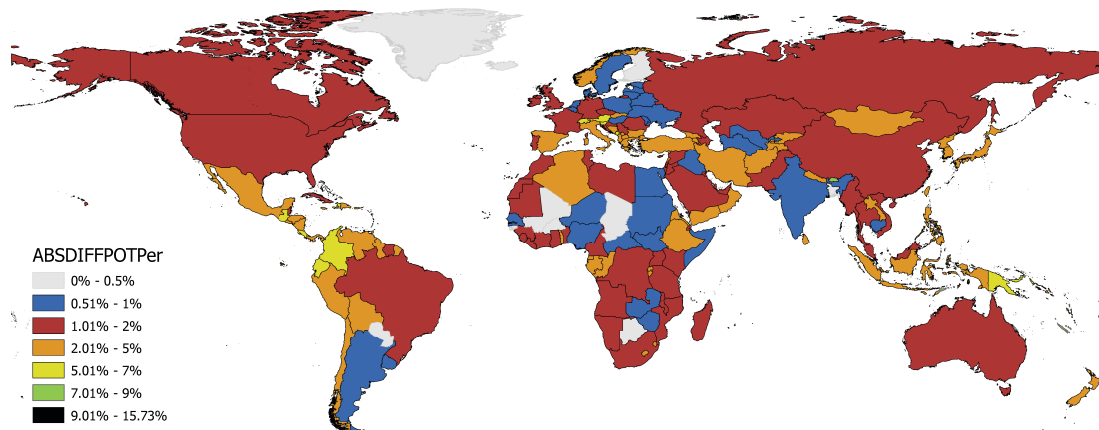


Figure A.2 | Absolute percentage difference in potential

The figure is a author generated visualisation of data representing absolute percentage difference in yearly potentials when using either maximum or minimum CF factor value inside an FN compared to mean statistic used in the study. Majority of the global countries have an absolute percentage difference between 0-2% when compared to their mean yearly potential. The countries having high absolute percentage difference are the ones that are located in a mountainous terrain. The range of the absolute percentage difference are the bounds of uncertainty for a country, within which the actual value is expected to fall depending on whether the FN having the deviation contains built-up area or not. On a global aggregated level, an absolute difference of $\pm 1\%$ is observed around mean yearly potential of 27 PWh.

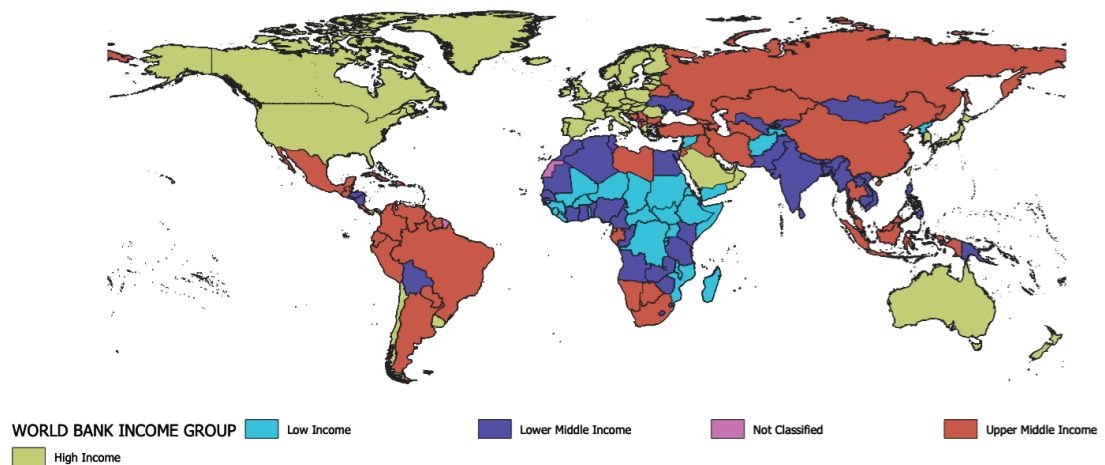


Figure A.3a | World Bank Income Groups

For the current 2021 fiscal year, low-income economies are defined as those with a GNI per capita, calculated using the World Bank Atlas method, of \$1,035 or less in 2019; lower middle-income economies are those with a GNI per capita between \$1,036 and \$4,045; upper middle-income economies are those with a GNI per capita between \$4,046 and \$12,535; high-income economies are those with a GNI per capita of \$12,536 or more. Mapping Data Source: World Bank, visualisation done by author.

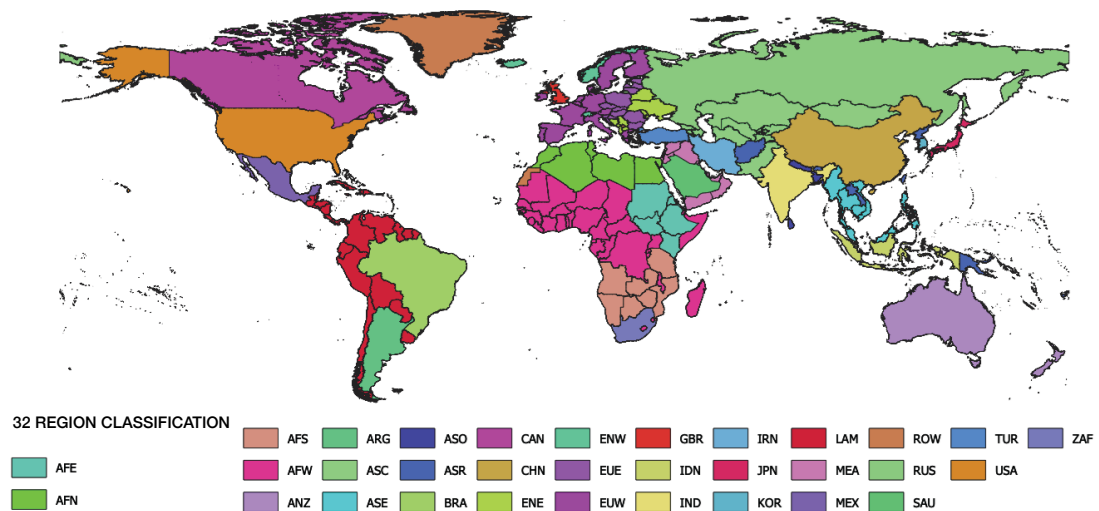


Figure A.3b | 32 Region global classification

The 32 region global map is a visualisation by author based on the regions description of CHIMERA project that is being executed as a collaboration project between University College Cork, Ireland, Tsinghua University, China and Peking University, China to design next generation global energy models with high temporal and spatial resolution. The regions are designed based on geographic continuity and sub regional uniqueness. These regions will act as a base unit for further work being done under the project.

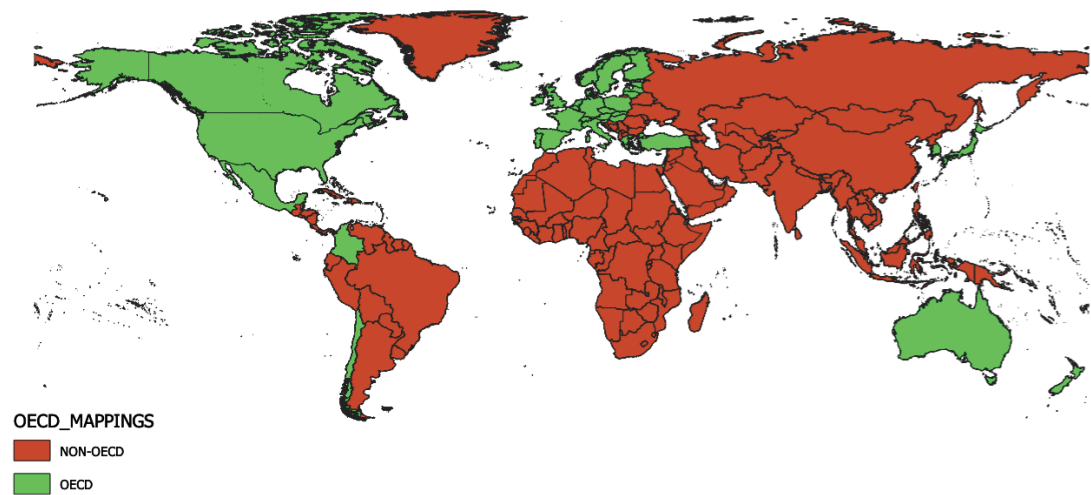


Figure A.3c | OECD country classification

The OECD classification is based on the global charter of Organisation for Economic Co-operation and Development group. The OECD classification is used to map OPEX and Discount Rates for the current research. Mapping Data Source: OECD, visualisation done by author.

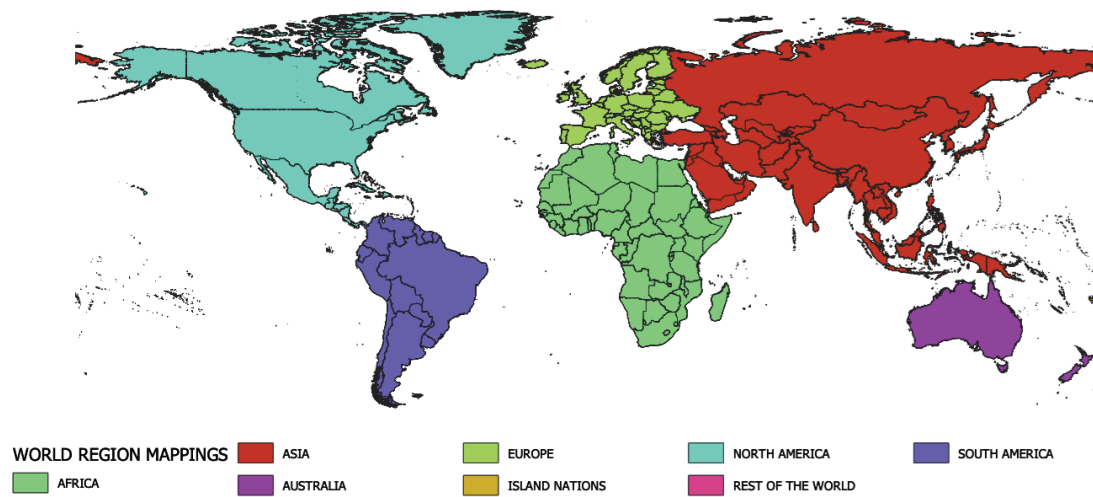


Figure A.3d | World Regions

The world region classification is an author generated visualisation based off assigning the countries to respective global continent with exception of Cyprus and Russia, which is assigned to Asia continent. The Island Nations region is assigned to small group of Island countries in Asia-Pacific region.

A.3 Supplementary Pseudocode

Algorithm 1: Data Preparation

Input:

FN: Fishnet Grid
BF: Building Footprint polygon (Vector)
RL: Road polyline (Vector)
BA: Built-up Area (Raster)
CF_M: Monthly Conversion Factor (Raster)
PPLN: Population count (Raster)

Output:

BF_{FN}: Aggregated Building Footprint area mapped to unique FN
RL_{FN}: Aggregated Road Length mapped to unique FN
BA_{FN}: Aggregated Built-up Area mapped to unique FN
CF_{M, FN}: Averaged Monthly Conversion Factor mapped to unique FN
PPLN_{FN}: Aggregated Population count mapped to unique FN

```
1: for each FN:                                     /* Iterate for each cell in Fishnet Grid*/
2:   if BA>0:                                         /* If built-up area exist in FN*/
3:     MASKFN = not (Geographic extent of BA in FN) /* Generate Masking layer*/
4:     BFFN = sum (Area of BF outside MASKFN)      /* Aggregate non-masked Building
                                                    Footprint area*/
5:     RLFN = sum (Length of RL outside MASKFN)    /* Aggregate non-masked length of
                                                    Roads*/
6:     PPLNFN = sum (Pixels of PPLN outside MASKFN) /* Aggregate non-masked Population
                                                    count*/
7:     BAFN = sum (PixelValue*PixelArea of BA)/100 /* Aggregate non-masked Built-up
                                                    area*/
8:     CFM, FN = mean (Pixels of CFM)             /* Average of Conversion Factor value
                                                    for each month*/
```

Algorithm 2: XGBoost Model Training and Estimation

Input:

BF_{FN}: Aggregated Building Footprint area mapped to unique FN
RL_{FN}: Aggregated Road Length mapped to unique FN
BA_{FN}: Aggregated Built-up Area mapped to unique FN
PPLN_{FN}: Aggregated Population count mapped to unique FN
S: Denotes samples extracted from full data

Output:

BFE_{FN}: Aggregated estimated Building Footprint area mapped to unique FN

Sample Fishnet Cell extraction

```
1: for each FN:                                     /* Iterate for each cell in Fishnet Grid*/
2:   if BFFN > 0:                                   /* If Aggregated Building Footprint area
                                                    exist in FN*/
3:     FNs = FN                                     /* FNs becomes sample FN for model
                                                    . . . . . */
```

Hyperparameter Optimisation (Aim is to reduce Mean Squared Error of the base model with each iteration)

```
1: for n:                                           /* n is the number of iterations*/
2:   XS = BFFNs                                   /* Set dependent variable for sample FNs */
3:   YS = (RLFNs, BAFNs, PPLNFNs)             /* Set independent variables dataframe for sample FNs */
4:   KSi = XSi, YSi                             /* Split data into 10 folds using shuffling, i is the ith fold */
5:   MSEi = XGBP(KSi)                             /* Calculate MSE for ith fold data using "P" parameters for
                                                    base XGBoost model*/
6:   MSEmean,t = mean(MSEi)                       /*Take mean of MSE for all 10 folds at t iteration number*/
7:   if MSEmean,t-1 > MSEmean,t:                   /*If MSE of t-1 iteration number is greater than MSE of t
                                                    iteration*/
8:     Choose the next best parameter combination based on predictive Tree Parzen
       Estimator
9:   save P                                           /*Save best parameter combination after n iterations*/
```

Estimation of Building Footprint Area per FN from trained model

```
1:  $X_s = BF_{FN_s}$  /* Set dependent variable for sample FNs */
2:  $Y_s = (RL_{FN_s}, BA_{FN_s}, PPLN_{FN_s})$  /* Set independent variables dataframe for sample FNs */
3: Model = XGBp ( $X_s, Y_s$ ) /* Train base XGBoost model using tuned parameters */
4:  $Y = (RL_{FN}, BA_{FN}, PPLN_{FN})$  /* Set independent variables dataframe for full set of FN */
5: if  $RL_{FN}$  and  $BA_{FN}$  and  $PPLN_{FN}$  is not null: /* If logical data exists within the FN */
6:    $BFE_{FN} = \text{Model}(Y)$  /* Use trained model to estimate aggregated building footprint area per FN */
7: save  $BFE_{FN}$  /* Save estimated Building footprint data for FN */
```

Algorithm 3: Calculation of Potentials and Costs

Input:

BFE_{FN}: Aggregated estimated Building Footprint area mapped to unique FN

CF_{M, FN}: Averaged Monthly Conversion Factor mapped to unique FN

A_P: Area required by each solar panel

RAF: Rooftop Availability Factor

CAPEX_{FN}: Aggregated Capital Expenditure mapped to unique FN

OPEX_{FN}: Aggregated Operation and Maintenance cost per year mapped to unique FN

DR_{FN}: Average Discount Rate mapped to unique FN

TL: Technology life of Rooftop Solar PV

Output:

SP_{M,FN}: Estimated monthly electricity generation potential mapped to unique FN

SP_{Y,FN}: Estimated yearly electricity generation potential mapped to unique FN

LCOE_{FN}: Estimated Levelised Cost of Electricity mapped to unique FN

Calculation of potential per FN cell

```
1: for each FN:                                     /* Iterate for each cell in Fishnet Grid*/
2:   for each M:                                     /* Iterate for each month*/
3:     if BFEFN>0:                                   /* If estimated aggregated Building Footprint area exist
4:       NPFN = (BFEFN*RAF)/AP                       /*calculate number of 1 kWp panels per FN*/
5:       SPM,FN = NPFN*CFM,FN                         /*Calculate monthly potential per FN*/
6:     SPY,FN = sum(SPM,FN)                             /*Calculate yearly potential per FN*/
7:   save SPY,FN,SPM,FN                               /*save SPY,FN,SPM,FN as Geopackage and csv file*/
7:   create Figure 5a using SPY,FN                     /*Use geomapped SPY,FN to create figure 5a */
```

Calculation of LCOE per FN cell

```
1: for each FN:                                     /* n is the number of iterations*/
2:   map CAPEX, OPEX and DR                           /* Map CAPEX, OPEX and DR based on FN
                                                         geolocation */
3:   CAPEXFN = CAPEX* NPFN                           /* Find total CAPEX using number of panels */
4:   OPEXFN = OPEX* NPFN                             /* Find total OPEX using number of panels */
5:   LCOEFN=function(CAPEXFN, OPEXFN,
                    DRFN, SPY,FN,TL)                 /* Calculate LCOE */
6:   save LCOEFN                                       /*save LCOEFN as Geopackage and csv file*/
7:   create Figure 5b using LCOEFN                   /*Use geomapped LCOEFN to create figure 5b
                                                         */
```

References Appendix A

- 1 Bódis, K., et al. (2019). "A high-resolution geospatial assessment of the rooftop solar photovoltaic potential in the European Union." *Renewable and Sustainable Energy Reviews* 114.
- 2 Gernaat, D. E. H. J., et al. (2020). "The role of residential rooftop photovoltaic in long-term energy and climate scenarios." *Applied Energy* 279.
- 3 Deng, Y. Y. et al. (2015) Quantifying a realistic, worldwide wind and solar electricity supply. *Global Environmental Change* 31, 239–252 (2015).
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- 13 Hong, T., et al. (2017). "Development of a method for estimating the rooftop solar photovoltaic (PV) potential by analyzing the available rooftop area using Hillshade analysis." *Applied Energy* 194: 320-332.
- 14 Yuan, J., et al. (2016). "A method to estimate the potential of rooftop photovoltaic power generation for a region." *Urban Climate* 17: 1-19.

Appendix B: Supplementary Information for Chapter 3

B.1 Supplementary Tables

Table B.1 | Base year layers used in this study along with their attributes and sources

Layer	Type	Region	Attribute	Format	Size
FN	Fishnet Grid	Global	~ 3 million polygons	Vector Polygon	N.A.
BF20	2020 Building Footprint	USA, Canada, UK, Australia, Africa	~ 700 million buildings	Vector Polygon	~100 GB
OSM_20	2020 Building Footprint	Rest of the world - OSM	~ 250 million buildings	Vector Polygon	~200 GB
PPLN20	2020 Population Count	Global	100m Resolution	Raster	~1GB
BU20	2020 Built-up Area	Global	100m Resolution	Raster	~3GB
RL20	Road Length	Global	~ 34 million km	Vector Polylines	~100 GB

Table B.2 | SSP derived layers used in this study along with their attributes and sources

Layer	Type	Region	Attribute	Format	Size
PPLNX,Y*	Future SSP derived griddled population count	Global	1/8 degree	Raster	N.A.
BUX,Y*	Future SSP derived griddled built-up extent	Global	1/8 degree	Raster	N.A.
GDPX,Y*	Future SSP derived country-wise GDP	Global	Country wise	Vector Polygon	N.A.

* where "X" is the SSP narrative number, "Y" is the year for which the respective metric is provided.

Table B.3 | Distribution and attribute of samples used for model training

Sample Areas	Input Rooftop Area (km ²)	# Individual Polygons
Australia	2,418	~10 million
UK	3,450	~33 million
USA	29,930	~ 144 million
Canada	2,500	~19 million
Africa	17,166	~300 million
OSM	21,000	~140 million

Table B.4 | Percentage distribution of assessed global gross rooftop area across SSPs and continents

Continents	2020	SSP1_2050	SSP2_2050	SSP3_2050	SSP4_2050	SSP5_2050
Africa	8.76	12.30	12.34	12.56	12.12	11.83
Asia	50.39	49.54	49.60	51.09	48.99	47.89
Australia	1.00	0.98	0.92	0.85	0.95	1.06
Europe	18.90	17.16	17.13	16.29	17.58	18.06
North America	15.50	14.99	14.97	13.90	15.39	16.34
Oceania	0.20	0.20	0.19	0.18	0.20	0.20
South America	5.26	4.84	4.84	5.12	4.78	4.63

Table B.5 | Absolute Growth of global gross rooftop area across SSPs and continents

Continents	SSP 1	SSP 2	SSP 3	SSP 4	SSP 5
Africa	1.71X	1.92X	1.79X	1.80X	2.06X
Asia	1.19X	1.34X	1.27X	1.27X	1.44X
Australia	1.19X	1.26X	1.07X	1.24X	1.60X
Europe	1.10X	1.23X	1.08X	1.21X	1.45X
North America	1.17X	1.31X	1.13X	1.29X	1.60X
Oceania	1.24X	1.31X	1.16X	1.28X	1.52X
South America	1.12X	1.25X	1.22X	1.18X	1.34X

Where X is the absolute increase in 2050 values over 2020 values

Table B.6 | Regional definitions of the 11 MESSAGEix-GLOBIOM Model

Regions	Definition	List of countries
NAM	North America	Canada, Guam, Puerto Rico, United States of America, Virgin Islands
WEU	Western Europe	Andorra, Austria, Azores, Belgium, Canary Islands, Channel Islands, Cyprus, Denmark, Faeroe Islands, Finland, France, Germany, Gibraltar, Greece, Greenland, Iceland, Ireland, Isle of Man, Italy, Liechtenstein, Luxembourg, Madeira, Malta, Monaco, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, United Kingdom
PAO	Pacific OECD	Australia, Japan, New Zealand
EEU	Central and Eastern Europe	Albania, Bosnia and Herzegovina, Bulgaria, Croatia, Czech Republic, The former Yugoslav Rep. of Macedonia, Hungary, Poland, Romania, Slovak Republic, Slovenia, Yugoslavia, Estonia, Latvia, Lithuania
FSU	Former Soviet Union	Armenia, Azerbaijan, Belarus, Georgia, Kazakhstan, Kyrgyzstan, Republic of Moldova, Russian Federation, Tajikistan, Turkmenistan, Ukraine, Uzbekistan
CPA	Centrally Planned Asia and China	Cambodia, China (incl. Hong Kong), Korea (DPR), Laos (PDR), Mongolia, Viet Nam
SAS	South Asia	Afghanistan, Bangladesh, Bhutan, India, Maldives, Nepal, Pakistan, Sri Lanka
PAS	Other Pacific Asia	American Samoa, Brunei Darussalam, Fiji, French Polynesia, Gilbert-Kiribati, Indonesia, Malaysia, Myanmar, New Caledonia, Papua, New Guinea, Philippines, Republic of Korea, Singapore, Solomon Islands, Taiwan (China), Thailand, Tonga, Vanuatu, Western Samoa
MEA	Middle East and North Africa	Algeria, Bahrain, Egypt (Arab Republic), Iraq, Iran (Islamic Republic), Israel, Jordan, Kuwait, Lebanon, Libya/SPLAJ, Morocco, Oman, Qatar, Saudi Arabia, Sudan, Syria (Arab Republic), Tunisia, United Arab Emirates, Yemen
LAM	Latin America and the Caribbean	Antigua and Barbuda, Argentina, Bahamas, Barbados, Belize, Bermuda, Bolivia, Brazil, Chile, Colombia, Costa Rica, Cuba, Dominica, Dominican Republic, Ecuador, El Salvador, French Guyana, Grenada, Guadeloupe, Guatemala, Guyana, Haiti, Honduras, Jamaica, Martinique, Mexico, Netherlands Antilles, Nicaragua, Panama, Paraguay, Peru, Saint Kitts and Nevis, Santa Lucia, Saint Vincent and the Grenadines, Suriname, Trinidad and Tobago, Uruguay, Venezuela
AFR	Sub-Saharan Africa	Angola, Benin, Botswana, British Indian Ocean Territory, Burkina Faso, Burundi, Cameroon, Cape Verde, Central African Republic, Chad, Comoros, Cote d'Ivoire, Congo, Democratic Republic of Congo, Djibouti, Equatorial Guinea, Eritrea, Ethiopia, Gabon, Gambia, Ghana, Guinea, Guinea-Bissau, Kenya, Lesotho, Liberia, Madagascar, Malawi, Mali, Mauritania, Mauritius, Mozambique, Namibia, Niger, Nigeria, Reunion, Rwanda, Sao Tome and Principe, Senegal, Seychelles, Sierra Leone, Somalia, South Africa, Saint Helena, Swaziland, Tanzania, Togo, Uganda, Zambia, Zimbabwe

B.2 Supplementary Figures

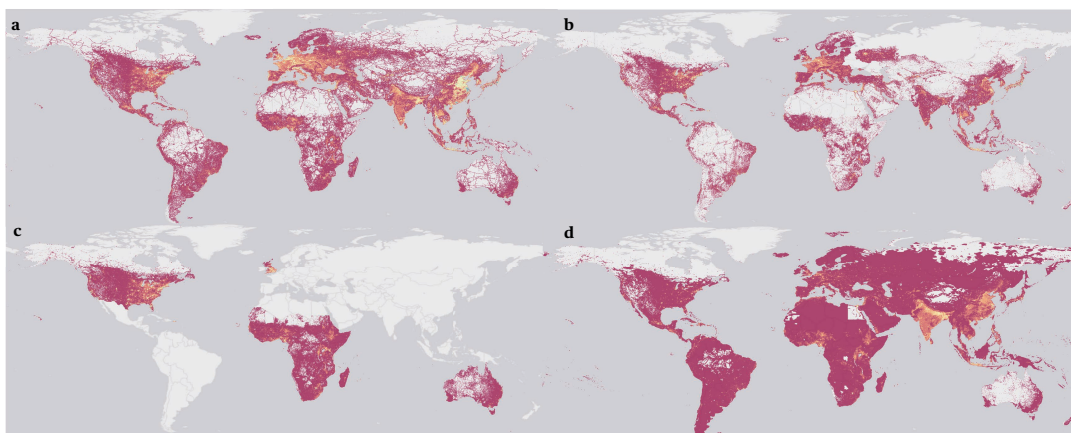


Figure B.1 | Spatial spread of the base input datasets

Global geo-mapped roads extracted from Open Street Maps, **a**. Global human made built-up areas extracted from Copernicus Land Monitoring Program GLC V3.1 2020, **b**. Building footprint polygons derived

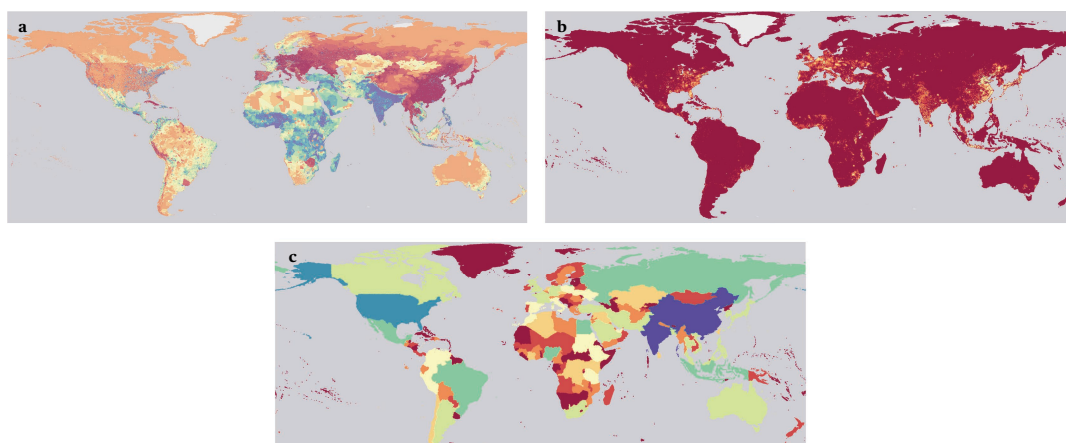


Figure B.2 | Relative change in metric for SSP2 derived datasets between 2020 and 2050

a, Global change in geo-mapped population. Red coloured areas have relatively lowest change in population between 2020 and 2050, with blue-coloured areas representing relatively highest change in population. **b**, Global change in geo-mapped built-up areas. Red coloured areas have relatively lowest change in Built-up area between 2020 and 2050, with yellow-coloured areas representing relatively highest change in Built-up area. **c**, country-wise change in GDP. Red coloured areas have relatively lowest growth in GDP between 2020 and 2050, with blue-coloured areas representing relatively growth in GDP.

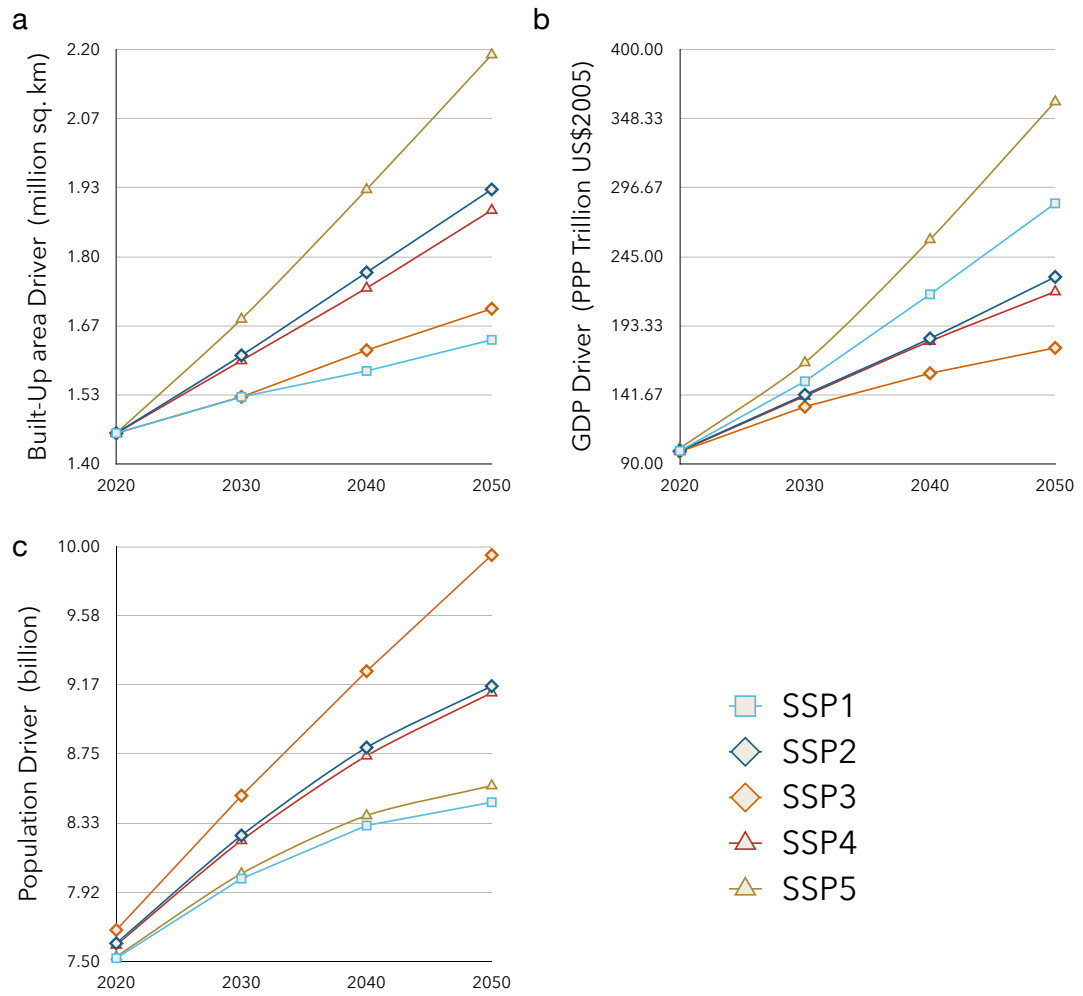


Figure B.3 | Global aggregated driver trajectories for M2 Model

a, Built-up area driver - $BU_{x,y}$ **b**, GDP driver - $GDP_{x,y}$ **c**, Population driver - $PPLN_{x,y}$

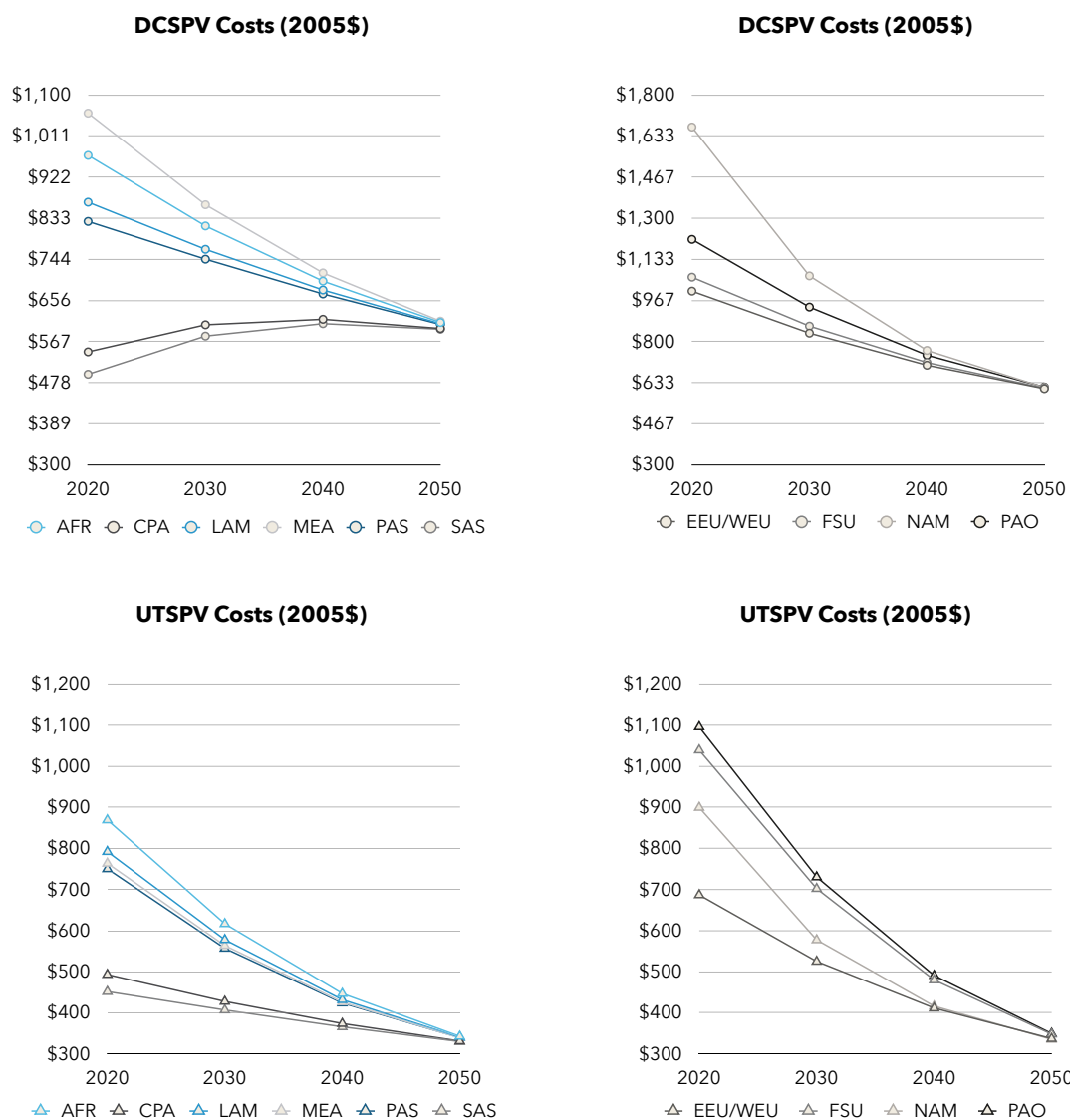


Figure B.4 | Cost trajectories for 11 global regions based on the technology topology

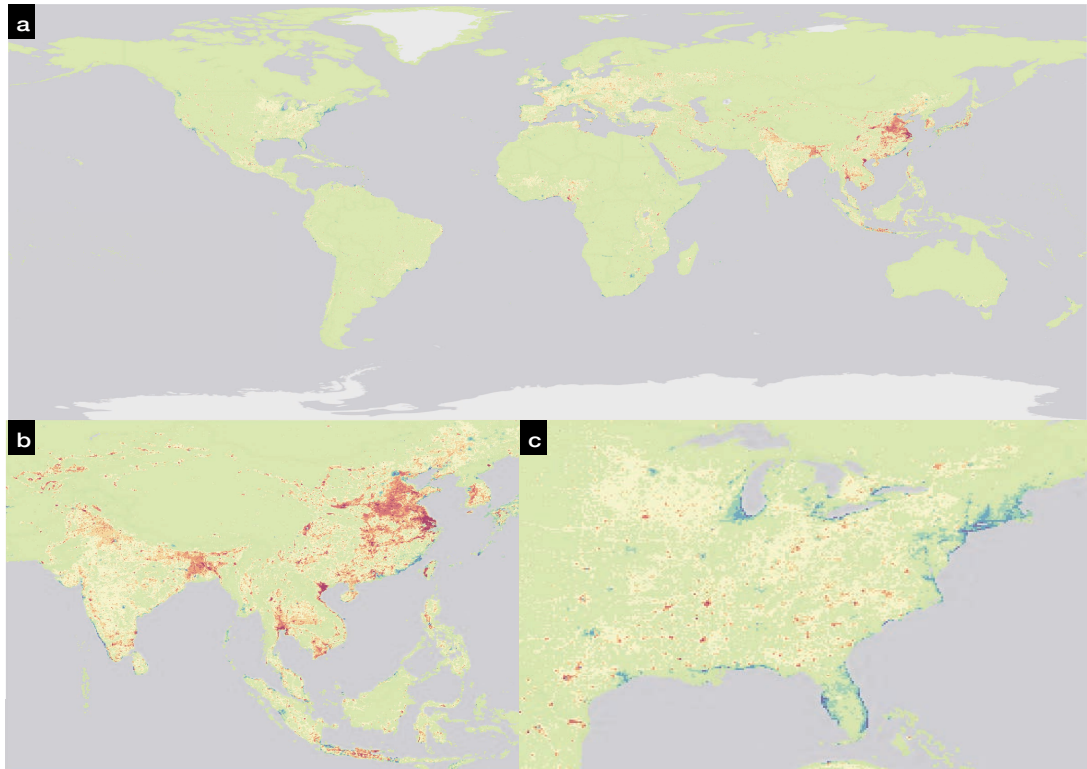


Figure B.5 | Discrepancies between BU20 layer and SSP derived $BU_{x,2020}$ layer

a, Global FN grid cell depicting the discrepancies between BU20 and $BU_{x,2020}$ layer. Red and orange coloured region FN grid cells have BU20 values more than $BU_{x,2020}$ dataset values while blue FN grid cells have $BU_{x,2020}$ values more than BU20 values. In general, the blue coloured FN grid cells signify overrepresentation of built-up area in $BU_{x,2020}$ layer and red coloured regions signify underrepresentation of built-up area. **b**, zoomed in region of Asia where red coloured FN grid cell are observed in East China with blue coloured grid cells being observed in coastal regions. **c**, zoomed in region of east coast of USA where blue colour FN grid cells are observed in coastal regions.

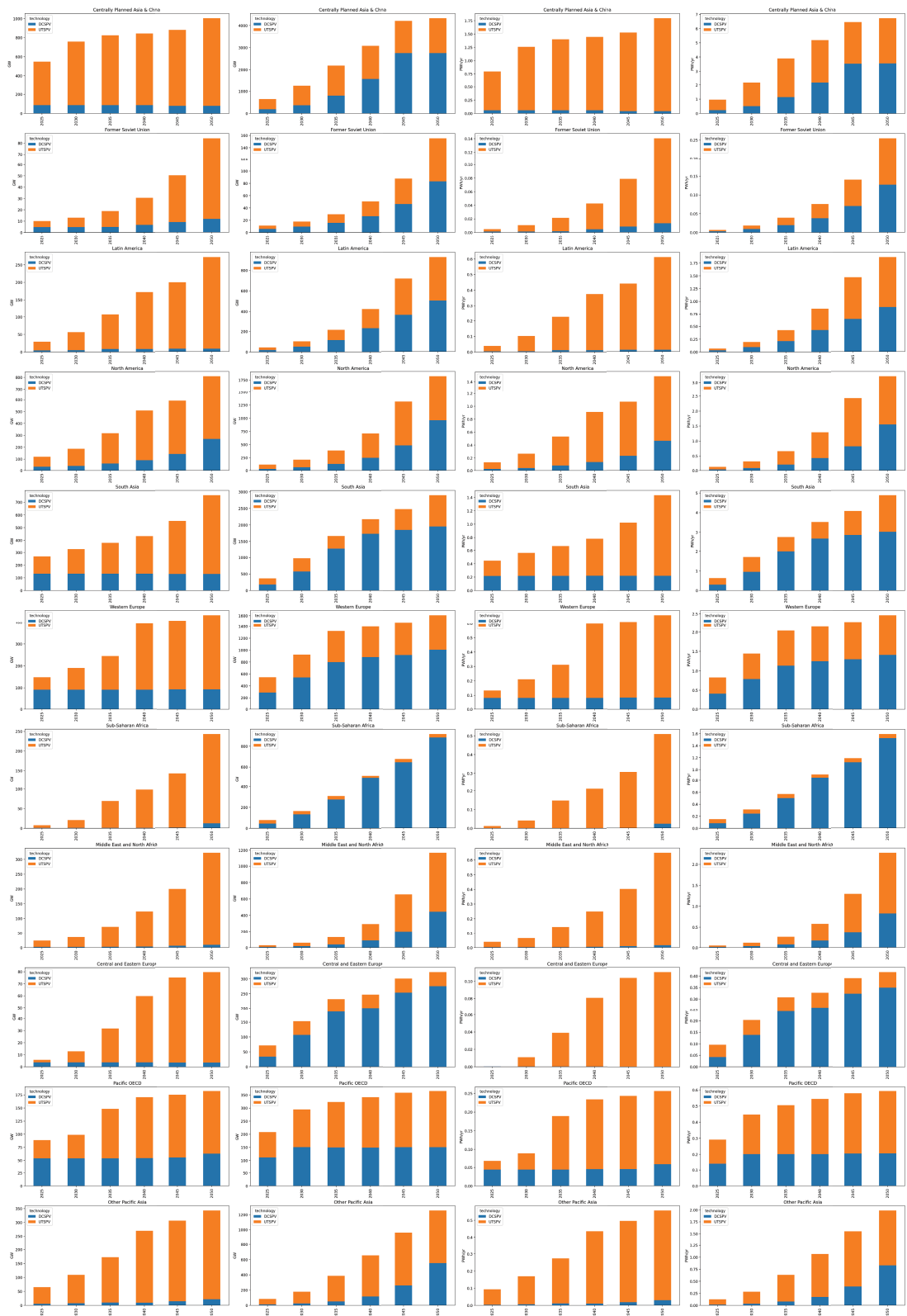


Figure B.6 | Capacity and Generation for C_{UTDC} and M_{UTDC} scenarios

a, Installed Capacity in GW for C_{UTDC} . **b**, Installed Capacity in GW for M_{UTDC} . **c**, Generation in PWh/yr for C_{UTDC} . **d**, Generation in PWh/yr for M_{UTDC} .

B.3 Technical validation

The datasets presented in this study have undergone end to end technical validation for the base year of 2020. The validation is performed for M1 and M2 model inputs, performance of M1 and M2 models, estimation validity of outputs of M1 and M2 models and finally verification of estimations generated by the M1 model. For datasets covering years 2030-2050, we unfortunately could not provide a true verification of validity of the results as the drivers used to estimate these values represent values in future which are difficult put an accuracy value on. The input validation of the base year datasets and SSP derived drivers are presented in Table B.7 as link to the validation reports generated by either the data providers or the peer reviewed publication which form the basis of the data. Due to the scale of the dataset, assumptions and the limitation of methods used, the big datasets used in this study are expected to have errors at a higher resolution when verifying at a per building level, but at an aggregated country/ regional spatial resolution these datasets have shown acceptable performance.

Table B.7 | Input data validation

Dataset	Format	Validation study link
Building Footprints	Vector	Heris, M.P, Foks, N.L., Bagstad, K.J. et al. A rasterized building footprint dataset for the United States. <i>Sci Data</i> 7, 207 (2020). https://doi.org/10.1038/s41597-020-0542-3
Population	Raster	Lloyd, C., Sorichetta, A. & Tatem, A. High resolution global gridded data for use in population studies. <i>Sci Data</i> 4, 170001 (2017). https://doi.org/10.1038/sdata.2017.1
Road	Vector	Barrington-Leigh, C., & Millard-Ball, A. (2017). The world's user-generated road map is more than 80% complete. <i>PloS one</i> , 12(8), e0180698. https://doi.org/10.1371/journal.pone.0180698
PVOUT	Raster	ESMAP. 2019. Validation Report: Global Solar Atlas 2.0 Validation Report. Washington, DC: World Bank.
Built-up area 2020	Raster	Tsendbazar, N.E., Tarko, A., Linlin, L., Herold, M., Lesiv, M., Fritz, S., Maus, V; (2020): Copernicus Global Land Service: Land Cover 100m: Version 3 Globe 2015-2019: Validation Report; Zenodo, Geneva, Switzerland, September 2020; doi: 10.5281/zenodo.3938974
SSP derived Built-up area 2020-2050	Raster	Gao, J., O'Neill, B.C. Mapping global urban land for the 21st century with data-driven simulations and Shared Socioeconomic Pathways. <i>Nat Commun</i> 11, 2302 (2020). https://doi.org/10.1038/s41467-020-15788-7
SSP derived Population 2020-2050	Raster	Jones, B. & O'Neill, B. C. Spatially explicit global population scenarios consistent with the Shared Socioeconomic Pathways. <i>Environ. Res. Lett.</i> 11, 084003 (2016). https://doi.org/10.1088/1748-9326/11/8/084003
SSP derived GDP 2020-2050	Dataset	Crespo Cuaresma, J. (2017). Income projections for climate change research: A framework based on human capital dynamics. <i>Global Environmental Change</i> , 42, 226–236. https://doi.org/10.1016/j.gloenvcha.2015.02.012

Learning accuracy of the M1 and M2 models are determined by the significance of the correlation between dependent and independent variables used to train the model. Further, a 10-fold cross validation strategy to expose the models to various combinations of input data to reduce model overfitting was used. Finally, the distribution of model output with respect to the dependent variables and spread of the errors were evaluated to choose the best model. Figure B.7 documents the results of these checks.

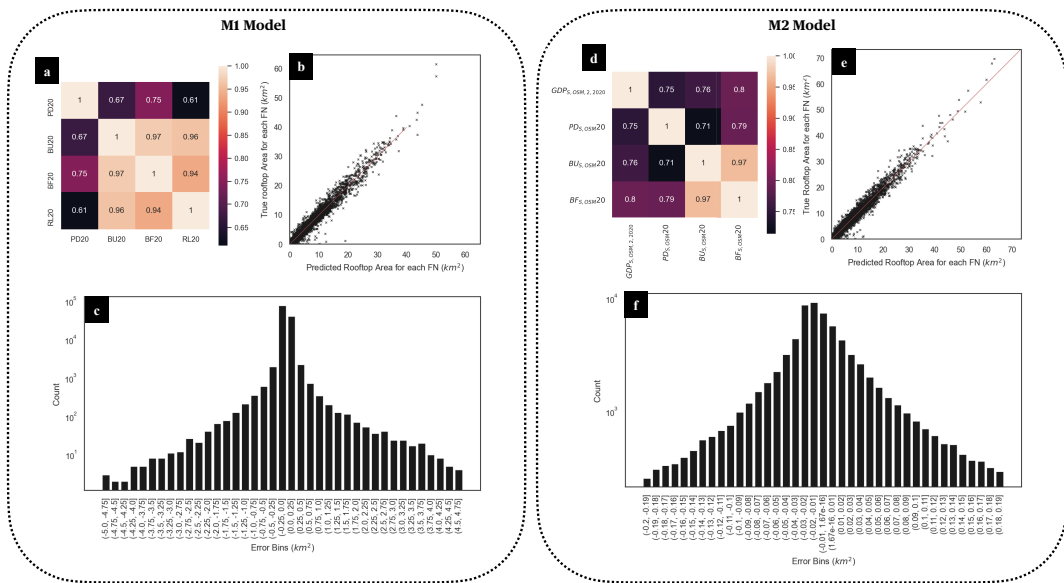


Figure B.7 | Performance metrics of M1 and M2 models

a, Correlation heatmap representing Pearson's correlation between pairs of independent and dependent variables of M1 model. High correlation can be observed for the depend variable (BF20) and independent variables (PD20, RL20, and BU20). **b**, graph representing relationship between M1 model's dependent variable and predicted values. High fidelity can be observed between dependent variable and predicted values. **c**, spread of absolute difference between dependent variable value and predicted value from M1 model at a per FN grid cell basis. Majority absolute error of $\pm 0.25 \text{ km}^2$ can be observed for a $1/8$ degree FN grid cell. **d**, Correlation heatmap representing Pearson's correlation between pairs of independent and dependent variables of M2 model. High correlation can be observed for the depend variable (BF_{S,OSM20}) and independent variables (PD_{S,OSM20}, GDP_{S,OSM2,2020}, and BU_{S,OSM20}). **e**, graph representing relationship between M2 model's dependent variable and predicted values. High fidelity can be observed between dependent variable and predicted values. **f**, spread of absolute difference between dependent variable value and predicted value from M2 model at a per FN grid cell basis. Majority absolute error of $\pm 0.05 \text{ km}^2$ can be observed for a $1/8$ degree FN grid cell with slight left skewness in the error distribution leading to model prediction showing slight underestimation of ground truth at FN grid cell level.

The final output of the M2 model ($BF_{X,Y}$) was further evaluated for discrepancies between aggregated country-wise input base year big data derived BF_{20} values and aggregated country-wise M2 models estimated outputs for SSP2 narrative in year 2020 ($BF_{2,2020}$). These evaluation were conducted by aggregating the FN grid cell values for those FN grid cell that fall within the geographic boundaries of the country being evaluated. Overall, we observed high fidelity between the ground truth and estimated values at a country level. On a higher spatial resolution, we also compared the sub country level estimations for USA based on ASHRAE climatic regions. Here also high fidelity was observed between ground truth and predicted values. This way, we could validate our results to a high degree of certainty by comparing results at sub-country level and country level. Table B.8 documents the results for sub-country level comparison and Table B.9 documents the comparison at city (Figure B.8), country and regional level.

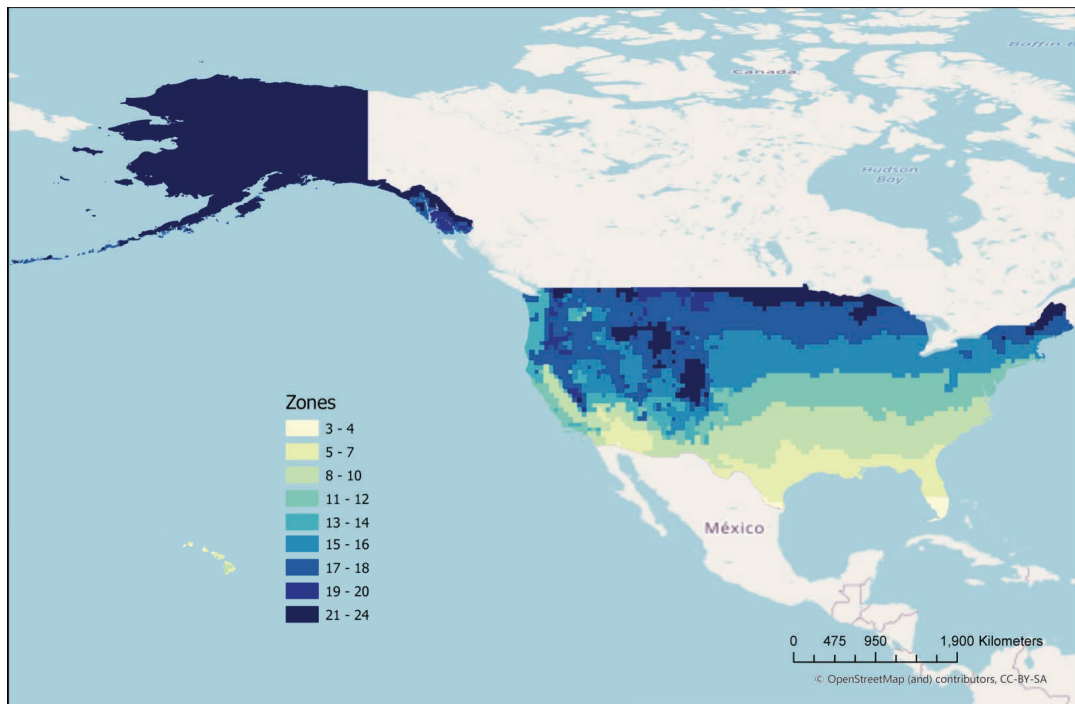


Figure B.8 | Map of climate zones over USA

Table B.8 | Result comparison of M2 Model's output at sub country level for USA (2020)

Climatic Zone	Ground Truth (km²)	M2 Model's output (km²)	Absolute percentage error
22	1.6	1.5	9.5
24	7.9	144.5	1,736.0
20	12.1	16.4	35.2
19	24.9	25.9	4.2
16	68.3	77.3	13.2
4	76.2	108.4	42.3
21	199.6	227.1	13.8
13	215.9	218.4	1.1
17	410.8	406.8	1.0
7	700.5	706.3	0.8
3	734.2	632.5	13.8
14	950.7	832.1	12.5
10	1,028.1	1,073.5	4.4
11	1,426.3	1,267.3	11.1
18	1,892.0	1,900.9	0.5
6	4,102.5	3,788.5	7.7
9	5,530.6	5,532.2	0.0
12	5,666.1	5,818.6	2.7
15	6,632.4	6,669.0	0.6
Total	29,680.5	29,447.1	0.8

Table B.9 | Result comparison of M2 Model's output at city, country and regional level

Country	Ground Truth (BF20) km²	M2 Model's Predicted value (2020) (km²)	Note
Australia	2,418	2,527	Seen data by model
UK	3,450	3,492	Seen data by model
USA	29,930	29,447	Seen data by model
Canada	2,500	2,753	Seen data by model
Africa	17,166	17,525	Seen data by model
OSM*	21,000	28,399	Seen data by model
Ireland	304	320	Not seen by model
Kansas	10	9	See Supplementary Figure B.9
Singapore	104	116	See Supplementary Figure B.9
Sydney	313	314	See Supplementary Figure B.9

* Input OSM Fishnet were not fully mapped in the same hence lower input aggregated area

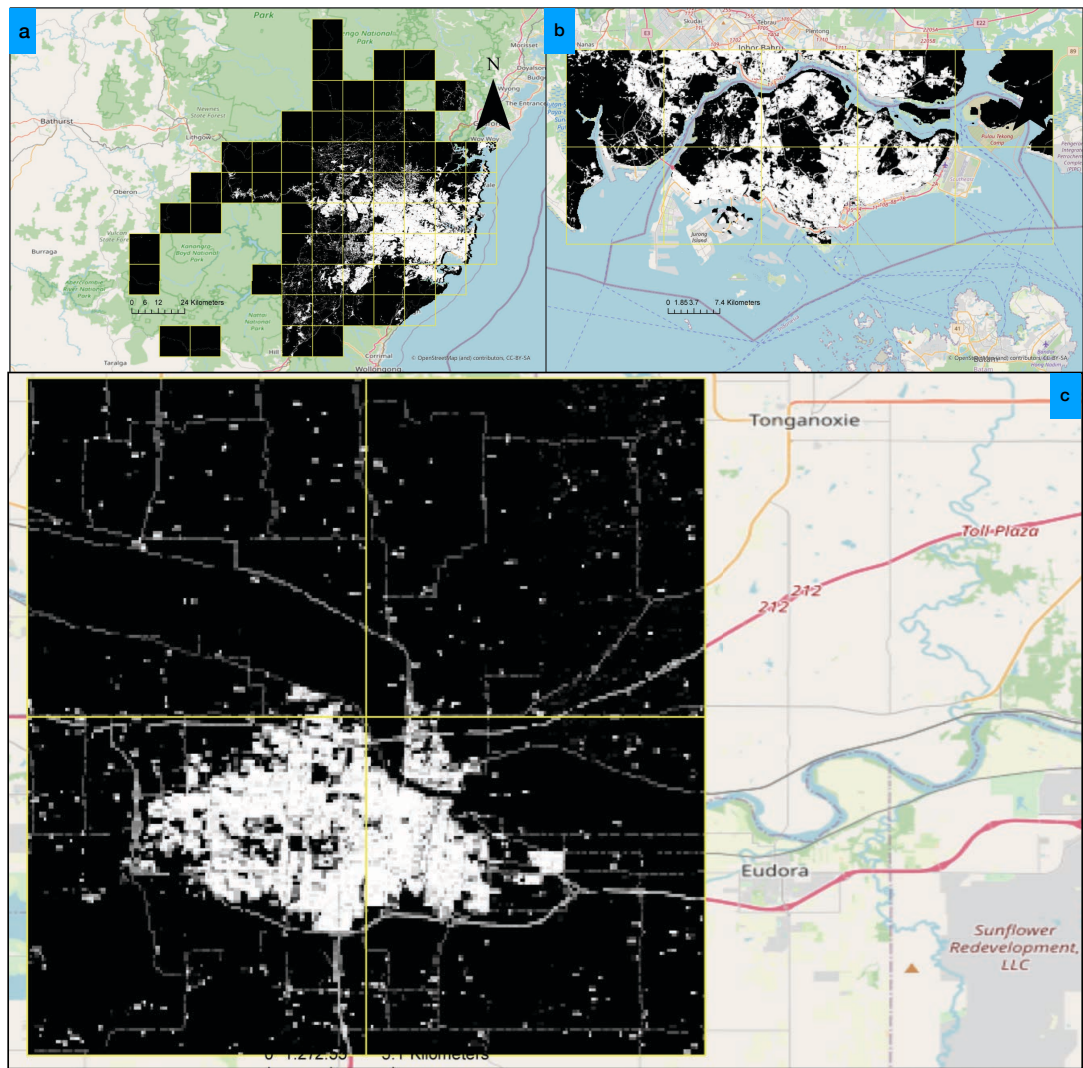


Figure B.9 | Sample boundaries for Table B.9

a, Boundary of test sample over greater Sydney region. The FN grid is marked with yellow colour, the black area is the non built-up area inside the FN tile and the white/grey area is the built-up area inside the FN tile. **b**, Boundary of test sample over Singapore/Malaysia region. The FN grid is marked with yellow colour, the black area is the non built-up area inside the FN tile and the white/grey area is the built-up area inside the FN tile. **c**, Boundary of test sample over Kansas region. The FN grid is marked with yellow colour, the black area is the non built-up area inside the FN tile and the white/grey area is the built-up area inside the FN tile. **Basemap**- Open Street Map contributors, **Built-up classification** - Copernicus GLC V3.1 2019.

B.4 Electricity substructure in MESSAGEix-GLOBIOM

The high resolution DCSPV potentials are aggregated for each country, and further for each model region. These DCSPV potentials are grouped into 11 categories based on the capacity factor, representing different available rooftop area (km²) based on the location. A 30% rooftop availability is taken into account when calculating these potential bins, meaning that up to 1/3 of the roof can be used for PV installation. For different availability factors the user needs to scale these potentials accordingly.

These resource potentials as available rooftop area are represented through the model parameter "renewable_potential", with each potential as a new "commodity" called "rooftop_area1" etc. Available DCSPV areas are not modelled by different "grades" to let the model link different DCSPV resource technologies to different potential commodities giving the user flexibility to control the uptake of each bin separately if needed.

A "renewable_capacity_factor" of 1 is taken into account for all potential bins, as the DCSPV capacity factor is modelled through resource technologies, called "solar_rt_res1" etc. Finally, the total installed capacity of DCSPV in different potential bins is equalised to the capacity of a PV panel technology called "solar_pv_RC". The PV panel exhibits all the technology parameters, such as growth rates, penetration values, etc. The following diagram (Figure B.10) shows the representation of these potential bins and respective resource technologies in the model.

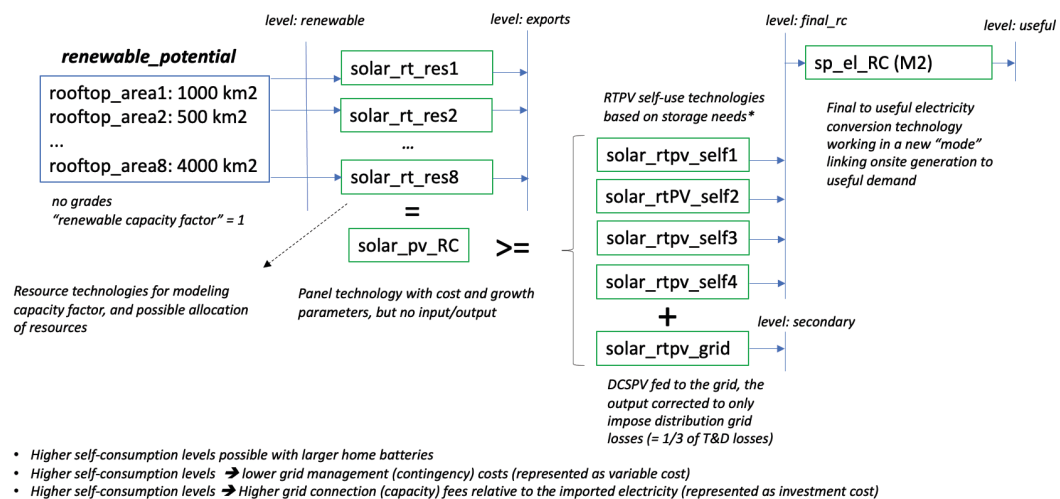


Figure B.10 | Representation of rooftop solar PV from resources to the panel technology, self-consumption, and fed to the grid

The total electricity generation of rooftop panel ("solar_pv_RC") is divided into two main parts: self-consumption in the building and the part fed to the central grid. Self-consumption of DCSPV is limited to a certain share, typically between 30-50% of total annual generation, depending on the size of the panel relative to the size of the annual load. For achieving higher levels of self-consumption, the building needs to be equipped with battery or other electricity storage options. It has been shown in the literature that self-consumption is one of the most favorable options for benefitting from distributed generation and reducing the grid management costs⁴. In a study by Lund⁵, the PV self-consumption ISO curves as a function of storage-to-PV capacity ratio is developed for different cities globally. The study shows that with almost a storage-to-PV capacity ratio (kWh/kWe) of 2, the prosumer can reach to self-consumption rates of up to 90%, depending on the location. Any storage capacity higher than this will improve the self-consumption very marginally, implying that the ratio of 2 can be considered as an optimal and reasonable sizing of storage and PV. This can be seen in Figure B.11 (left).

These self-consumption curves are reproduced by simplified stepwise curves for the model, including four self-consumption levels (Figure B.11 (right)). The first level does not require any storage, while higher consumption levels (2-4) require a certain level of storage capacity in the building. The capacity ratios are converted to activity ratio in the model to allow for a more convenient use of "relation_activity", without the need for vintaging for self-consumption technologies. The rest of the onsite DCSPV generation that is fed to the grid (via technology "solar_rtpv_grid"). This ensures that the distribution grid losses caused by the electricity from buildings back to the grid are taken into account. Moreover, the part PV generation fed to the grid is modeled similar to the utility scale solar PV in terms of systems integration challenges depending on the penetration levels, i.e., grid contingency costs, curtailment rates, flexibility needs, and contribution to the reserve margin capacity.

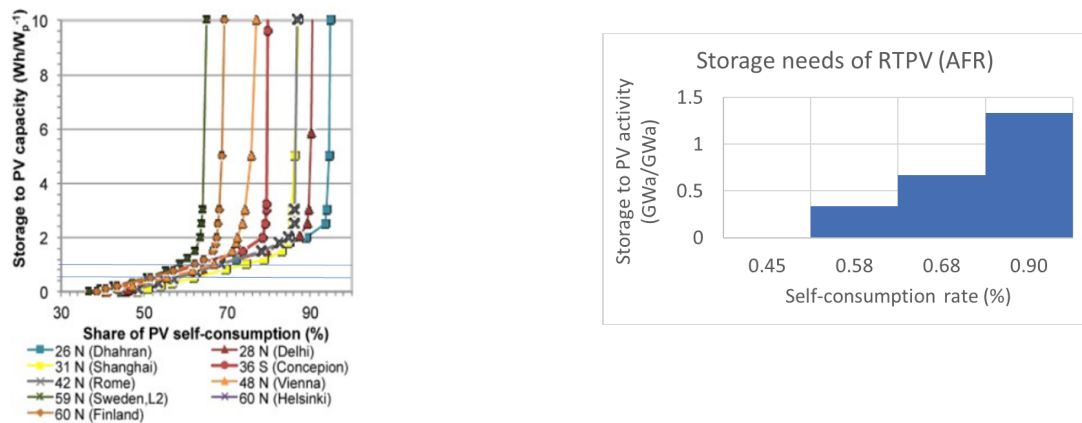


Figure B.11 | Rooftop PV self-consumption curves based on storage capacity onsite for different locations.

Reproduced from Lund PD (2018)

References Appendix B

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Appendix C: Supplementary Information for Chapter 3

C.1 Supplementary Tables

Table C.1 | Passenger data-series statistics

Series	Statistic	YEAR	Transport Metric (millions)	GDP 2005\$ PPP (Billion)	Persons (Thousands)
AP	count	544.00	544.00	544.00	544.00
AP	mean	2,007.66	97,249.60	1,550.26	116.37
AP	min	2,000.00	115.00	9.00	0.28
AP	25%	2,004.00	7,695.25	186.50	8.28
AP	50%	2,008.00	29,058.00	579.00	27.27
AP	75%	2,012.00	100,975.50	1,666.25	63.42
AP	max	2,015.00	1,452,002.00	16,568.00	1,397.03
RaP	count	1,498.00	1,498.00	1,498.00	1,498.00
RaP	mean	1,999.80	45,772.17	892.53	71.50
RaP	min	1,980.00	4.00	4.00	0.36
RaP	25%	1,993.00	1,159.25	66.00	4.81
RaP	50%	2,001.00	6,216.50	220.00	9.96
RaP	75%	2,008.00	17,910.25	888.00	48.81
RaP	max	2,015.00	1,196,060.00	16,568.00	1,397.03
RoP	count	1,298.00	1,298.00	1,298.00	1,298.00
RoP	mean	1,999.65	382,123.40	980.03	80.49
RoP	min	1,980.00	20.00	4.00	0.27
RoP	25%	1,993.00	15,365.00	68.25	5.13
RoP	50%	2,000.00	71,187.00	240.50	10.29
RoP	75%	2,007.75	284,328.75	1,121.75	56.45
RoP	max	2,015.00	15,415,000.00	16,568.00	1,397.03

Table C.2 | Goods data-series statistics

Series	Statistic	YEAR	Transport Metric (millions)	GDP 2005\$ PPP (Billion)	Persons (Thousands)
AG	count	1,516.00	1,516.00	1,516.00	1,516.00
AG	mean	1,999.25	1,817.33	936.09	84.22
AG	min	1,980.00	0.00	3.00	0.27
AG	25%	1,992.00	16.69	74.00	4.68
AG	50%	2,000.00	220.85	238.50	10.30
AG	75%	2,007.00	1,372.09	964.50	50.95
AG	max	2,015.00	40,617.74	16,568.00	1,397.03
RaG	count	1,530.00	1,530.00	1,530.00	1,530.00
RaG	mean	1,999.78	140,001.62	913.48	71.53
RaG	min	1,980.00	16.00	4.00	0.36
RaG	25%	1,993.00	2,440.50	67.25	4.68
RaG	50%	2,001.00	9,908.00	220.00	9.96
RaG	75%	2,008.00	24,335.50	888.00	48.81
RaG	max	2,015.00	2,946,579.00	16,568.00	1,397.03
RoG	count	1,451.00	1,451.00	1,451.00	1,451.00
RoG	mean	1,999.97	176,716.24	944.59	74.00
RoG	min	1,980.00	23.00	4.00	0.28
RoG	25%	1,993.00	8,292.50	63.00	4.57
RoG	50%	2,001.00	20,821.00	219.00	9.95
RoG	75%	2,008.00	125,558.00	1,026.00	51.23
RoG	max	2,015.00	5,953,486.00	16,568.00	1,397.03
MI	count	1,475.00	1,475.00	1,475.00	1,475.00
MI	mean	2,007.60	788,097.36	737.17	63.34
MI	min	2,000.00	369.71	4.00	0.28
MI	25%	2,004.00	29,686.87	62.00	4.75
MI	50%	2,008.00	108,659.79	214.00	16.94
MI	75%	2,012.00	516,718.17	587.00	47.90
MI	max	2,015.00	20,869,365.19	16,568.00	1,397.03

Table C.3 | Learning Phase Hyperparameters (Historical and Short-term)

				Number of Neurons					
Series	Hyperopt Iteration Number	Epoch	Layers	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
AG	372	10	6	2,650	1,400	200	750	1,300	200
AP	386	10	6	2,250	750	2,450	1,600	800	500
RaG	462	30	6	900	800	1,000	750	1,500	650
RaP	268	10	6	450	1,450	850	2,700	2,850	1,500
RoG	404	10	6	1,400	400	800	200	1,600	700
RoP	81	10	6	300	1,900	1,950	2,950	3,000	550
MI*	388	10	6	650	1,700	1,700	1,000	500	2,150

Table C.4 | Firing Phase Hyperparameters (Historical and Short-term)

				Number of Neurons			
Series	Hyperopt Iteration	Epoch	Layers	Layer 1	Layer 2	Layer 3	Layer 4
AG	372	800	4	300	2,750	1,850	1,750
AP	386	800	4	2,750	450	900	1,700
RaG	462	800	4	2,200	400	450	2,800
RaP	268	750	4	800	1,850	300	700
RoG	404	650	4	450	2,000	2,100	1,750
RoP	81	700	4	450	1,900	1,950	700
MI*	388	700	4	1,750	1,150	850	2,750

Table C.5 | Learning Phase Hyperparameters (Decadal)

				Number of Neurons					
Series	Hyperopt Iteration Number	Epoch	Layers	Layer 1	Layer 2	Layer 3	Layer 4	Layer 5	Layer 6
AP	436	10	6	100	1,450	900	2,650	1,100	2,300
RaP	321	10	5	1,600	1,750	1,500	2,150	1,400	N.A.
RoP	83	50	5	1,100	1,300	1,400	2,900	600	N.A.

Table C.6 | Firing Phase Hyperparameters (Decadal)

				Number of Neurons			
Series	Hyperopt Iteration	Epoch	Layers	Layer 1	Layer 2	Layer 3	Layer 4
AP	436	650	4	1,300	350	200	2,750
RaP	321	750	4	850	400	1,500	1,650
RoP	83	350	4	1,850	300	200	2,150

Table C.7 | Regional level model evaluation (arranged by MAE)

Historical Evaluation						Short-term evaluation			
Series	Framework	R ²	MAE	RMSE	% Over Actual	Framework	Absolute Error	Absolute Percentage Error	MAE
AP	TrebuNet	0.97	57,982	74,708	0.76	TrebuNet	-332,542	4.44	166,271
AP	LSTM	0.71	187,057	225,158	5.20	BiGRU	-452,085	6.03	226,042
AP	BiGRU	0.75	187,078	209,304	6.50	BiLSTM	-515,424	6.88	257,712
AP	BiLSTM	0.73	188,377	214,895	6.38	GRU	-725,083	9.68	362,542
AP	GRU	0.67	207,135	239,437	6.27	ANN	-729,644	9.74	364,822
AP	ANN	0.56	242,429	275,100	-9.04	LSTM	-743,241	9.92	371,620
RoP	BiGRU	0.99	240,146	320,523	-0.17	BiGRU	-573,593	4.21	301,518
RoP	BiLSTM	0.99	257,977	329,763	-0.23	BiLSTM	-594,773	4.37	304,709
RoP	TrebuNet	0.96	518,592	596,715	5.65	TrebuNet	1,288,864	9.47	644,432
RoP	GRU	0.94	525,919	780,063	-1.02	GRU	3,149,034	23.14	1,641,243
RoP	LSTM	0.92	578,491	892,372	-0.92	ANN	3,638,309	26.73	1,819,154
RoP	ANN	0.90	691,897	986,430	7.43	LSTM	4,067,736	29.89	2,033,868
RaP	BiGRU	0.84	36,366	43,378	3.60	TrebuNet	64,219	4.94	32,110
RaP	BiLSTM	0.78	41,414	51,329	4.48	ANN	-219,071	16.85	109,535
RaP	TrebuNet	0.83	41,501	45,425	5.29	BiGRU	478,500	36.80	260,572
RaP	GRU	0.62	57,160	67,832	6.76	BiLSTM	482,970	37.15	268,421
RaP	LSTM	0.61	59,210	68,729	7.10	GRU	491,165	37.78	272,149
RaP	ANN	0.04	105,547	107,893	-13.45	LSTM	542,085	41.69	278,898
AG	TrebuNet	0.99	2,064	2,678	-0.57	LSTM	-1,225	0.63	1,921
AG	BiGRU	0.97	3,122	4,105	-1.69	GRU	-3,653	1.88	2,794
AG	BiLSTM	0.97	3,287	4,283	-1.60	BiGRU	6,967	3.58	3,484
AG	ANN	0.94	4,815	6,109	-7.09	TrebuNet	5,321	2.73	4,473
AG	LSTM	0.79	9,213	11,393	10.41	BiLSTM	9,113	4.68	4,556
AG	GRU	0.76	9,883	12,156	11.94	ANN	24,500	12.59	12,250
RaG	BiGRU	0.98	80,086	105,949	0.20	GRU	744,907	12.01	372,453
RaG	TrebuNet	0.97	118,654	141,165	3.38	BiLSTM	414,050	6.68	386,091
RaG	ANN	0.91	153,763	231,316	4.80	LSTM	801,724	12.93	400,862
RaG	BiLSTM	0.82	268,386	321,570	8.79	BiGRU	825,304	13.31	412,652
RaG	LSTM	0.78	289,437	354,009	9.67	TrebuNet	835,648	13.48	417,824
RaG	GRU	0.74	324,291	390,759	11.23	ANN	1,924,480	31.04	962,240
RoG	TrebuNet	0.95	166,025	263,449	-0.92	TrebuNet	-643,460	8.53	321,730
RoG	ANN	0.79	389,483	531,614	6.94	ANN	1,348,904	17.89	674,452
RoG	BiGRU	0.81	417,701	508,952	-4.40	BiLSTM	2,285,150	30.31	1,142,575
RoG	BiLSTM	0.75	485,643	587,690	-4.39	GRU	2,326,022	30.85	1,163,011
RoG	LSTM	0.73	517,323	609,446	-2.80	BiGRU	2,401,689	31.85	1,200,845
RoG	GRU	0.71	526,371	631,393	-4.43	LSTM	2,702,335	35.84	1,351,167

* Green cells are the TrebuNet models and Red cells are the top performing models in respective data-series. The errors are in either Billion TKM or Billion PKM based on the data-series.

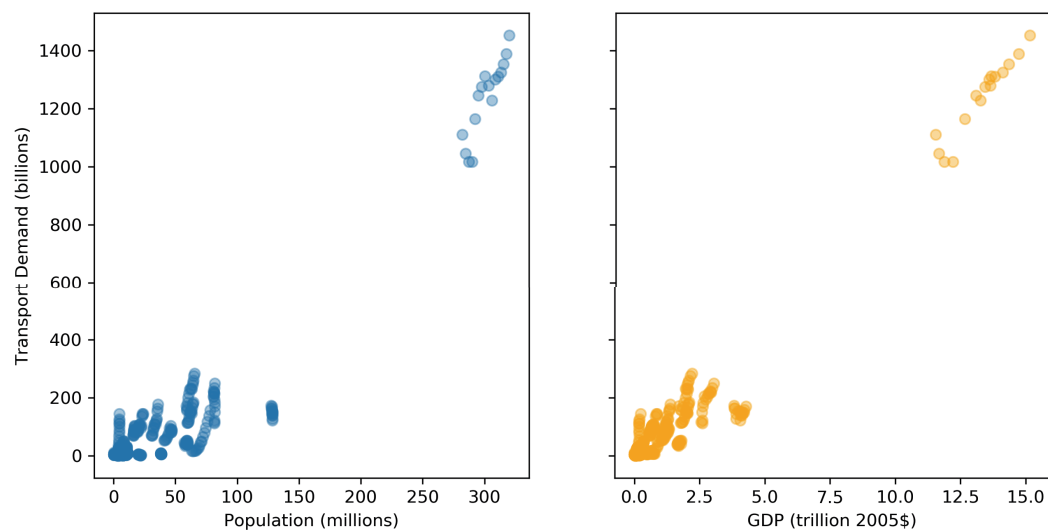
Table C.8 | Country level model evaluation (arranged by MAE)

Historical Evaluation						Short-term evaluation			
Series	Framework	R ²	MAE	RMSE	% Over Actual	Framework	Absolute Error	Absolute Percentage Error	MAE
AP	TrebuNet	0.995	9,443	17,548	0.76	TrebuNet	-332,542	4.4	23,960
AP	XGB	0.994	12,089	18,455	-0.64	ANN	-729,644	9.7	30,164
AP	ANN	0.987	17,060	28,146	-9.04	XGB	-1,041,317	13.9	35,667
AP	REG	0.966	29,243	45,018	0.05	REG	-450,508	6.0	41,356
RoP	XGB	0.999	18,988	28,297	-0.12	TrebuNet	1,288,864	9.5	45,762
RoP	TrebuNet	0.992	23,736	70,149	5.65	XGB	999,328	7.3	50,820
RoP	ANN	0.984	43,475	102,791	7.43	REG	2,714,427	19.9	71,940
RoP	REG	0.973	58,412	133,710	0.40	ANN	3,638,309	26.7	82,096
RaP	XGB	0.996	2,446	4,491	0.38	TrebuNet	64,219	4.9	4,525
RaP	TrebuNet	0.995	2,584	4,859	5.29	ANN	-219,071	16.8	5,491
RaP	ANN	0.983	4,333	8,842	-13.45	XGB	100,640	7.7	6,362
RaP	REG	0.322	22,556	55,237	-1.41	REG	-571,485	44.0	19,014
AG	TrebuNet	0.988	225	544	-0.55	TrebuNet	5,321	2.7	636
AG	XGB	0.988	343	558	0.04	XGB	-3,254	1.7	683
AG	ANN	0.961	541	992	-7.07	ANN	24,500	12.6	865
AG	REG	0.948	741	1,149	-0.18	REG	30,318	15.6	998
RaG	TrebuNet	0.997	6,320	18,297	3.38	TrebuNet	835,648	13.5	19,953
RaG	XGB	0.999	6,496	11,021	-0.20	XGB	637,788	10.3	24,027
RaG	ANN	0.993	13,134	30,125	4.80	ANN	1,924,480	31.0	36,703
RaG	REG	0.878	70,604	124,111	1.30	REG	3,980,951	64.2	88,569
RoG	TrebuNet	0.995	10,695	37,421	-0.92	XGB	-551,941	7.3	24,591
RoG	XGB	0.999	10,885	17,787	-0.17	TrebuNet	-643,460	8.5	43,422
RoG	ANN	0.980	24,952	73,266	6.94	ANN	1,348,904	17.9	47,162
RoG	REG	0.899	89,682	163,202	0.43	REG	4,330,219	57.4	126,012

* Green cells are the TrebuNet models and Red cells are the top performing models in respective data-series. The errors are in either Billion TKM or Billion PKM based on the data-series.

C.2 Supplementary Figures

AP



AG

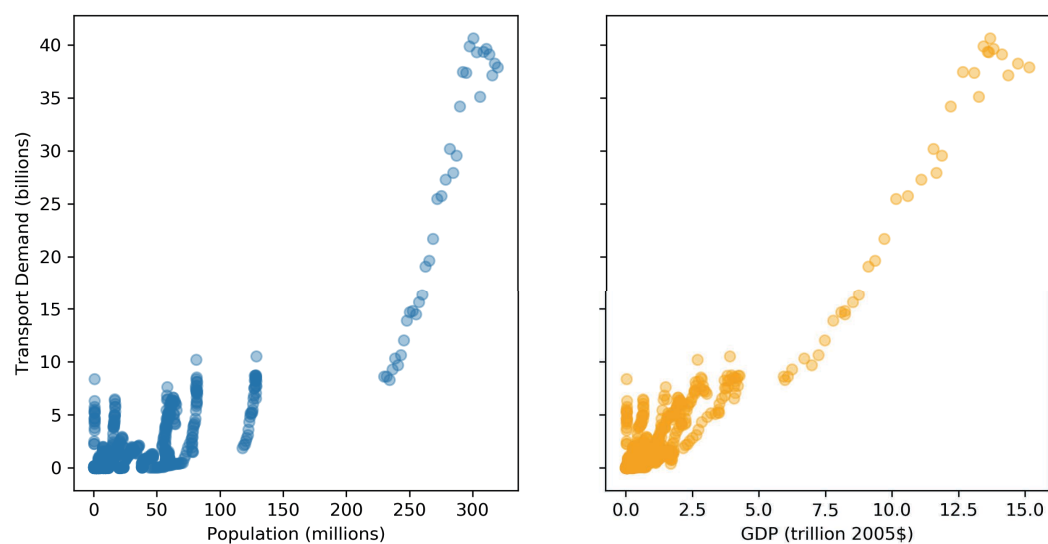


Figure C.1 | Aviation Mode historical data
Historical relationship between Energy service demand, population and GDP in aviation mode of transportation for passenger and freight types

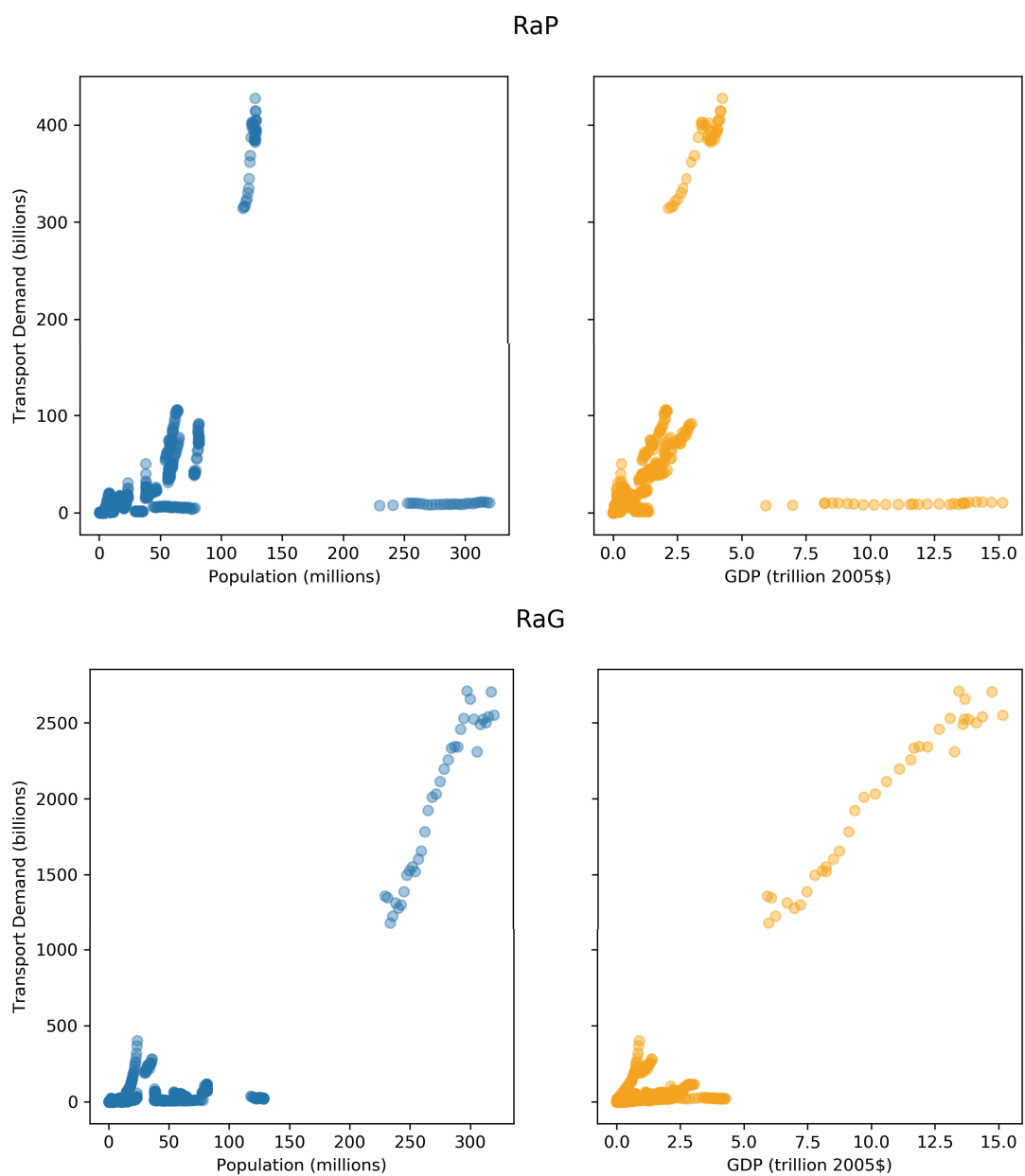


Figure C.2 | Rail Mode historical data.

Historical relationship between Energy service demand, population and GDP in rail mode of transportation for passenger and freight types

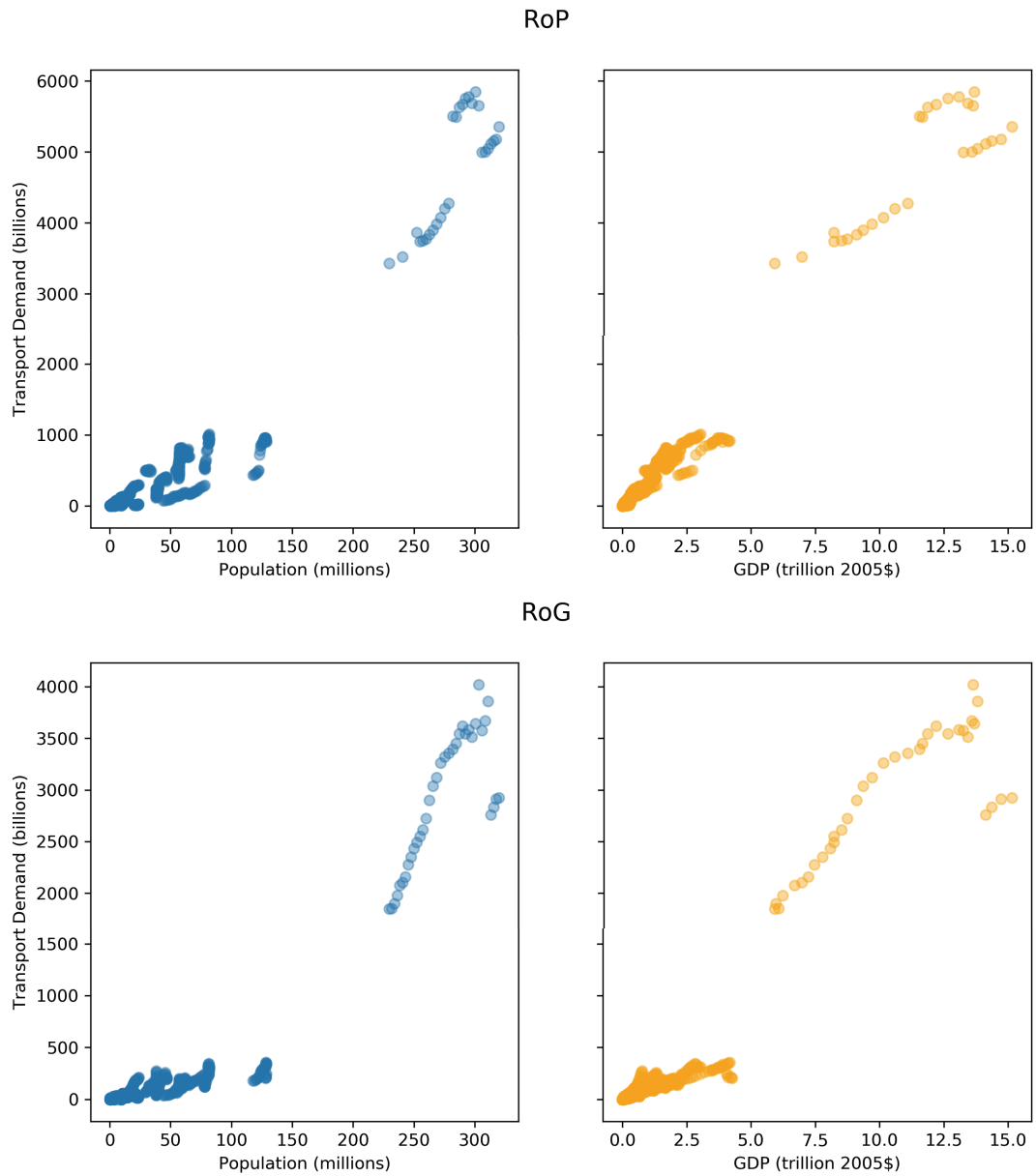


Figure C.3 | Road Mode historical data.

Historical relationship between Energy service demand, population and GDP in road mode of transportation for passenger and freight types

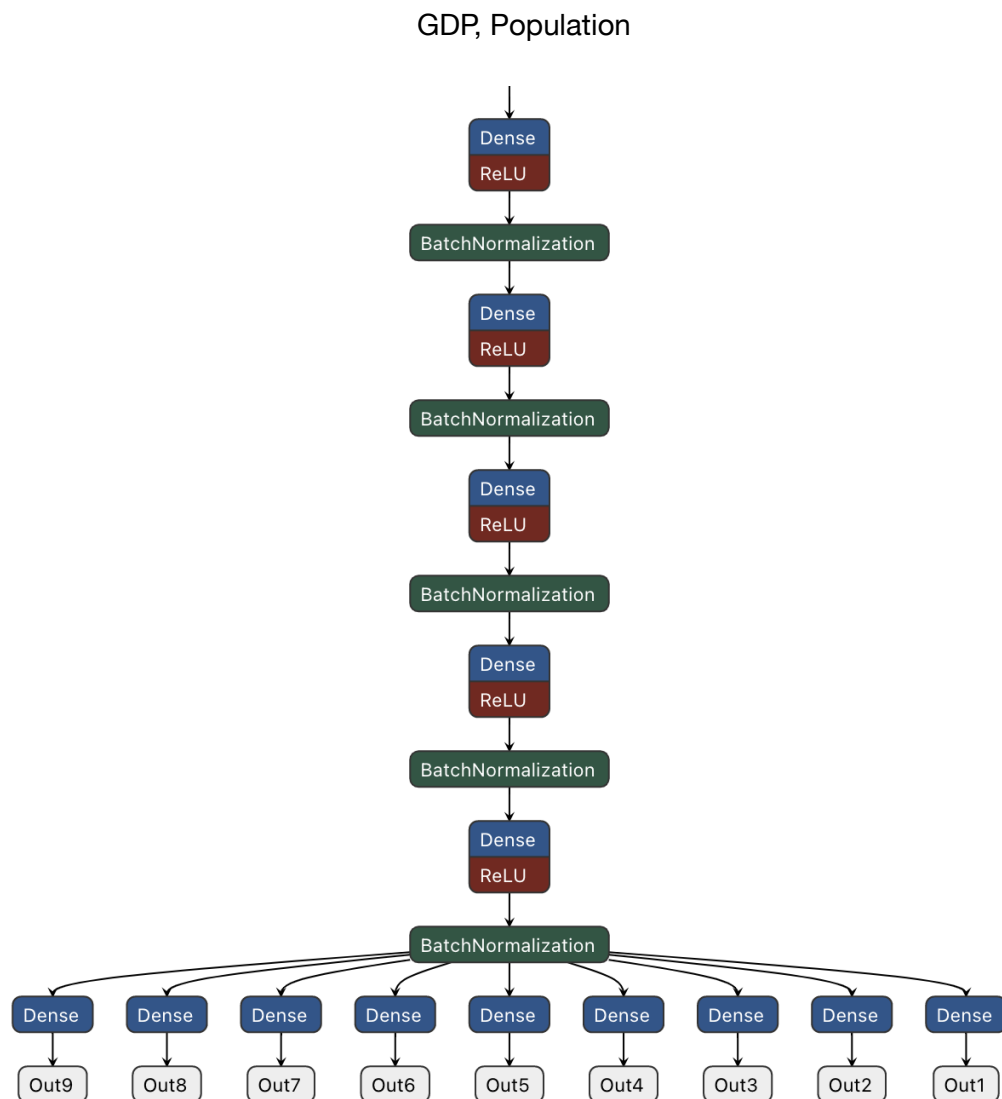


Figure C.4 | Learning Phase Model arrangement

Flowchart depicting data flow in the densely connected layers. The inputs to the layer are GDP and Population drivers and the output is in form of the energy service demand broken down into nine quantiles. Some data- series will have 6 layers instead of 5. Layer numbers are determined during hyperparameter optimisation.

1/5 of the data with 9 columns configuration into each parallel model.
This process is repeated 5 times for 5 fold CV

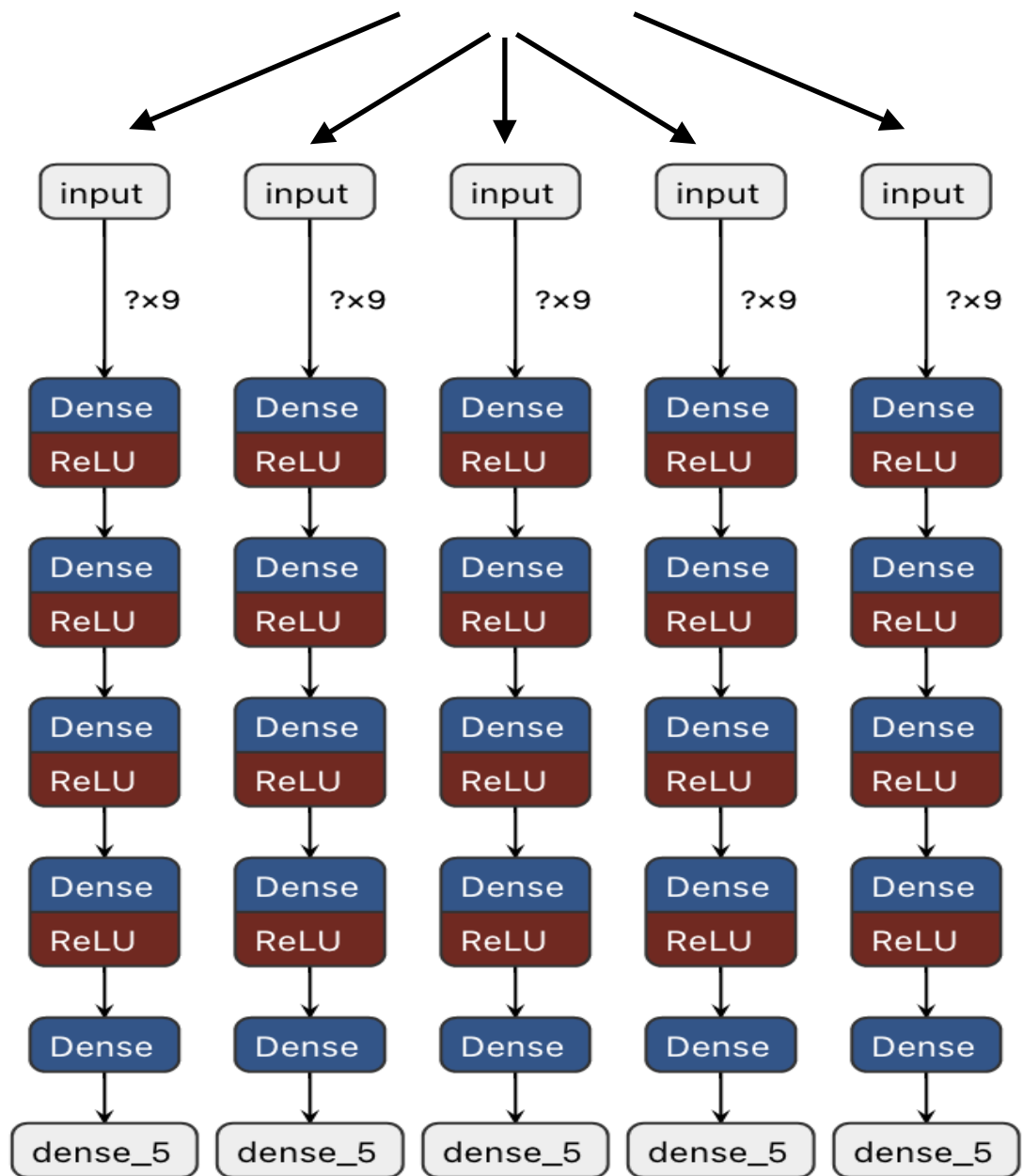


Figure C.5 | Firing Phase Model arrangement

Flowchart depicting data flow in the densely connected layers. The inputs to the layers are the energy service demands spanning nine quantiles created by the learning phase. Each input pipeline has 1/5 of the input data randomly selected to create 5 fold cross validation.

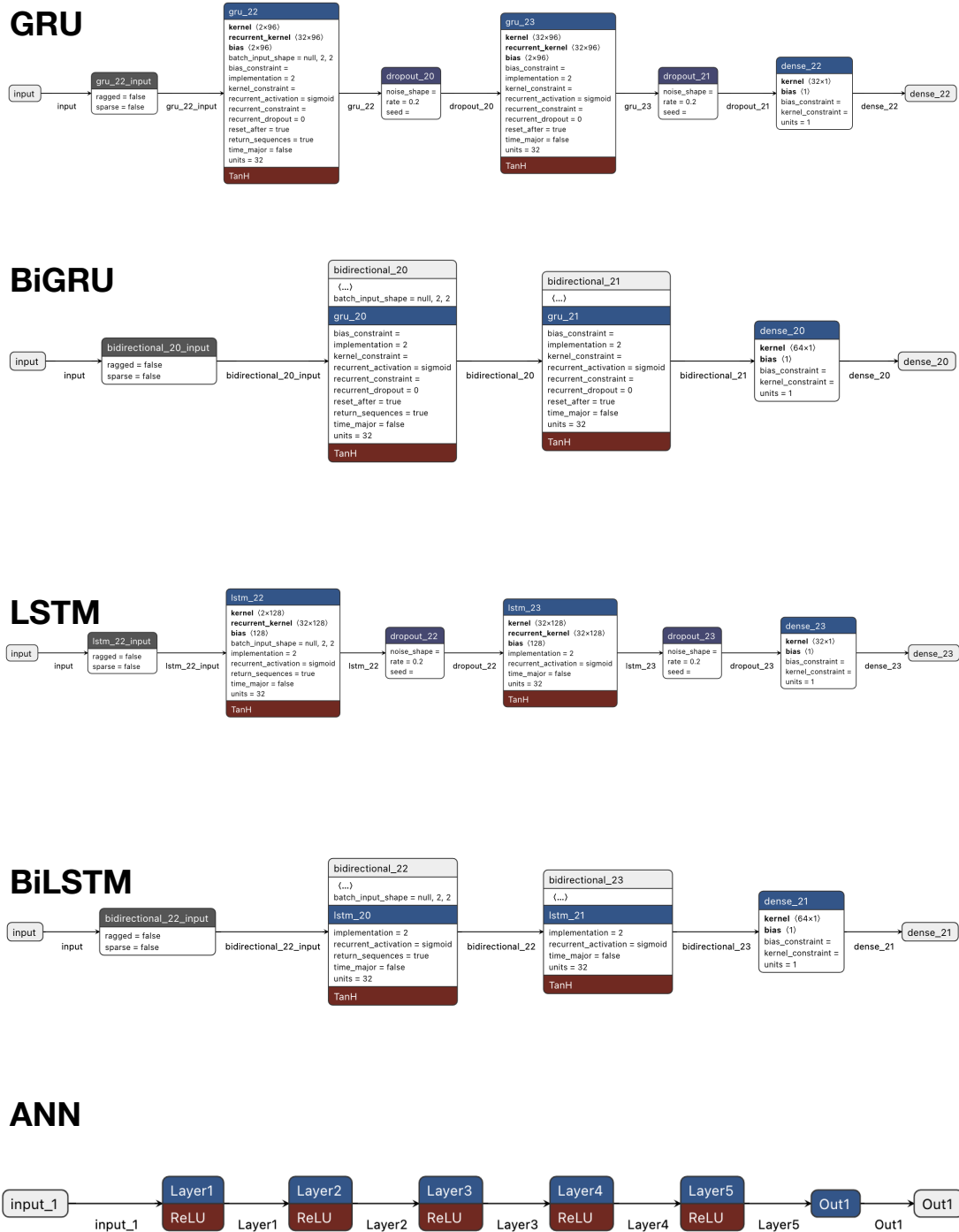


Figure C.6 | ANN and RNN model configuration .

Flowcharts depicting the structure of ANN and RNN based models namely GRU, BiGRU, LSTM, BiLSTM. Red cell represents the transfer functions. Blue cells are the layer names. Grey cells are the inputs/outputs.

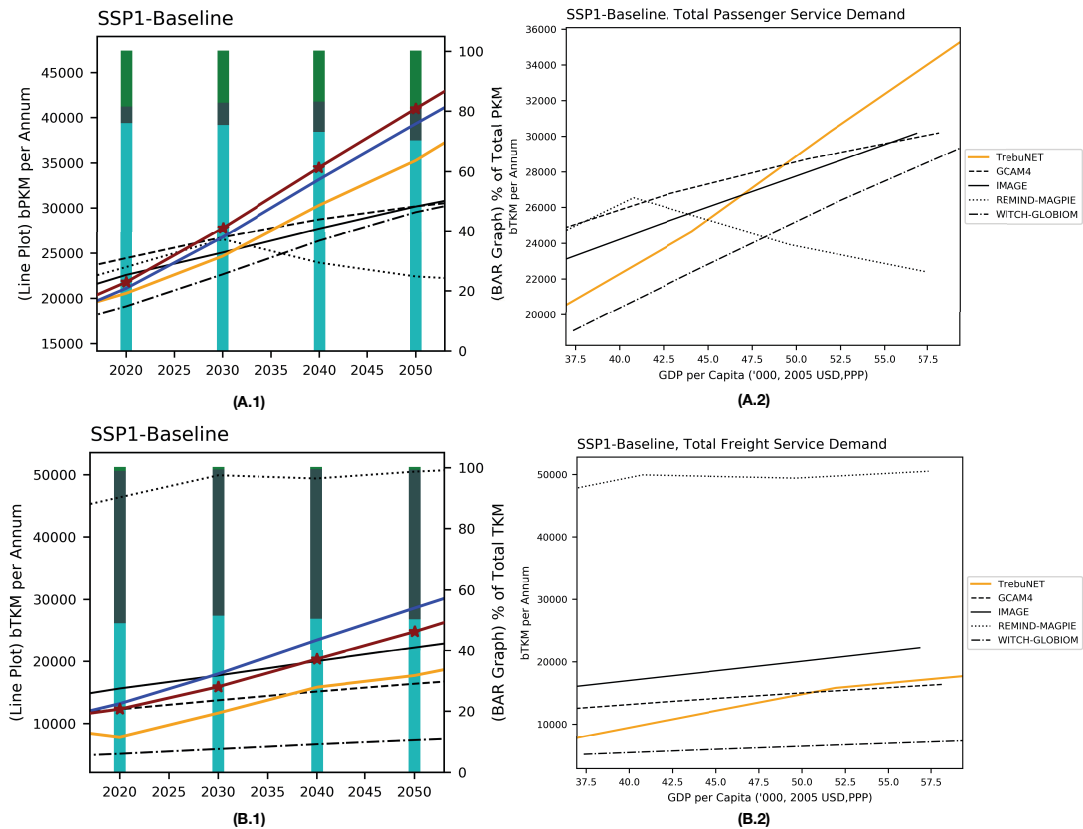


Figure C.7 | Medium Term Projection .

A, SSP1 transport energy service demand projections in Billion Passenger Kilometres units (A.1) and saturation curves (A.2) for passenger mode of transport for OECD countries with TrebuNet model and IAM comparisons. **B**, SSP1 transport energy service demand projections in Billion Tonnes Kilometres units (B.1) and saturation curves (B.2) for freight mode of transport for OECD countries with TrebuNet model and IAM comparisons

C.3 Power consumption statistics

As the aim of the research is to generate energy service demands, we also calculated the energy required to generate our transport service demands¹. The energy demand is calculated for single hyperparameter optimisation run followed by training run on the best-chosen hyperparameter. Here we only calculated the power consumed by the NVIDIA 2080ti and 1060ti GPUs. It was observed that an average power draw of 220 W occurred during the hyperparameter optimisation runs. Total time taken to complete hyperparameter optimisation runs was 70 hours. This results in circa 15.4 units of electricity being used for hyperparameter optimisation runs for all the data series. It is pertinent to know that each series were run multiple times during prototyping. On an average each series were run for five times to validate the results. Thus, total circa 77 units of electricity was used by GPU during this exercise. With a carbon intensity of 453 gCO₂/unit of electricity in Ireland for 2019, total CO₂ released into the atmosphere during this research was circa 35 kg. On top of this displays, CPU and other system components also add-on to the power requirements and hence result in higher CO₂ emissions than one showed here.

References Appendix C

- 1 Strubell, E., Ganesh, A. & McCallum, A. Energy and Policy Considerations for Deep Learning in NLP. (2019) .

Annex

This Annex documents the report that was developed in collaboration with Irish Solar Energy Association. The report which is based on the outputs of chapter 4 summarises the rooftop solar PV potential in Republic of Ireland disaggregated by counties. It further goes into economic and carbon mitigation potential analysis of rooftop solar PV with insights into how this technology can directly address energy security and mitigate energy poverty for different deployment scales and scenarios. Here, the report is presented as is in its final published form.



INTRODUCTION

WHAT DID THIS STUDY SET OUT TO DO?

This study quantifies the available residential solar photovoltaic rooftop capacity and associated annual electricity potential in Ireland for the first time using satellite imagery and weather data.

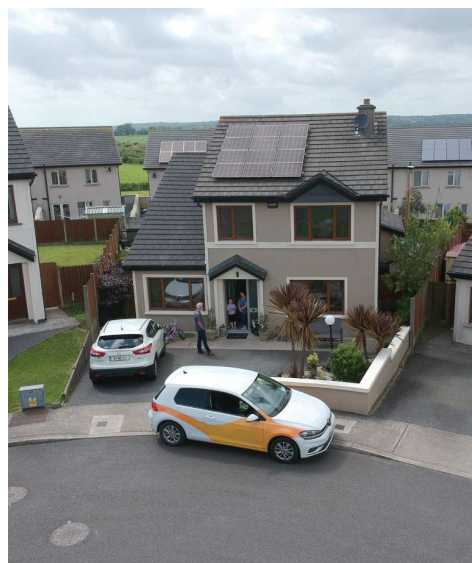
WHY IS THIS IMPORTANT?

This allows us to understand how we can use rooftops in Ireland to produce electricity and reduce both emissions and energy bills for families.

AND WHAT SCENARIOS DID YOU INVESTIGATE?

The next 3 slides explain the insights and results we found for 3 scenarios where we assume:

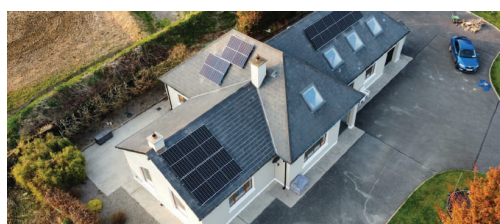
- 6 Solar Panels on each suitable roof
- 10 Solar Panels on each suitable roof
- Maximum Theoretical potential on each roof as an exploratory scenario



FOREWORD BY ISEA

This report is being published at an inflection point for both energy producers and consumers.

Energy bill increases have been compounded by the war in Ukraine and its impact on fossil markets. Irish citizens will be entitled to payment for exporting power they generate themselves and rooftop solar planning restrictions are due to be eased. The EU Solar Energy Strategy sets out a growth trajectory for solar PV with provision for all new residences to have rooftop solar PV from 2029.



As this analysis shows, there are significant potential financial savings for people from their rooftops. Beyond the positive impact on bills, solar PV provides an option for people to directly participate in the battle against climate change. Solar panels could be the entry point for many people on their sustainability journey.

About 24,000 homes have already begun this transition. As this report shows, the rooftops of Ireland have substantial potential.

Many jobs will be needed to deliver this solar opportunity. These roles traverse a range of activities across the trades and business. These are purposeful jobs with real meaning.

Enabling participation in the energy transition will only not create employment, but ensure that people are included in Ireland's decarbonisation journey.



WHY SOLAR IN IRELAND

Ireland is known more for wind and waves rather than sunshine, but advances in solar technology and reductions in cost now make it an attractive technology for residential electricity generation in Ireland.

Solar panels that produce electricity are known as solar photovoltaic (PV) modules. These panels generate electricity when exposed to light and since 2010 solar PV has been the fastest growing power generation technology worldwide. Solar PV systems produce electricity that can be used to power your home and heat water. Solar PV systems will still function on overcast days in Ireland although not at their maximum rated capacity. Solar PV systems are rated in kilowatts (kW). A 1kW solar PV system would require 2-3 solar panels on a roof and will generate most of its electricity between April to September.

The deployment of residential solar PV in Ireland addresses key energy and climate issues such as Electricity Affordability, Climate Action and Energy Security.



It does this by:

SAVING MONEY FOR HOUSEHOLDS: A typical household in Dublin with 2.4 kW of solar panels could generate over one third of their annual electricity and save 380€/year in electricity bills with the system paying back for itself in 7 years. Today most modern panels will last for more than 25 years, and cumulative savings are significant. These savings can be increased if the household has an electric vehicle allowing cheap charging of the car throughout the day.

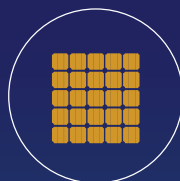
INCREASING SECURITY OF SUPPLY: At the same time fossil fuel use with the power sector is reduced and this reduces emissions and increases the security of supply.

REDUCING GREENHOUSE GAS EMISSIONS: Ireland has committed to delivering one of the world's most ambitious emission reduction targets of a 51% reduction by 2030. Ireland has one of the highest reliance on natural gas within the power system in Europe and delivering on Solar PV will help meet these targets.

PUTTING SIX SOLAR [2.4 KW] PANELS ON EVERY SUITABLE HOME



1 million homes have potential for six panels



Equating to 2.5 GW of Capacity or 21% of current power system size



Producing 22% of all residential demand | 1.8 TWh



Meeting 6% of Renewable Electricity Target



Reducing 95,000 tonnes of CO₂ emissions

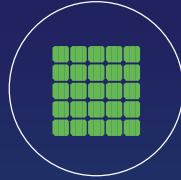


Saving 380€ on annual electricity bills

PUTTING TEN SOLAR PANELS [3.4KW] ON EVERY SUITABLE HOME



1 million homes have potential for ten panels



Equating to 3.6 GW of Capacity or 30% of current power system size



Producing 25% of all residential demand | 2.2 TWh



Meeting 8% of Renewable Electricity Target



Reducing 135,000 tonnes of Carbon Dioxide Emissions



Saving 450€ on a Family's annual electricity bill

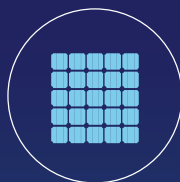
MAXIMUM POTENTIAL ON EVERY SUITABLE HOME



*In this scenario all rooftops are assumed to be structurally suitable for PV, whereas in the 2 previous scenarios we assumed 15% of rooftops were not suitable. This is why the number of homes has increased.



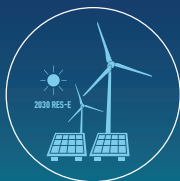
Over 1.3 million homes have roof space for solar panels*



Equating to 13 GW of Capacity or 113% of current power system size



Producing 36% of all residential demand | 3.1 TWh



Meeting 19% of Renewable Electricity Target

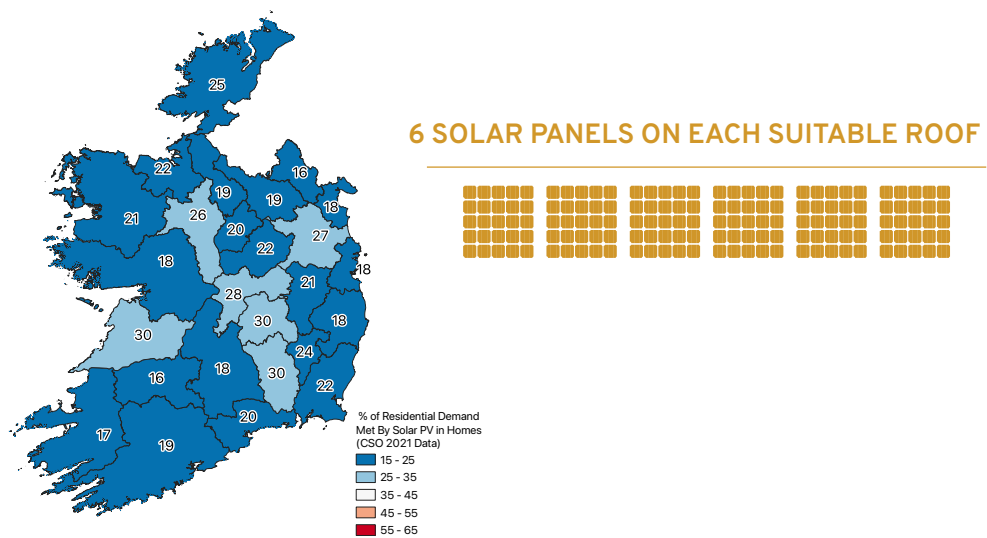


Reducing 306,000 tonnes of CO₂ emissions

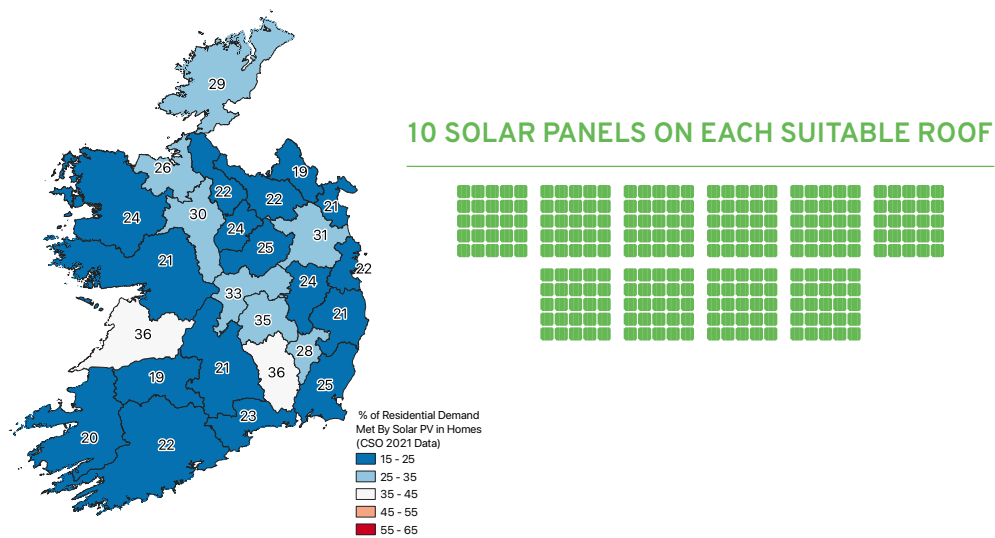


Saving €500+ on annual electricity bills

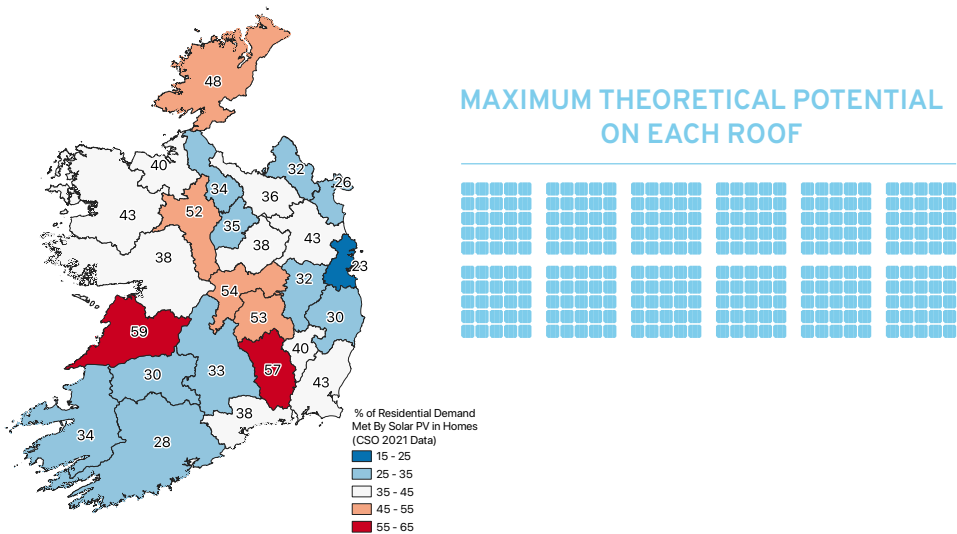
COUNTY LEVEL FINDINGS (% OF ANNUAL RESIDENTIAL DEMAND MET BY SOLAR ROOFTOP PV)



COUNTY LEVEL FINDINGS (% OF ANNUAL RESIDENTIAL DEMAND MET BY SOLAR ROOFTOP PV)



COUNTY LEVEL FINDINGS (% OF ANNUAL RESIDENTIAL DEMAND MET BY SOLAR ROOFTOP PV)



FAQ'S

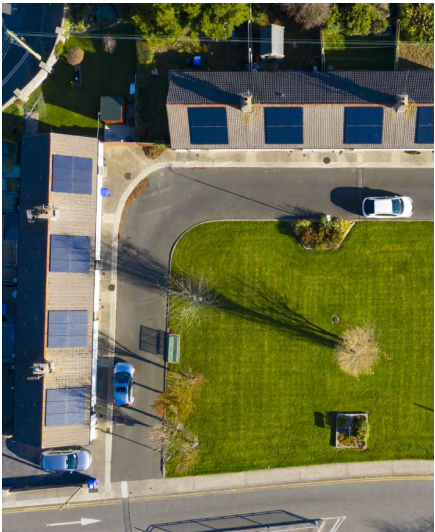


Photo Credit: 3 Counties Energy Agency (3cea)

WHO WROTE THIS REPORT? This report was written by Siddharth Joshi and Paul Deane from the MaREI centre which is the Science Foundation Ireland Research Centre for Energy, Climate and Marine, coordinated by the Environmental Research Institute (ERI) at University College Cork. Graphic design and layout was done by Karen O'Callaghan also with the MaREI centre.

WHO FUNDED THIS REPORT AND WHY? This report was funded by the Irish Solar Energy Association (ISEA). ISEA was established in 2013 to advance a policy and regulatory landscape promoting solar as a leading renewable energy technology that will decarbonise Ireland's electricity system, and contribute to a successful and strong clean economy.

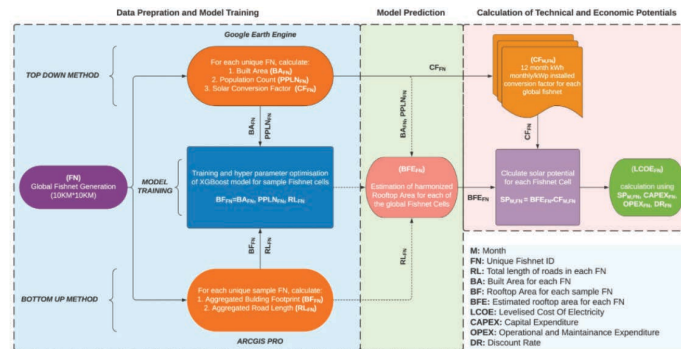
WHAT ARE THE MAIN STRENGTHS OF THE ANALYSIS? The analysis undertakes a high-resolution assessment of rooftop solar photovoltaics potential in Ireland using big data, machine learning and geospatial analysis. This allows us to get a detailed understanding of the actual potential for rooftop solar PV in Ireland.

WHAT ARE THE MAIN WEAKNESSES OF THE ANALYSIS? The analysis does not consider any local constraints such as access to rooftops, shade from trees or nearby buildings or local electricity grid constraints for exports. We do assume that 15% of all available homes are unsuitable for rooftop solar PV due to structural issues.

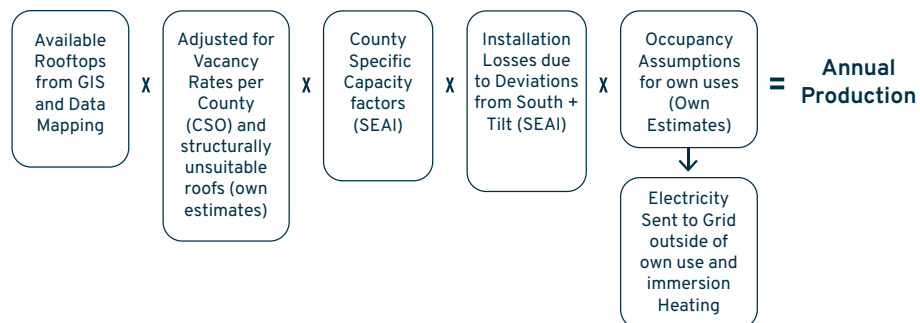
APPENDIX

The framework developed in this study starts with data preparation and mapping of various geospatial metrics to both Top down and Bottom up pathways. The machine learning model is trained and used to estimate BFEFN values from BAFN, PPLNFN, and RLNF values (See image for explanation of terms and link to research paper below). Next, the BFEFN values are used to calculate the technical potential (SP) with the aid of the conversion factors (CF). Finally, the calculated potential dataset is used to map the potential by county with costs determined using SEAI's solar calculator which is available online <https://www.seai.ie/tools/solar-electricity-calculator/>

Model parameters and regional mappings are provided in [High resolution global spatiotemporal assessment of rooftop solar photovoltaics potential for renewable electricity generation | Nature Communications](#)



CALCULATION SUMMARY





 **MaREI**
Energy · Climate · Marine

 **ISEA**
Irish Solar Energy Association

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