INTRODUCTION TO DIGITAL TWINS, MODELS AND PARAMETER ESTIMATION

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SUMMARY

The report introduces the concept of digital twins in the built environment. It identifies that data and models that feed on this data are crucial for building a digital twin. The models are classified based on the modelling method as white box, grey box and black box models and based on the modelling problem as forward and inverse models. The report explains each of these models to throw light on how to choose a model based on the data available and the kind of objective to be achieved. The objectives can be performance prediction, parameter estimation, control, optimisation and fault detection and diagnosis. The next part of the report briefly explains the parameter estimation models. The parameter estimation models are essentially grey-box models. They are useful while making retrofit decisions as they help characterise the existing house and also, check the effectiveness of a proposed retrofit option. The report elucidates how the choice of data and the choice of the thermal network configuration influence the estimated parameters. It also further explains why detailed measurements are required to validate parameter estimation models. The last part of the report shortly describes the behavioural models, the challenges in implementing them and the importance of including them to reduce the performance gap. The report includes a few examples of behavioural models from scientific literature highlighting the data used, the modelling approach and the occupant behaviour studied. In conclusion, the report highlights the importance of data to build a digital twin of a residential building. Leveraging data available from smart meters and home automation systems is the first step to getting closer to achieving such a digital twin.

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1. INTRODUCTION

1.1 Goal of this report

Various beta versions of digital twins are already in circulation among companies and the scientific literature also describes various methods for building such twins. However, there is no overview available of which models to use for which purposes and with what type of data. The aim of this report is therefore to mobilize this existing knowledge so that it can be used for further design of digital twins. What data-driven analysis methods are already available for testable performance assessment? The idea is that potential energy savings can be identified much more efficiently with digital twins than with current models and expensive inspections. The basic principle of a digital twin is that it is (continuously) calibrated with 'machine learning' methods. This means "smart metering" and home automation environments for "on-line" automated calibration of the twins are a must.

As it will be seen later, digital twins are enhanced from Building Information Models (BIM) and used for energy use prediction, especially that of electrical consumption. However, nowadays, applications are starting to be developed for heating and cooling prediction, fault diagnosis and continuous commissioning and digital building inspection, allowing for digital parameter estimation.
This report aims to provide a preliminary understanding of the models used to develop digital twins while focussing on models used for parameter estimation. A quick introduction to behavioural models is also given.

Section 3 establishes a basic understanding of a digital twin and the importance of models and data to develop a digital twin. Since digital twins do not have a stringent definition, a comparison is done with Building Information Models (BIM) to establish its applicability in buildings. Section 4 describes the models and data used for developing digital twins in particular, the white, grey and black box models and, the forward and inverse models. This section aims to define these models so that identification and application of these models become easier for future research. Section 5 briefly describes the models applicable for parameter estimation. Parameter estimation models use on-board monitored data and help to characterise existing buildings which can help in making an informed retrofit decision. And also, these models have a potential to accurately predict the as- built parameters which are required as essential inputs for other models such as prediction, optimisation, control and fault detection and diagnosis models. Section 6 very briefly describes the different models used for accounting occupant behaviour.

2. DIGITAL TWINS

The term "Digital Twin" was conceived to be first presented in 2002 by Michael Grieves during his lecture at the University of Michigan on product lifecycle management (Grieves & Vickers, 2016). It saw its first uses by NASA (Piascik, et al., 2012), (Glaessgen & Stargel, 2012). And, ever since its inception, there have been immense advances in computational power, sensor technologies and semantic technologies. Along with these advancements, the digital twin concept witnessed many definitions according to the areas of its application (Wagner, et al., 2019). Table 1 lists the different but not the only definitions of digital twins. The definitions are adapted to a general context; however, references are given for the actual definitions.

Table 1. Definitions of digital twins

Glaessgen & Stargel (2012) while envisioning a digital twin for NASA and U.S. Air force vehicles	*"Digital twin is an integrated multi-physics, multi-scale, probabilistic simulation of a complex product and uses the best available physical models, sensor updates, etc., to mirror the life of its corresponding twin."*
Grieves & Vickers (2016) while introducing digital twins to mitigate unpredictable, undesirable emergent behaviour in complex systems	*"The digital twin is a set of virtual information constructs that fully describes a potential or actual physical manufactured product from the micro atomic level to the macro geometrical level. At its optimum, any information that could be obtained from inspecting a physical manufactured product can be obtained from its Digital Twin."*
Batty (2018) while explaining the concept of digital twin	*"A digital twin is a mirror image of a physical process that is articulated alongside the process in question, usually matching exactly the operation of the physical process which takes place in real-time"*
IBM (2021)	*"A digital twin is a virtual representation of an object or a system that spans its lifecycle, is updated from real-time data, and uses simulation, machine learning and reasoning to help decision-making."*

In short, to build a digital twin of a building, two essential components are required: on-board monitored data and models which can feed on this data. Khajavi et al. (2019) brought out the meaning of a digital twin clearly by comparing it to the Building Information Modelling (BIM). The BIM models are mostly used in the design and construction phase of buildings for resource efficiency enhancement, knowledge exchange and facilitate architects, engineers and other associated entities to avoid costly design mistakes. BIMs most often use the Computer Aided Design software (CAD). On the other hand, digital twins employ real- time data from a functioning building to carry out simulations, analyse data irregularities and perform energy optimisation, predictive maintenance and fault detection and diagnosis. Thus, ultimately leading to the improvement of the building's interaction with the environment and the users. Moreover, since digital twins employ data monitored during the use phase of the building, digital twins can provide valuable inputs during retrofit by detecting existing flaws and opportunities for improvement. This advantage of digital twins is particularly in line with the parameter estimation models that will be discussed in the later part of the report. It is also important to note that even though BIM is embedded with useful data, existing buildings without BIM can benefit from the implementation of digital twins through installations of sensors and smart meters. Khajavi et al. (2019) illustrated the development of digital twins using Figure 1.

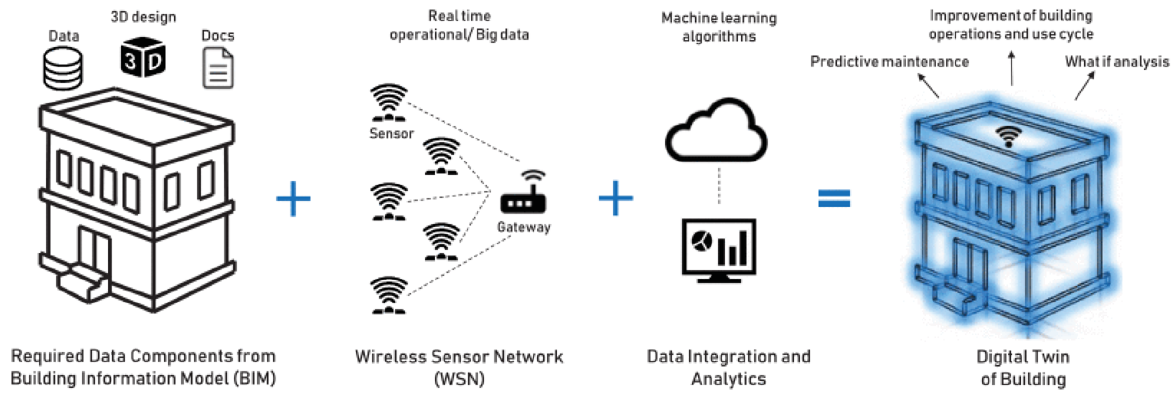


Figure 1. The construction of a digital twin as taken from (Khajavi, Motlagh, Jaribion, Werner, & Holmström, 2019)

Furthering the digital twin development presented in Figure 1, Qiuchen Lu et al. (2020) developed a hierarchical digital twin system architecture for buildings and is represented in Figure 2. The data acquisition layer is the foundation of the digital twin. This includes data collected from sensors, smart meters, construction files, etc. The transmission layer transfers the collected data from the buildings to the higher layers for analysis. The digital model layer consists of the existing models of the building (Eg., BIM) and is supplemented with additional information like data from weather stations to support the next layers. The data/model integration layer is where the actual data analysis takes place with suitable models. The service layer represents the possible aims of the analysis: to provide comfort, energy savings and optimal performances.

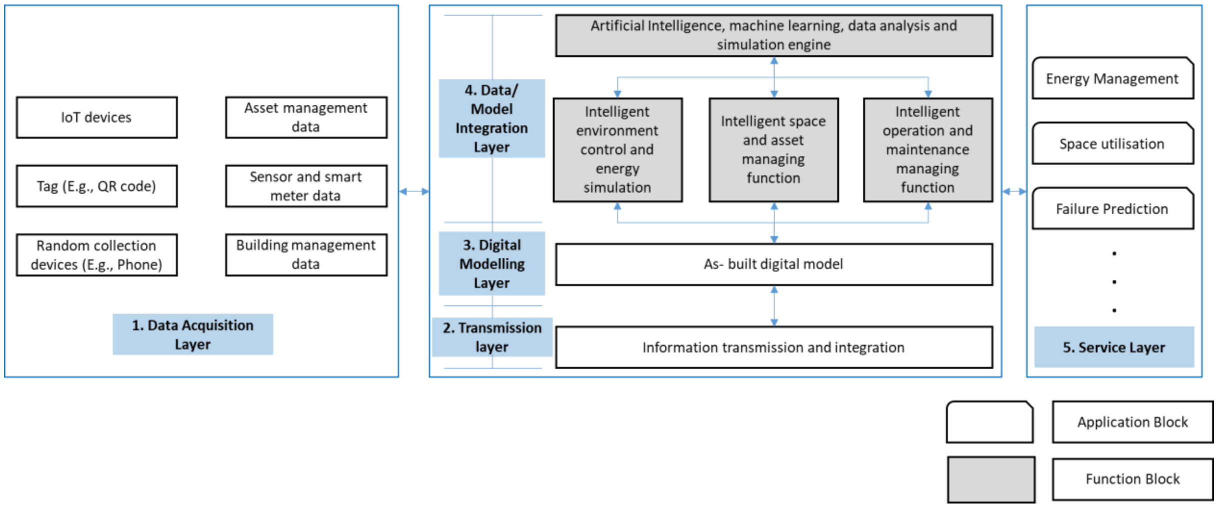


Figure 2. Dynamic digital twin of a building

Having established the concept of digital twins and how it can be developed for residential buildings, it becomes important to introduce the models that can build the digital twins.

3. MODELS FOR ENERGY APPLICATIONS IN BUILDINGS

Digital twins are constructed using models and models are fed by data. Hence, it is important to describe what models and data are used in the building environment. For the ease of understanding, the models are broadly classified based on the modelling method and the modelling problem.

3.1 Classification based on the modelling method

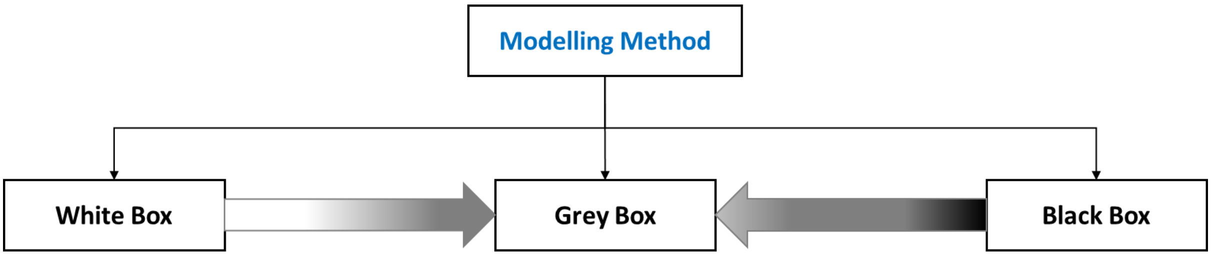


Figure 3. Classification based on the modelling method

3.1.1 White box models

The white box models are generally termed as models based on known physics. This definition is imprecise and does not in essence capture the applicability and the limitations of the white box models. Therefore, a model is a white box model when (Ghiaus, 2014), (Boodi et al., 2018):

1. The structure of the model is known and is developed from fundamental laws of physics, thermodynamics, and heat transfer;
2. And the model parameters (the thermo-physical characteristics of the building) are well known and used as inputs to the model.

Kroll (2000) referred white box models as axiomatic, rigorous or models based on energy, mass and momentum conservation principles. The main steps involved in a detailed white box model are explained in the figure below (Wang, Yan, & Xiao, 2012). The weather conditions include the outdoor air temperature, solar irradiation, etc. The building description is the thermo-physical characteristics obtained from construction files and the building geometry. The system blocks concentrate on the performance of the air handling and distribution system and the control of air temperature and humidity. While the components block are the HVAC components which includes their type, size and performance characteristics. The plant analysis block calculates the gas and electricity requirements for the components. The energy performance indicators can be the energy consumption, CO_2 emission, etc.

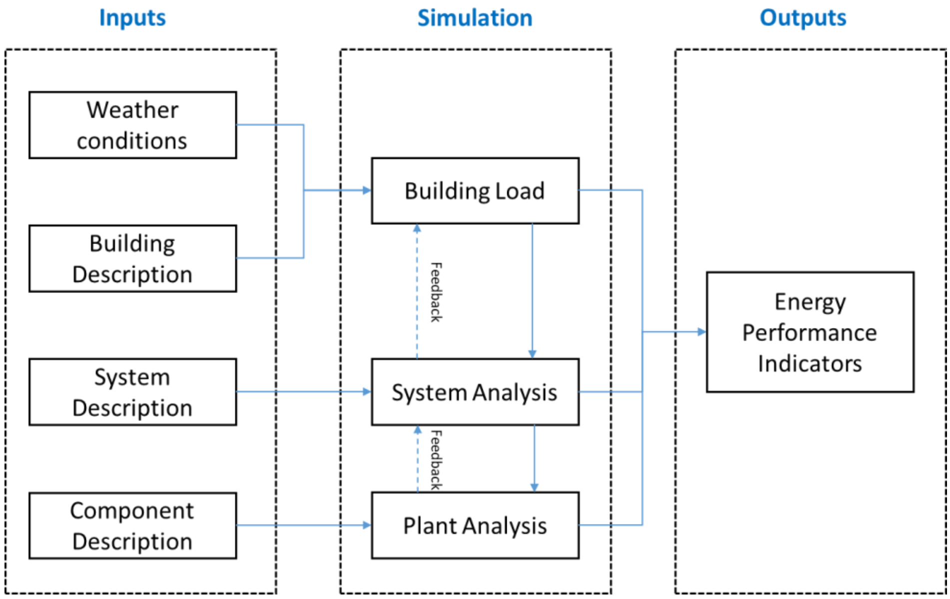


Figure 4. Steps involved in a white box model

The simulation itself can be carried out in two ways (Boodi et al., 2018):

1. Directly using well established simulation tools such as DOE-2 (Birdsall, Buhl, Ellington, Erdem, & Winkelmann, 1990), BLAST (Building Systems Laboratory, 1999), EnergyPlus (Crawley, et al., 2001) and TRNSYS (Solar Energy Laboratory, 2000) based on state space equations.
2. Developing models that employ simplified state space equations and lumped resistance and capacitance modelling, sometimes referred to as RC models in literature. These models have been used in buildings since the 1980s and possibly before that in other applications. (Fraisse, Viardot, Lafabrie, & Achard, 2002), (Hudson & Underwood, 1999) are some of the preliminary works done using lumped parameter modelling. These papers help provide a basic understanding to develop these RC models for buildings.

There is no fundamental difference between both ways of doing, except that in the first one these well-established tools have been validated extensively using for instance the BESTEST procedure (Judkoff & Neymark, 1995). The BESTEST allows for testing the outcomes of the components and subsystem models under specified conditions, i.e., with well-determined input data. RC models typically use the same type of equations but are in general less extended and/or less well validated.

To give an example, most well-established simulation tools would typically model the transient heat transfer in all different layers of a wall (e.g., concrete/insulation/gypsum), while in RC model the wall would be considered as one node with equivalent overall properties. Sometimes, even the transient behaviour would not be modelled.

Finally, it should be noted that the term 'RC model' is quite confusing as the well-established tools are nothing else than an extended and complex version of RC models.

Advantages of white box models are their accuracy when all inputs are well determined and their explanatory power, by which they allow for prediction of the output (e.g. energy usage) when the input is changed (like insulating a wall).

A big disadvantage is that it is almost impossible in real life to determine accurately enough all needed inputs. For example, to simulate a wall in an existing building, a destructive inspection would be needed to determine accurately all materials and their thickness; air velocities should be measured to estimate the convective heat transfer coefficient etc. Because of this lack of accuracy in the inputs, the predictions made by the model may be very inaccurate; leading to the so-called prediction gap (IEBB report Task 1.1), (Brom, 2020).

3.1.2 Black box models

The black box models can be referred to as data-driven or statistical or empirical models. The black box model uses mathematical equations from statistics to relate influential inputs (E.g., weather, occupancy) to the outputs. The source of data for these models can be on-board monitored data from the sensors and smart meters, data simulated from the simulation tools listed in the previous section, survey or standard data from public benchmark datasets (Boodi et al. 2018). These models do not require the building description which are often unavailable or not reflective of the as- built characteristics.

These models are purely based on (advanced) statistical methods, often referred to as machine learning. Just like in classic statistics, the algorithms basically look for correlations between variables and based on that, they automatically set up a model representing the data, like a regression model. There is therefore no underlying building model.

(Wei, et al., 2018) classified and detailed the data-driven black models based on their application for either predicting energy demands or profiling the energy consumption patterns using classification methods. Figure 5 elucidates the different types of methods used in both the above cases. For a short definition of these methods, see Appendix A.

Please note that the classification presented in figure 5 may sometimes be a bit confusing as some of the methods like ANN or GA or even regression models may also be used in combination with a building model supporting the analysis, becoming this way a grey-box model, see section 4.1.3 and 5.2.2.

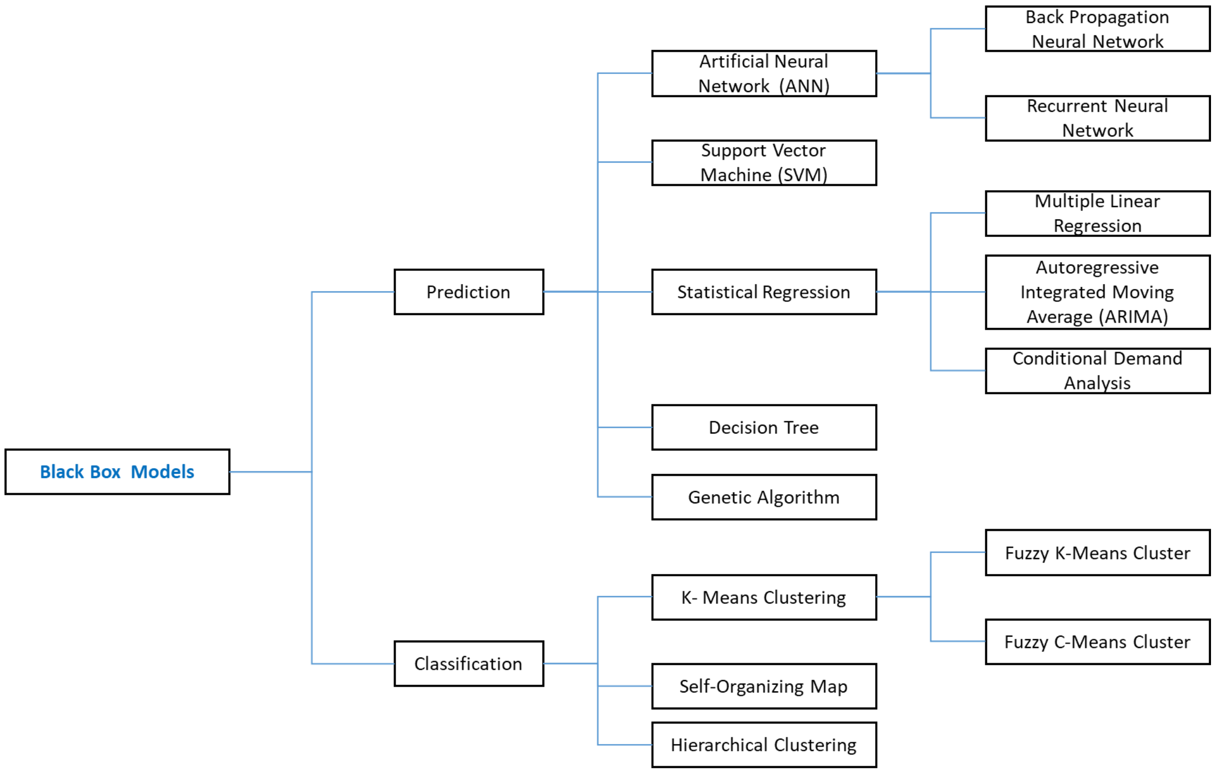


Figure 5. Black box models classified (Wei, et al., 2018)

The review paper by Amasyali & El-Gohary (2018) illustrates studies that used the above listed black box models for various applications relating to energy in buildings. The paper lists the studies conducted along with the building type, data used with the type and granularity, the purpose of the study and the performance of the models. Black box models used for parameter estimation are introduced in section 5.

The main advantage of black box models is that they are purely based on data and do not require any model. They offer a powerful way to classify large bunches of data and to analyse correlations and patterns. They are also reasonably successful in predicting energy use patterns.

Their biggest disadvantage is that they offer little possibility to steer and control the systems they are describing and to propose improvements to the system. For instance, there are well predicting black box energy models based on weather data and building's indoor temperature and opening times, very useful for instance to determine peak loads and quantities of energy to be bought (López, 2017). However, these variables do not give any clue how to decrease building's energy use nor do they allow for predicting the effect of renovation parameters like adding insulation or changing a ventilation or lighting system.

3.1.3 Grey box models

The disadvantages of the black and the white box models are overcome by using the grey box models. The grey box models are based on known physics and as well use real-time data.

Grey box models are generally defined as a combination of black box and white box models. This definition is ambiguous in distinguishing when a white box and a black box model become grey. Using some inspirations from (Kroll, 2000), the figure below shows how to arrive to a grey box model from a black box and white box model.

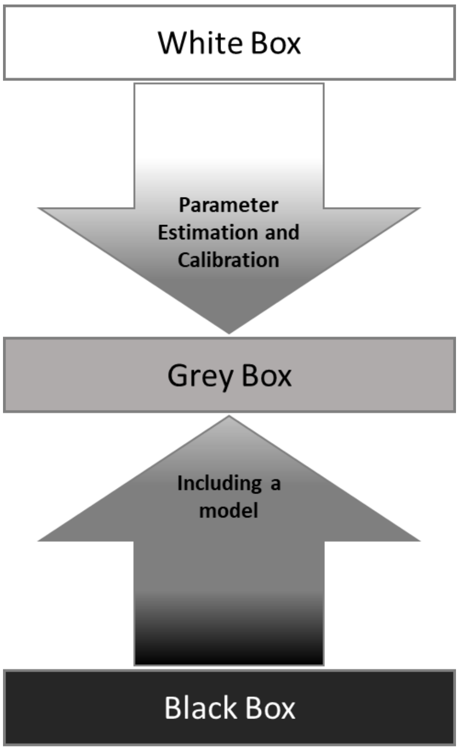


Figure 6. Arriving to a grey box model

A model becomes a grey box model:

1. When simulation models (white box models) explained in 4.1.1 are calibrated with real-time monitored data to obtain results close to the actual performance of the buildings (Raftery, Keane, & O'Donnell, 2011), (Y.Heo, R.Choudhary, & G.A.Augenbroe, 2012). These calibration models are particularly useful to generate probabilistic predictions of retrofit performance to support decision making. The calibration process is based on monitored input and output data fed to the model to estimate parameters which are otherwise unknown (Bacher & Madsen, 2011), (Deconinck & Roels, 2016), (González et al., 2018), (Rasooli & Itard, 2020), (Wang & Xu, 2006), (Rouchier, 2018), (Reynders, Diriken, & Saelens, 2014) and (Jiménez, Madsen, & Andersen, 2008). Because the availability of very detailed data on all components is limited or even impossible to get, simple white box models (referred to as RC models) are generally preferred. Section 4 of this report elaborates the parameter estimation models.

2. When data-driven models (black box models) explained in 4.1.2 are (partly) supported by explicit models (equations) with a physical meaning (Kroll, 2000). For instance, Jiménez, Madsen, & Andersen (2008) used an ARMAX (Auto-Regressive Moving Average) model to give a physical interpretation to the data and ultimately estimate parameters (see Appendix B for more details). Or genetic algorithms or regression models in which the variables are chosen based on prior knowledge from heat transfer models (see section 5.2.2).

   Ultimately, there is a continuous gradation of models between white and black. We will use the term Grey Box Model as a container definition for all models making use of a combination of physical and data-driven models.

3.1.4 Summary of the modelling methods

Table 2 summarizes the advantages and disadvantages of the previously discussed modelling methods.

Table 2. Applicability and limitations of the modelling methods

	White Box	Grey Box	Black Box
Advantages	1. These models are developed based on known physics, hence, results can be interpreted in physical terms 2. Training data is not required 3. Computational time increases with the model complexity	1. These models are also developed based on known physics, hence, results can be interpreted in physical terms 2. Enjoys the benefit of simple physics 3. Computational time is generally quick	1. The results are obtained heuristically, hence, these models can be used where complex relationships cannot be established based on known physics. 2. The computational time is quick except in the case of SVM. 3. The development time of these models is short 4. Accurate results can be obtained given that the data quality is good
Disadvantages	1. The detailed parameters are often not possible to obtain and also, if obtained they are not reflective of the as- built characteristics leading to poor model performance. 2. These models are computationally complex to be used for online use	1. Although, grey box models have the benefit of both black box and white box models, the selection of suitable model structure is still difficult. Lower order models do not reflect the true building and higher order models may be undetermined and lead to multiple solutions.	1. Difficulty to interpret in physical terms 2. Training data collected over longer duration is required 3. The performance of the black box models rely on the quality of the data collected. 4. Regression models may exhibit low accuracy 5. Models are not flexible, in the sense, when retrofits are made or when applied to a different building, re-training of the model is required.

3.2 Classification based on the modelling problem

The models in general consists of four parts: the inputs, the outputs, the parameters and the model structure (Wang, Yan, & Xiao, 2012), (Ghiaus, 2014). How the inputs and outputs to the model are selected depends on what kind of calculation needs to be achieved.

Inputs are also referred to as 'independent variables' and outputs as 'dependent variables'. The parameters are the 'weights' attributed to the independent variables.

For instance, In the equation,

$y = ax_1 + bx_2 + cx_3 + d$

y is the dependent variable (the output); x_1, x_2 and x_3 are the independent variable (the inputs) and a, b, c and d are the parameters.

As another example, the temperature in a building may be governed by an equation like:

$Q_{heating} = \rho CV \frac{dT}{dt} + (\rho CV + \sum UA)\, T - (\rho CV + \sum UA)\, T_{outdoor} - Q_{sol} - Q_{int}$

In this case, the dependent variable is $Q_{heating}$, the independent variables are T (indoor temperature), T_{oudoor}, Q_{sol} (Solar energy) and Q_{int} (Internal heat gains) and all the others are parameters.

1. Therefore, the inputs can be the influential factors (e.g., temperatures, solar radiation, internal hat load) or command required to reach a set- point (Eg., set point temperature) in the case of a control problem.
2. The outputs can be the energy performance indicators or temperature like in case of a temperature control problem.
3. The parameters are the thermo-physical characteristics of the buildings.
4. And the model structure can be obtained through known physics or heuristically.

Having established the four parts of a model, Ghiaus (2014) classified models as forward models (Direct or Simulation or Straight forward models) and inverse models. Figure 7 gives an overview of this classification.

Forward Models- When inputs and parameters of a model are known and used to obtain outputs, it is called forward modelling. It is a straightforward approach.

Inverse Models- 1. When measured inputs and outputs are used to obtain building parameters which are otherwise unknown 2. And, when the desired set-point (output) is known and the input to achieve this set point is estimated, it is called an inverse modelling approach.

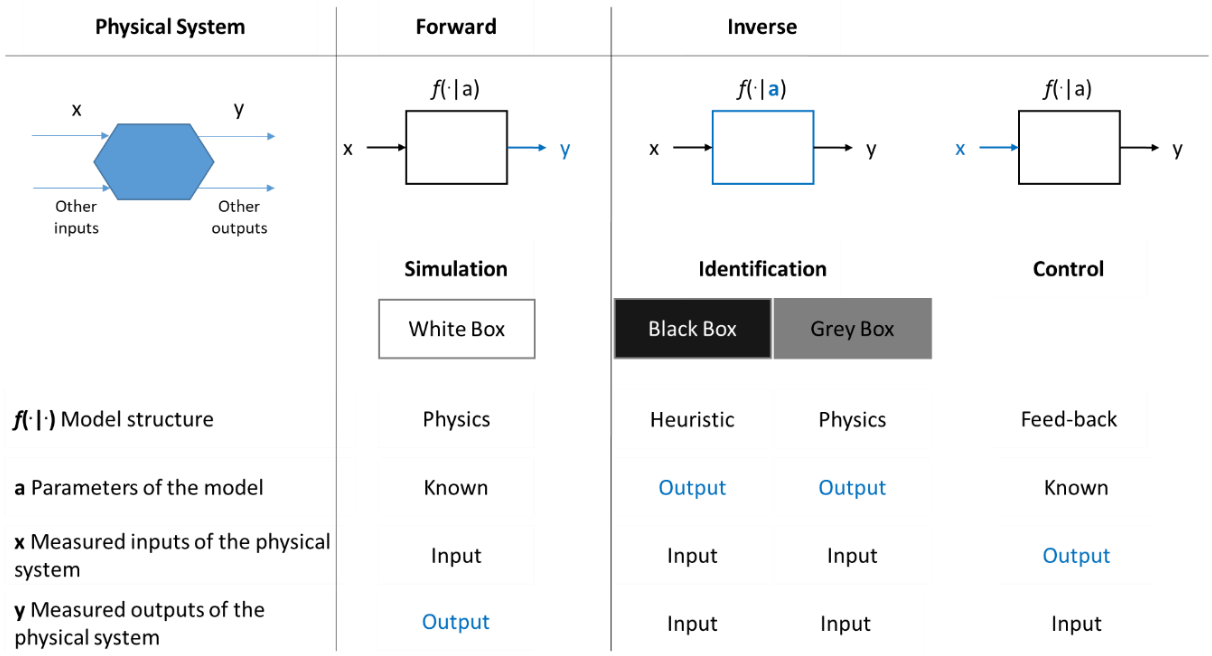


Figure 7. Forward modelling vs inverse modelling (Ghiaus, 2014)

4. PARAMETER ESTIMATION

4.1 Introduction

These days, dwellings are moving towards the goal of improved energy performance through optimal operation and control. With the increasing presence of sensors and smart meter data in dwellings, this goal is becoming more and more practically attainable. But for an accurately functioning optimisation or control model, a proper system identification model becomes an essential foundation. Bloem (1994) described system identification as the estimation of building characteristics in a dynamic model. Therefore, 'parameter estimation', 'system identification' and 'determination of the characteristics of the buildings' is considered synonymous throughout this report. And building parameters or characteristics means the thermo-physical characteristics (it may also be occupant behaviour) of the buildings throughout this report.

Infiltration rate, ventilation flow rate, types of glazing, glazing area, the resistance of the building envelope to conduct heat between its two surfaces and, the capacitance of the building envelope to store heat are some parameters that help characterise a building. Unfortunately, theoretical values obtained from construction files, standards and product information do not often reflect the as-built characteristics (Deconinck & Roels, 2016). Thus, the estimation of these parameters is paramount to establish the heat dynamics of the buildings for future energy performance modelling. In addition to adequately representing the heat dynamics of the buildings, it is also important that these models are simple and work with minimal computational effort for ease of application. Such models can be developed from observed input and output data of the buildings.

Once the system identification model is established, the model can then be used for various applications. Bacher & Madsen (2011) developed a system identification model that can be used for indoor climate control, forecasting of energy consumption for heating and accurate description of energy performance in buildings. Prívara, et al. (2013) pointed out that for a proper functioning Model Predictive Controller (MPC), a model which is reasonably simple and establishes the heat dynamics fairly is required. Reynders, Diriken, & Saelens (2014) stated that a robust system identification model is required for the development and evaluation of demand-side management control strategies. Kim et al. (2018) specified that system identification models were required for optimally operating Heating Ventilation and Air conditioning (HVAC) systems using prediction of future loads and for monitoring building energy performance. Rasooli & Itard (2018) indicated the criticality of estimating these parameters to support decision and policy making by the governments. Senave et al. (2019) stated that understanding the thermal behaviour of the building envelope is one of the initiators to implement energy-saving strategies such as increasing energy efficiency and transitioning to renewable energy. Moreover, since these models characterise existing buildings, the effectiveness of a proposed retrofit can be evaluated. Thus, enabling dwellings to function in a cost-effective and energy efficient manner while reducing the retrofit requirements.

A kind of reverse modelling is known for a long time at component level and applied in many measuring methods. For instance, the ISO method (ISO9869-1, 2014) for in-situ measurement of wall's thermal resistance is based on such a method: by measuring for a long period, surface temperatures and heat fluxes, the heat resistance can be determined by an inverse model. See Appendix C for explanation. The measurement methods suffer limitations such as the need for special measurement equipment, cost, intrusiveness, measurement duration of more than a day and limited number of parameters it can estimate. These limitations can be overcome by models that use on-board monitored data to estimate parameters.

Having recognised the importance of the system identification models and the limitations of measurement methods in the built environment, it becomes essential to divulge the parameter estimation models that have been developed thus far, the kind of data that feeds such models and the validation techniques.

4.2 Models used thus far for parameter estimation

Parameter estimation of buildings is an inverse problem as described in section 4.2. Up until now, several different models were studied to approach the parameter estimation problem. The choice of modelling methods depends on the extensiveness of the data available, parameters to be estimated, duration of the measured data, granularity and the modelling approach (stationary or dynamic analysis) itself.
The succeeding sections briefly describe models used for parameter estimation along with their applicability and limitations. A greater emphasis is given to grey box models. It is because of their physical interpretability, flexibility which allows for different modelling approaches (e.g., Inverse Modelling), versatility which allows these models to be developed using any preferred coding language (e.g., Python, MATLAB) and simplicity.

4.2.1 Grey Box Models for Parameter Estimation

Table 3. Grey box models described

Model	Data- Driven + Physics
Parameters	Estimated
Inputs	Measured
Outputs	Measured

Auto regressive models such as the AutoRegressive Moving Average (ARMAX) model which are normally referred to as black box models can be physically interpreted making them grey box models. This is achieved by representing the auto regressive model equations in the form of state space equations (Jiménez, Madsen, & Andersen, 2008). Thus, making them grey box models in a way. Senave et al. (2019) and Deconinck & Roels (2016) used AutoRegressive with eXogenous inputs model to achieve this physical interpretation. See Appendix B for more explanation.

Another approach to developing an inverse grey box model to estimate parameters is described below in steps. This is particularly described because research as a part of IEBB is expected to be carried out using this method. It is illustrated with an example adopted from (Rasooli & Itard, 2020):

1. Obtain the measured inputs and the outputs of the building. For instance, outdoor air temperature (T_{out}^{∞}), space heating consumption ($\dot{Q}_H$) and global horizontal irradiation (P_{sol}) were considered as inputs and the indoor air temperature as the output (T_{in}^{∞}).
2. Choose a thermal network model that would adequately capture the heat dynamics of the building with the available data. For instance, 1R1C lumped parameter model was used by Rasooli & Itard (2020) and models of increasing complexity was used by Bacher & Madsen (2011).

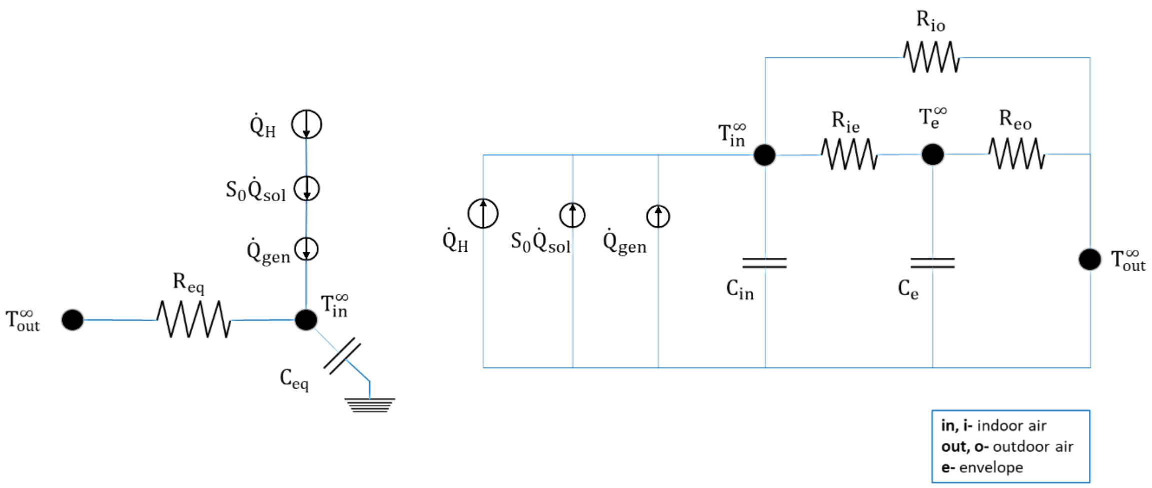


Figure 8 A lumped parameter 1R1C model on the left and 3R2C model on the right

3. Derive the building's governing equations and feed it the with the measured inputs and outputs. For instance, Rasooli & Itard (2020) used the following equation for 1R1C model:

$$R_{eq}^{-1}[T_{out}^{\infty} - T_{in}^{\infty}] - C_{eq}\left[\frac{\partial T_{in}^{\infty}}{\partial t}\right] + \eta.[\dot{Q}_H] + S_0.[P_{sol}] + S_1 = 0$$

Similarly, for 3R2C model, the following set of equations can be used:

$$R_{ie}^{-1}[T_e^{\infty} - T_{in}^{\infty}] + R_{io}^{-1}[T_{out}^{\infty} - T_{in}^{\infty}] - C_{in}\left[\frac{\partial T_{in}^{\infty}}{\partial t}\right] + \eta.[\dot{Q}_H] + S_0.[P_{sol}] + S_1 = 0$$

$$R_{ie}^{-1}[T_{in}^{\infty} - T_e^{\infty}] + R_{eo}^{-1}[T_{out}^{\infty} - T_e^{\infty}] - C_e\left[\frac{\partial T_e^{\infty}}{\partial t}\right] = 0$$

4. Determine the parameters which satisfy the whole set of equations by launching an optimization problem to obtain the parameter values. In our illustration, the parameters included the global heat loss coefficient (R_{eq}^{-1}), global capacitance

(C_{eq}), a constant that accounted for the fraction of solar irradiation entering the building (S_0) and another constant which accounted for the internal heat gains (S_1).

a. Define an objective function for the optimisation problem. Here, Rasooli & Itard (2020) used an objective function so as to minimise the Root Mean Square Error (RMSE) between the measured and the predicted indoor air temperature. While Bacher & Madsen (2011) used maximum likelihood of estimated parameters. Also, for obtaining reliable parameter estimates, a logical upper and lower bound for each of the parameters was defined as constraints.
b. Solve the optimisation problem with an algorithm that estimates the parameters. Rasooli & Itard (2020) used a Genetic Algorithm (GA) and Bacher & Madsen (2011) used a Bayesian approach to estimate the parameters. The optimisation was run several times until the parameter with the lowest RMSE value (objective function) and maximum likelihood of parameters respectively was obtained.

4.2.1.1 The choice of models

The choice of a thermal network model is important to reflect the true system. Raillon (2020) stated that the quantity and the quality of input and output data determines the complexity of the thermal model. While a first order lumped parameter model is a simplified representation, a complex model like a white box model, results in multiple solutions and may require unrealistic quantity of data to become structurally identifiable. A question then arises: *How to choose an appropriate thermal network configuration based on the available data and without compromising the accuracy of the estimated parameters?* Bacher & Madsen (2011) described a forward selection of models from the simplest to the most complex based on the likelihood ratio test. An observation from the conducted literature study shows that a large number of studies include the 3R2C model for their parameter estimation. Table 4 summarises the different inverse grey box models which start with a choice of thermal network models and finish with an optimisation algorithm to determine optimal parameters.

Table 4. Summary of models used for parameter estimation

Paper	System	Thermal Network Configuration	Objective Function	Estimation Algorithm	Software Used
(Penman, 1990)	A primary school with a total floor area of 780m², UK	3R2C	Minimising the sum of the squares of the residuals	Gauss-Newton	FORTRAN
(Wang & Xu, 2006)	50 floors commercial building, Hong Kong china	3R2C external wall 3R2C roof 2R2C internal mass	-Minimising Root Mean Square Error (RMSE)	Genetic Algorithm	Not specified
(Bacher & Madsen, 2011)	Unoccupied. Experimental house, Demark	Forward selection from simple to complex models based on likelihood ratio tests	Maximum likelihood estimation of parameters	Bayesian Approach	CTSM toolbox -R
(Reynders, Diriken, & Saelens, 2014)	2 detached single family dwellings with different insulation levels	1R1C 3R2C 4R3C 6R4C 8R5C	Maximum likelihood estimation of parameters	Bayesian Approach	CTSM toolbox -R
(Harb, Boyanov, Hernandez, Streblow, & Müller, 2016)	2 office (33140 m² & 9032m²) and 1 residential building (2564m²)	3R2C 1R2C 4R2C 8R3C	Minimising the sum of the squares of the residuals	Interior Point	MATLAB
(González, Brown, Gabe-Thomas, Lovett, & A.Coley, 2018)	1000 simulated buildings based on real surveys, London	1R 1R1C 2R1C 2R2C 3R2C 1R1CThermalMass 2R1CThermalMass 2R2CThermalMass	-Minimising error	Simplex	Not specified
(Dimitriou, K.Firth, M.Hassan,	11 detached dwellings, UK	3R2C	Minimising the sum of the	Generalised Reduced	MS Excel

Paper	System	Thermal Network Configuration	Objective Function	Estimation Algorithm	Software Used
& Kane, 2020)			squares of the residuals with constraints	Gradient algorithm	
(Rasooli & Itard, 2020)	Occupied residential house, The Netherlands	1R1C	-Minimising Root Mean Square Error (RMSE) -along with upper and lower bound constraints	Genetic Algorithm	MATLAB

4.2.1.2 The choice of data

Senave et al. (2019) concluded in their study that the choice of data analysis had a lesser influence on the estimated parameters in comparison to the kind of data used. From this literature study, it can be seen that the most commonly used input data include gas consumption, solar irradiation and outdoor air temperature and in the case of output data, indoor air temperature is used.

It then becomes important to assess: *What kind of data is required for parameter estimation?* Should all inputs and outputs of the heat balance equation be measured or, is it possible to make nearly the same estimates based on logical assumptions?
In case of indoor air temperature, most studies assume a single zone and assume the indoor air temperature to be an average or a volume weighted average of the temperatures measured in different rooms. Such assumptions can give rise to uncertainties (Rasooli & Itard, 2020), (Senave, Roels, Verbeke, Lambie, & Saelens, 2019).

Rasooli & Itard (2020) and Jurado López (2017) included global horizontal irradiation data measured by closest possible KNMI (Royal Netherlands Meteorological Institute) weather station in the modelling. Solar gains are highly influenced by the orientation of the windows and the presence of surrounding objects that obstruct irradiation. Thus, by using solar irradiation data measured on-site and by incorporating orientation- specific solar irradiation data in the model instead of the global horizontal irradiation, the prediction of the building parameters can be improved. This is especially crucial when internal conditions of the buildings are to be predicted in summer. Table 5 summarises the data that fed the grey box models.

Table 5. Summary of data used for inverse models

Paper	Input Data	Output data	Time Interval	Kind of data
(Penman, 1990)	1. Heat gains which included space heating, solar, electrical and metabolism 2. Outdoor air temperature	Indoor air temperature	30 minutes	Measured
(Wang & Xu, 2006)	1. Fixed ventilation rate 2. Outdoor air temperature 3. Global irradiance 4. Internal gains	Indoor air temperature	Not specified	Measured
(Bacher & Madsen, 2011)	1. Outdoor air temperature 2. Heat input from electrical 3. Global irradiance	Indoor air temperature	5 minutes	Measured
(Reynders, Diriken, & Saelens, 2014)	1. Outdoor air temperature 2. Constant Ground temperature 12°C 3. Solar gains 4. Internal gains 5. Heat gains from the radiator	-Indoor air temperature -heat flux to different building components	10 minutes	Simulated IDEAS library - Modelica
(Harb, Boyanov, Hernandez, Streblow, & Müller, 2016)	1. Space heating gas consumption 2. Global irradiance 3. Outdoor air temperature	Indoor air temperature	1 min- 1 hr	Measured
(González, Brown, Gabe-Thomas, Lovett, & A.Coley, 2018)	1. Indoor air temperature 2. Outdoor air Temperature 3. Electricity 4. Gas use		Not specified	Simulated
(Rasooli & Itard, 2020)	1. Space heating gas consumption 2. Global irradiance 3. Outdoor air temperature	Indoor air temperature	Hourly	Measured

Paper	Input Data	Output data	Time Interval	Kind of data
(Dimitriou, K.Firth, M.Hassan, & Kane, 2020)	1. Outdoor air Temperature 2. Gas use (not aggregated) 3. Electricity 4. Heat Loss due to infiltration	1. Indoor air temperature 2. Envelope temperature	Not specified	Measured

4.2.1.3Parameters estimated and the validation methods

Gori & Elwell (2018) studied the importance of quantifying the error associated with the estimated parameter for informed decision making and quality assurance. Although, many studies estimated parameters that were found to be consistent with the construction data, there is a scope for improvement to widen its applicability to more residential buildings. The starting point of which would be the methods of validation. There are different ways of validating: The first one is to look at the quality of the fit (e.g RMSE). In that case, the objective function and the validation function are identical. Second, a better way of validation is to use different subsets of data (different periods) for the validation. Third, the parameters can be validated against known values from construction documents or by experts. Finally, and most convincing, the parameters can be measured in-situ. This last point is extremely important in the research phase to demonstrate the quality of the method. The very need for system identification models is to obtain parameters reflective of the as-built characteristics. Hence, for this sake, during a monitoring campaign aimed at validating the approach, it becomes vital to include detailed measurements such as infiltration, ventilation flow rates and heat flux. Table 6 details the parameters estimated, and the validation methods used in different studies.

4.2.1.4 Enriching parameter estimation with additional data

González et al. (2018) remarked that aggregated gas (space heating gas consumption separated from the total gas consumption) data, infiltration and ventilation flow rate measurements were needed to improve the estimations of the heat transfer coefficients, especially in the winter. And, including surface temperature measurements during monitoring campaigns can help improving the resolution of the models from 1R1C to higher order models, leading to detailed yet reliable parameter estimations. Thus, leading to the question: *Can detailed measurements help in improving parameter estimation models and obtain more detailed parameters? (and can this additional information be kept to a minimum?)*

Table 6. Summary of estimated parameters and validation methods

Paper	Estimated parameters[1]	Validation Method
(Penman, 1990)	1. Thermal Resistance 2. Capacitance of the indoor air and building envelope	1. RMSE
(Wang & Xu, 2006)	1. Capacitance of the internal mass 2. Thermal resistance	Comparison with two operation periods from summer (2 weeks) and winter (one week)
(Bacher & Madsen, 2011)	1. Thermal Resistance 2. UA-value 3. Capacitance 4. Time constants 5. Area- window and envelope	1. Auto- correlation of residuals 2. Cumulated Periodogram
(Reynders, Diriken, & Saelens, 2014)	1. UA- value 2. ventilation losses 3. Indoor air capacity 4. Capacity of envelope, internal walls and floors	Comparison between observed and predicted output data 1. RMSE 2. Auto- correlation of residuals 3. Model performance for day ahead predictions 4. Physical interpretation of the parameters
(Harb, Boyanov, Hernandez, Streblow, & Müller, 2016)	1. Heat Loss Coefficients 2. Capacitance 3. Time constants	1. RMSE 2. Measure data from 2 other buildings
(González, Brown, Gabe-Thomas, Lovett, & A.Coley, 2018)	1. Heat Loss Coefficient 2. Time constants	Measured data from 6 real houses Internal temperatures (3rooms) External Temperatures

- [1] The heat loss coefficient or the UA value of the building determines the rate of heat flow through the buildings' envelope when a temperature difference exists between the indoor air and the outdoor air under steady state conditions
- Thermal resistance (R) is a heat property and a measurement of a temperature difference by which an object or material resists a heat flow.
- Thermal mass or thermal capacitance (C) is a property of the mass of a building which enables it to store heat, providing "inertia" against temperature fluctuations.
- The time constant is a measure of how quickly the interior of the building responds to a temperature differential between inside and outside.

Source: Passive and Low Energy Ecotechniques (PLEA), the proceedings of the Third International PLEA Conference held in Mexico City, Mexico on August 6-11, 1984.

Paper	Estimated parameters[1]	Validation Method
		Electricity use Aggregated gas use CO_2 concentration Blue prints
(Dimitriou, K.Firth, M.Hassan, & Kane, 2020)	1. Resistance of envelope 2. Boiler efficiency 3. Window area 4. Capacity of internal mass 5. Capacity of building envelope 6. Node positioning 7. Air Change per Hour (ACH) 8. Node positioning	1. RMSE
(Rasooli & Itard, 2020)	1. Global heat loss coefficient 2. Global capacitance 3. Fraction of solar irradiation entering the building 4. Internal heat gains	1. Estimation of parameters in different periods 2. Evaluation based on construction data

4.2.2 Black box modelling approach for parameter estimation: A contradiction

The black box models are generally considered as purely data driven models. Table 7 shows the studies that used a modelling approach represented in Figure 5 (black box models classified). While taking a closer look at the table 7, it can be seen that although the studies used a black box modelling approach, the data used for the models are indeed similar to the data used in the previous section: grey box modelling approach. To explain it further, the estimated parameters in these studies are heat loss coefficient and gain factor. By principle, these parameters are related to indoor and outdoor air temperature, heat supplied and irradiation in the heat balance equation. And the studies in table 7 use this exact data for the parameter estimation. In a way, contradicting the definition of a black box model i.e., the models are exclusively based on input- output relationships established using statistical techniques and have no prior knowledge of the internal workings. Hence, it can be argued that black box models in this context are in fact grey box. Therefore, they should be classified as grey box models.

However, it should be noted that there is literature addressing black box models in their true sense for occupant behaviour which will be presented in the next section very briefly and even more addressing energy and performance prediction which will be presented in the Task 1.4 report of IEBB.

Table 7. A statistical approach to estimate parameters

Paper	System	Modelling approach	Data used	Parameters estimated
(Olofsson & Andersson, 2002)	Single family dwelling, Sweden	Feed- forward back propagation neural network	1. Outdoor air temperature 2. Indoor air temperature 3. Electrical load 4. Heat supplied	1. Heat loss coefficient 2. Gain factor
(Lundin, Andersson, & Östin, 2004)	Test cell	Artificial Neural Network with the back propagation algorithm	1. Outdoor air temperature 2. Indoor air temperature 3. Electrical load 4. Heat supplied	1. Heat loss coefficient 2. Heat capacity 3. Gain factor
(Martínez-Comesaña et al., 2020)	Public library with three floors, Spain	1. Extreme Gradient Boosting 2. Support Vector Regression 3. Multi- Layer Perceptron Neural Network	1. Outdoor air temperature 2. Global Irradiation 3. Heating demand 4. Indoor air temperatures	Heat loss coefficient

5. BEHAVIOURAL MODELLING

It is widely accepted that occupant behaviour is one of the sources of uncertainty in the predicted performance, leading to a gap between the actual and predicted performance (Brom, 2020). This is particularly crucial during the building design and retrofit since occupant behaviour is known to influence the adaptability and implementation of building technologies (Li, Yu, Haghighat, & Zhang, 2019), (Olivia Guerra Santin, 2009). Yan et al. (2017) defined occupant behaviour as the presence, movements and interaction of the occupants with the building energy devices and systems. And from the literature study conducted, it can be seen that occupant behaviour can be modelled using sensor data, smart meter data, data regarding the buildings, data from survey and weather data.

Increasing efforts are being taken to model energy related occupant behaviour to address the problem of uncertainty in performance calculations. One such effort was taken by the International Energy Agency (IEA): EBC Annex 66, "Definition and simulation of occupant behaviour in buildings" (Yan, et al., 2017), (IEA, 2018). The aim of annex 66 was to reduce the performance gap by modelling occupant behaviour quantitatively, integrating the models with building performance simulation programs, and demonstrating the methodology through case studies. (IEA, 2018) can be accessed for a detailed reading.

Annex 66 was followed up by the IEA EBC Annex 79: "Occupant-centric building design and operation" (O'Brien, et al., 2020), (EBC, 2018). The annex 79 will address the problems of oversimplifying or ignoring the impacts of occupant behaviour on the building energy performance throughout its entire operation by introducing data- driven occupant modelling and occupant- centric building design. Annex 79 recognises the importance of machine learning techniques fed by real- time data to study occupant behaviour which is in line with our aim of building digital twins using such techniques. Annex 79 will continue to build up until 2023.

While there is a huge potential for behavioural modelling using real- time data and machine learning techniques, there are challenges that need to be overcome for their practical implementation. O'Brien et al. (2020) identified these challenges and also recommended actions which are presented in Table 8 and Figure 9.

Table 8. Challenges and actions: data- driven modelling (O'Brien, et al., 2020)

Challenges	Actions
1. Lack of scalable data collection solutions	1. Developing new occupancy data collection methods including scalable data sources such as mobile position and social media.
2. Lack of clear understanding of the different methods used for occupant presence and action modelling	2. Conducting a literature review of the methods used. 3. Developing an application guideline for the entire process from the collection of in situ occupant-centric sensing data to the visualization of data and outcomes
3. Lack of availability of open data and experience using open data 4. Lack of structured metadata to support releasing and using open data 5. And handling of privacy issues when releasing data	4. Developing a community platform to share open data and code for modelling occupant behaviour and actions. 5. Supporting the platform by creating metadata schemas for annotating data and querying data for various use cases. 6. Anonymizing methods for pre-processing released data to improve occupant/participant privacy. 7. Building a research community by holding data competitions among researchers and people from practice 8. Creating awareness about the released data and code.

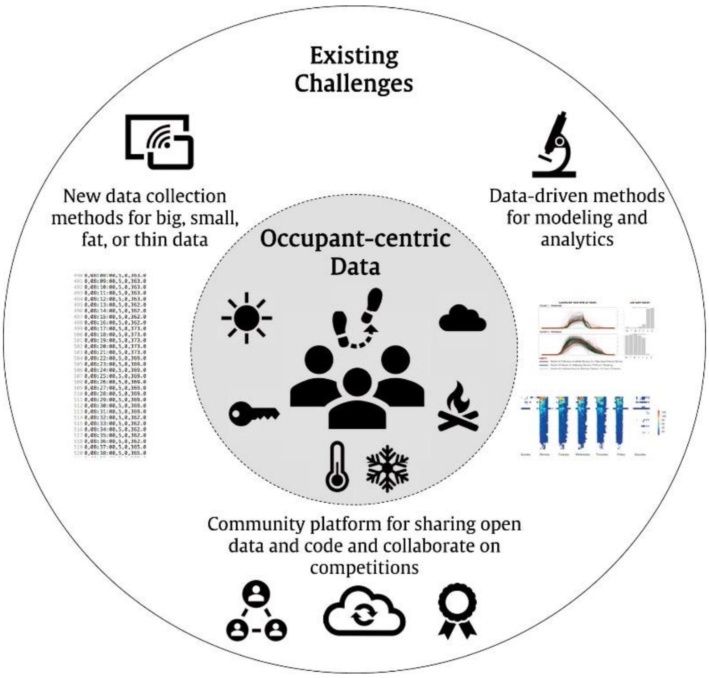


Figure 9. Challenges and actions: data- driven modelling (O'Brien, et al., 2020)

Having introduced the importance of behavioural modelling, the studies that are focusing on behavioural modelling integration and the challenges involved, the report now aims to introduce specific studies that used data- driven approaches to study occupant behaviour. It is important to note that this is not an extensive literature study and only strives to establish with few examples that the black box modelling approach is being used in these studies. In this view, Table 9 tries to illustrate the different occupant behaviour that are being studied, the modelling approach used, and the data employed. For a more comprehensive list of studies, review by Yan et al. (2017), last chapter of Ioannou (2018) and Dai, Liu, & XinZhang (2020) can be referred.

Table 9. Behavioural models

Paper	System	Data- driven modelling approach	Data studied	Behaviour Studied
(Haldi & Robinson, 2008)	8 office buildings, Sweden	Logistic Regression	1. Clothing 2. Activity level 3. Thermal sensation 4. Preference 5. Indoor air temperature 5. Outdoor air Temperature 6. Adaptive activities exercised (see paper for detailed data)	Predicting occupants' actions to adapt both personal (clothing, activity and drinks) and environmental (windows, doors, fans and blinds) characteristics as a function of both internal and external temperature.
(Andersen, Toftum, Andersen, & Olesen, 2009)	Residential buildings, Denmark 933 respondents in summer 636 respondents in winter	Logistic Regression	1. Outdoor air temperature 2. Solar Radiation 3. Survey results 4. Dwelling characteristics	Occupant behaviour 1. Window-open/closed, 2. Heating on/off 3. Lighting on/off 4. Solar shading in use or not
(Andersen, Olesen, & Toftum, 2011)	15 dwellings, Demark	Linear Regression	1. Survey 2. Indoor air temperature 3. Indoor RH 4. Illumination in Lux 5. CO_2 6. Outdoor air temperature 7. Outdoor RH 8. Wind speed	Occupants' interactions with thermostatic radiator valves

Paper	System	Data- driven modelling approach	Data studied	Behaviour Studied
			9. Irradiation 10. Window position (open/closed) 11. Heating set-point on thermostatic radiator valves	
(D'Oca & Hong, 2015)	16 private offices with single or double occupancy in a multi-storey building, Frankfurt, Germany	3 step processes: Decision tree, rule induction and cluster analysis	10 min data over two years 1. Occupancy state 2. Time of day 3. Day of week 4. Season of year 5. Window Change	Occupancy schedule patterns
(Markovic, Grintal, Wölki, Frisch, & Treeck, 2018)	52 single or double occupied offices, RWTH Aachen University's Building, Germany	Deep feed forward neural network	1. Presence 2. CO_2 3. RH 4. Indoor air temperature 5. Outdoor air temperature 6. Wind speed 7. Irradiation 8. Window position 9. Rain droplets (see paper for detailed data)	Window opening
(Hao, Hejiang, Junjie, & Shen, 2019)	6 residential apartments, China	1. Logistic Regression 2. XGBoost	1. Indoor air temperature 2. Indoor RH 3. Indoor CO_2 concentration 4. Indoor PM2.5[2] concentration	Window behaviour of the occupants

[2] PM- Particulate Matter

Paper	System	Data- driven modelling approach	Data studied	Behaviour Studied
			5. Outdoor air temperature 6. Outdoor RH 7. Outdoor PM2.5 concentration 8. Outdoor PM10 concentration 9. Rainfall.	

6. CONCLUSION

The report introduced the concept of digital twins in the built environment. It established that digital twins are built on real-time monitored data and models that use this data for specific objectives. These objectives are performance prediction, parameter estimation, control, optimisation and fault detection and diagnosis. Furthering this establishment, the report gave an overview of the model concepts that can be used to meet the above objectives. The models were classified based on the modelling methods as white box, grey box and black box models, and based on the modelling problems as forward and inverse models.

White box models on their own do not require real-time monitored data. However, white box models can be calibrated with real-time data, making them grey box models and used in the building of a digital twin. However, to reduce computation time and because most of the input data needed by white box model cannot be easily monitored, there is a strong preference for using simple models, like the so-called RC models.

The black box models were defined as models which are purely data- driven and based on statistical approach. The relationship between the measured data is established through correlation and the underlying logic is unknown preliminarily. Some black box modelling approaches were then listed. However, it was established that these modelling approaches may not be strictly black box and gradate towards grey box models. It was illustrated with few examples from parameter estimation models.

Then, the report introduced the parameter estimation models. Parameter estimation models are essentially grey box models. These models were recognised as an essential foundation for performing energy and thermal comfort objectives in the building. These models were also found to be particularly useful for making informed decisions during the retrofit. The report then laid out the various studies conducted to estimate parameters, in particular the grey box modelling approach. The measurement method was also included in the appendix of the report because the measurements are done in actual buildings. This means, that the data resulting from such measurements are reflective of the actual building and in a way be used in the building of the digital twins.

During, the literature study of the parameter estimation models, focus was placed on the choice of models, data, parameters estimated and the validation methods. It was identified that the monitored data played a crucial role in determining the choice of models and the accuracy of the estimated parameters. It was particularly evident when studies conducted on similar systems used different thermal network configuration models and estimated less detailed to detailed parameters of varying accuracy.

The last part of the report briefly described behavioural models, the challenges in implementing them and the importance of including them to reduce the performance gap. The report also saw the potential of black box models to study occupant behaviour.

As consistent with the rest of the report, it was seen that data was again a crucial part of developing such behavioural models.

In conclusion, sensors and smart meters are increasingly installed in residential houses. This allows models such as the parameter estimation models to reach closer to practical application in the residential scenario. But in the view of developing a digital twin of a house, can data from the existing sensors and smart meters be sufficient? Can models feeding a digital twin be improved by including more detailed data? If so, what kind of data is required in addition to the existing sensor and smart meter data?

7. REFERENCES

Amasyali, K., & El-Gohary, N. M. (2018). A review of data-driven building energy consumption prediction studies. *Renewable and Sustainable Energy Reviews, 81*, 1192-1205.

Andersen, R. V., Olesen, B. W., & Toftum, a. J. (2011). Modelling occupants' heating set-poibt preferences. *12th Conference of International Building Performance Simulation Association.* Sydney: Proceedings of Building Simulation.

Andersen, R. V., Toftum, J., Andersen, K. K., & Olesen, B. W. (2009). Survey of occupant behaviour and control of indoor environment in Danish dwellings. *Energy and Buildings, 41*(1), 11-16.

Atsonios, I. A., Mandilaras, I. D., Kontogeorgos, D. A., & Founti, M. A. (2017, November 1). A comparative assessment of the standardized methods for the in–situ measurement of the thermal resistance of building walls. *Energy and Buildings, 154*, 198-206.

Bacher, P., & Madsen, H. (2011). Identifying suitable models for the heat dynamics of buildings. *Energy and Buildings, 43*, 1511-1522.

Bagheri, A., Feldheim, V., & Ioakimidis, C. S. (2018). On the Evolution and Application of the Thermal Network Method for Energy Assessments in Buildings. *Energies, 11*(4).

Batty, M. (2018). Digital twins. *Environment and Planning B: Urban Analytics and City Science , 45*(5), 817-820.

Birdsall, B., Buhl, W. F., Ellington, K. L., Erdem, A. E., & Winkelmann, F. C. (1990). *Overview of the DOE-2 building energy analysis program, Version 2. 1D.* Lawrence Berkeley Lab., CA (USA).

Bloem, J. (1994, July). Application of System Identification for Thermal Characterisation of Building Components. *IFAC Proceedings Volumes, 27*(8), 247-252.

Boodi, A., Beddiar, K., Benamour, M., Amirat, Y., & Benbouzid, M. (2018). Intelligent Systems for Building Energy and Occupant Comfort Optimization: A State of the Art Review and Recommendations. *Energies, 11*.

Brom, P. v. (2020). *Energy in dwellings*. Delft, The Netherlands: TU Delft BK.

Building Systems Laboratory. (1999). *BLAST 3.0 Users Manual.* Department of Mechanical and Industrial Engineering, Building Systems Laboratory, University of Illinois,Urbana-Champaign, IL.

Crawley, D. B., Lawrie, L. K., Winkelmann, F. C., Buhl, W., Huang, Y., Pedersen, C. O., . . . Glazer, J. (2001). EnergyPlus: creating a new-generation building energy simulation program. *Energy and Buildings, 33*(4), 319-331.

D'Oca, S., & Hong, T. (2015). Occupancy schedules learning process through a data mining framework. *Energy and Buildings, 88*, 395-408.

Dai, X., Liu, J., & XinZhang. (2020). A review of studies applying machine learning models to predict occupancy and window-opening behaviours in smart buildings. *Energy and Buildings, 223*.

Deconinck, A.-H., & Roels, S. (2016). Comparison of characterisation methods determing the thermal resistance of buildings components from on-site measurements. *Energy and Buildings*.

Dimitriou, V., Firth, S. K., Hassan, T. M., Kane, T., & Coleman, M. (2015). Data-driven simple thermal models: The importance of the parameter estimates. *6th International Building Physics Conference, IBPC* (pp. 2614-2619). Leicestershire, United Kingdom: Energy Procedia.

Dimitriou, V., K.Firth, S., M.Hassan, T., & Kane, T. (2020, September 15). The applicability of Lumped Parameter modelling in houses using in-situ measurements. *Energy and Buildings, 223*.

EBC, I. (2018). *Occupant behaviour- centric building design and operation EBC Annex 79.* IEA. Retrieved from https://www.dropbox.com/s/hqehzws95es90sy/2018-10-10%20EBC%20Annex%2079%20Proposal%20final%20version.pdf?dl=0

Fraisse, G., Viardot, C., Lafabrie, O., & Achard, G. (2002). Development of a simplified and accurate building model based on electrical analogy. *Energy and Buildings, 34*(10), 1017-1031.

Ghiaus, C. (2014, September 1). Linear algebra solution to psychometric analysis of air-conditioning systems. *Energy, 74*, 555-566.

Glaessgen, E. H., & Stargel, D. (2012). The Digital Twin Paradigm for Future NASA and U.S. Air Force Vehicles. *53rd Structures, Structural Dynamics, and Materials Conference: Special Session on the Digital Twin.* Honolulu, Hawaii.

González, A. P., Brown, M., Gabe-Thomas, E., Lovett, T., & A.Coley, D. (2018). The reliability of inverse modelling for the wide scale characterization of the thermal properties of buildings. *Journal of Building Performance Simulation, 11*(1), 65-83.

Gori, V., & Elwell, C. A. (2018, May 15). Estimation of thermophysical properties from in-situ measurements in all seasons: Quantifying and reducing errors using dynamic grey-box methods. *Energy and Buildings, 167*, 290-300.

Grieves, M., & Vickers, J. (2016). Digital Twin: Mitigating Unpredictable, Undesirable Emergent Behavior in Complex Systems. In *Transdisciplinary Perspectives on Complex Systems* (pp. 85-113). Springer.

Haldi, F., & Robinson, D. (2008). On the behaviour and adaptation of office occupants. *Building and Environment, 43*(12), 2163- 2177.

Hao, M., Hejiang, S., Junjie, L., & Shen, W. (2019). Developing window behavior models for residential buildings using XGBoost algorithm. *Energy and Buildings, 205*.

Harb, H., Boyanov, N., Hernandez, L., Streblow, R., & Müller, D. (2016, April 1). Development and validation of grey-box models for forecasting the thermal response of occupied buildings. *Energy and Buildings, 117*, 199-207.

Hedegaard, R. E., & Petersen, S. (2017). Evaluation of Grey-Box Model Parameter Estimates Intended for Thermal Characterisation of Buildings. *11th Nordic Symposium on Building Physics, NSB2017* (pp. 982-987). Trondheim, Norway: Energy Procedia.

Hudson, G., & Underwood, C. (1999). A simple building modelling procedure for MATLAB/ SIMULINK. *Proceedings of the 6th International Conference on Building Performance Simulation*, (pp. 777-783). Kyoto, Japan.

IBM. (2021). *What is a digital twin?* (IBM) Retrieved April 20, 2021, from https://www.ibm.com/topics/what-is-a-digital-twin

IEA. (2018). *International Energy Agency, EBC Annex 66: Definition and Simulation of Occupant Behavior in Buildings.* The Regents of the University of California (through Lawrence Berkeley National Laboratory) and Tsinghua University, China. Retrieved from https://annex66.org/sites/default/files/2018FinalReport/Annex%2066%20Final%20Report%20-%20read.pdf

Ioannou, A. (2018). *Thermal comfort and energy related occupancy behavior in Dutch residential dwellings.* Delft, The Netherlands: TU Delft.

ISO9869-1. (2014, August). *Building Elements—In-Situ Measurement of Thermal Resistance and Thermal Transmittance - Part 1: Heat Flow Meter Method.* Retrieved 2021, from ISO: https://www.iso.org/standard/59697.html

Jiménez, M., Madsen, H., & Andersen, K. (2008). Identification of the main thermal characteristics of building components using MATLAB. *Building and Environment, 43*, 170-180.

Judkoff, R. D., & Neymark, J. S. (1995). A Procedure for Testing the Ability of Whole Building Energy Simulation Programs to Thermally Model the Building Fabric. *Journal of Solar Energy Engineering, 117*, 7-15.

Khajavi, S. H., Motlagh, N. H., Jaribion, A., Werner, L. C., & Holmström, J. (2019). Digital Twin: Vision, Benefits, Boundaries, and Creation for Buildings. *IEEE Access, 7*, 147406-147419.

Kim, D., Cai, J., E.Braun, J., & B.Ariyur, K. (2018, May 15). System identification for building thermal systems under the presence of unmeasured disturbances in closed loop operation: Theoretical analysis and application. *Energy and Buildings, 167*, 359-369.

Kramer, R., Schijndeln, J. v., & Schellen, H. (2012). Simplified thermal and hygric building models: A literature review. *Frontiers of Architectural Research*, 318-325.

Kroll, A. (2000). Grey box models: concepts and application. In *New frontiers in computer intelligence and its applications* (pp. 42-51). Amsterdam: IOS Press.

Langevin, J., L., J. W., & Gurian. (2015). Simulating the human-building interaction: Development and validation of an agent-based model of office occupant behavior. *Building and Environment, 88*, 27-45.

Li, J., Yu, Z. (., Haghighat, F., & Zhang, G. (2019). Development and improvement of occupant behavior models towards realistic building performance simulation: A review. *Sustainable Cities and Society, 50*.

López, C. J. (2017). *Data-driven Predictive Control for Heating Demand in Buildings.* Delft: TU Delft.

Lundin, M., Andersson, S., & Östin, R. (2004, September). Development and validation of a method aimed at estimating building performance parameters. *Energy and Buildings, 36*(9), 905-914.

Markovic, R., Grintal, E., Wölki, D., Frisch, J., & Treeck, C. v. (2018). Window opening model using deep learning methods. *Building and Environment, 145*, 319-329.

Martínez-Comesaña, M., Febrero-Garrido, L., Granada-Álvarez, E., Martínez-Torres, J., & Martínez-Mariño, S. (2020). Heat Loss Coefficient Estimation Applied to Existing Buildings through Machine Learning Models. *Applied Sciences*.

Mejri, O., Peuportier, B., & Guiavarch, A. (2013). Comparison of different methods for estimating the building envelope thermal characteristics. *13th Conference of International Building Performance Simulation Association*, (pp. 630-635). Chambéry, France.

O.M.Brastein, D.W.U.Perera, C.Pfeifer, & N.-O.Skeie. (2018, June 15). Parameter estimation for grey-box models of building thermal behaviour. *Energy and Buildings, 169*, 58-68.

O'Brien, W., Wagner, A., Schweiker, M., Mahdavi, A., Day, J., Kjærgaard, M. B., . . . Berger, C. (2020). Introducing IEA EBC annex 79: Key challenges and opportunities in the field of occupant-centric building design and operation. *Building and Environmnet, 178*.

Olivia Guerra Santin, L. I. (2009). The effect of occupancy and building characteristics on energy use for space and water heating in Dutch residential stock. *Energy and buildings, 41*(11), 1223-1232.

Olofsson, T., & Andersson, S. (2002). Overall heat loss coeffcient and domestic energy gain factor for single-family buildings. *Building and Environment*, 1019-1026.

Penman, J. (1990). Second Order System Identification in the Thermal Response of a Working school. *Building and Environment, 25*(2), 105-110.

Petojević, Z., Gospavić, R., & Todorović, G. (2018, October). Estimation of thermal impulse response of a multi-layer building wall through in-situ experimental measurements in a dynamic regime with applications. *Applied Energy, 228*, 468-486.

Piascik, B., Vickers, J., Lowry, D., Scotti, S., Stewart, J., & Calomino, A. (2012). *Materials, Structures, Mechanical Systems, and Manufacturing Roadmap.* Washington, DC : National Aeronautics and Space Administration (NASA).

Prívara, S., Cigler, J., Váňa, Z., Oldewurtel, F., Sagerschnig, C., & EvaŽáčeková. (2013, January). Building modeling as a crucial part for building predictive control. *Energy and Buildings, 56*, 8-22.

Qiuchen Lu, A., Parlikad, A. K., Woodall, P., Ranasinghe, G. D., Xie, X., Liang, Z., . . . Schooling, J. (2020). Developing a Digital Twin at Building and City Levels: Case Study of West Cambridge Campus. *Journal of management in Engineering, 36*(3).

Raftery, P., Keane, M., & O'Donnell, J. (2011). Calibrating whole building energy models: An evidence-based methodology. *Energy and Buildings, 43*(9), 2356-2364.

Raillon, L. (2020). *Experimental identification of physical thermal models for demand response and performance evaluation.* Lyon: l'INSA de Lyon.

Rasooli, A., & Itard, L. (2018). In-situ characterisation of walls' thermal resistance: An extension to the ISO 9869 standard method. *Energy & Buildings*, 374-383.

Rasooli, A., & Itard, L. (2020). Determination of buildings' global parameters through inverse modelling and on-board monitored data. In A. Rasooli, *In-Situ Determination of Buildings' Thermo-Physical Characteristics* (pp. 147-184). Delft: Architecture and the Built Environment, TU Delft.

Reynders, G., Diriken, J., & Saelens, D. (2014, October). Quality of grey-box models and identified parameters as function of the accuracy of input and observation signals. *Energy and Buildings, 82*, 263-274.

Rokach, L., & Maimon, O. (2005). Clustering Methods. In *The data mining and knowledge discovery handbook* (pp. 321-352). Retrieved from https://link-springer-com.tudelft.idm.oclc.org/chapter/10.1007/0-387-25465-X_15#citeas

Rouchier, S. (2018, May 1). Solving inverse problems in building physics: An overview of guidelines for a careful and optimal use of data. *Energy and Buildings, 166*, 178-195.

Senave, M., Roels, S., Verbeke, S., Lambie, E., & Saelens, D. (2019). Sensitivity of characterising the heat loss coefficient through on-board monitoring: A case study analysis. *Energies, 12*(3322).

Solar Energy Laboratory. (2000). *TRNSYS Version 15 User Manual and Documentation.* Solar Energy Laboratory, Mechanical Engineering Department, University of Wisconsin, Madison, WI.

Tabatabaei, S. A., Ham, W. V., Klein, M. C., & Treur, J. (2017). A Data Analysis Technique to Estimate the Thermal Characteristics of a House. *Energies.*

VirginiaGori, & Elwell, C. A. (2018, May 15). Estimation of thermophysical properties from in-situ measurements in all seasons: Quantifying and reducing errors using dynamic grey-box methods. *Energy and Buildings, 167*, 290-300.

Wagner, R., Schleich, B., Haefner, B., Kuhnle, A., Wartzack, S., & Lanza, G. (2019). Challenges and Potentials of Digital Twins and Industry 4.0 in Product Design and Production for High Performance Products. *Procedia CIRP, 84*, 88-93.

Wang, S., & Xu, X. (2006, April). Simplified building model for transient thermal performance estimation using GA-based parameter identification. *International Journal of Thermal Sciences, 45*(4), 419-432.

Wang, S., Yan, C., & Xiao, F. (2012). Quantitative energy performance assessment methods for existing buildings. *Energy and Buildings, 55*, 873-888.

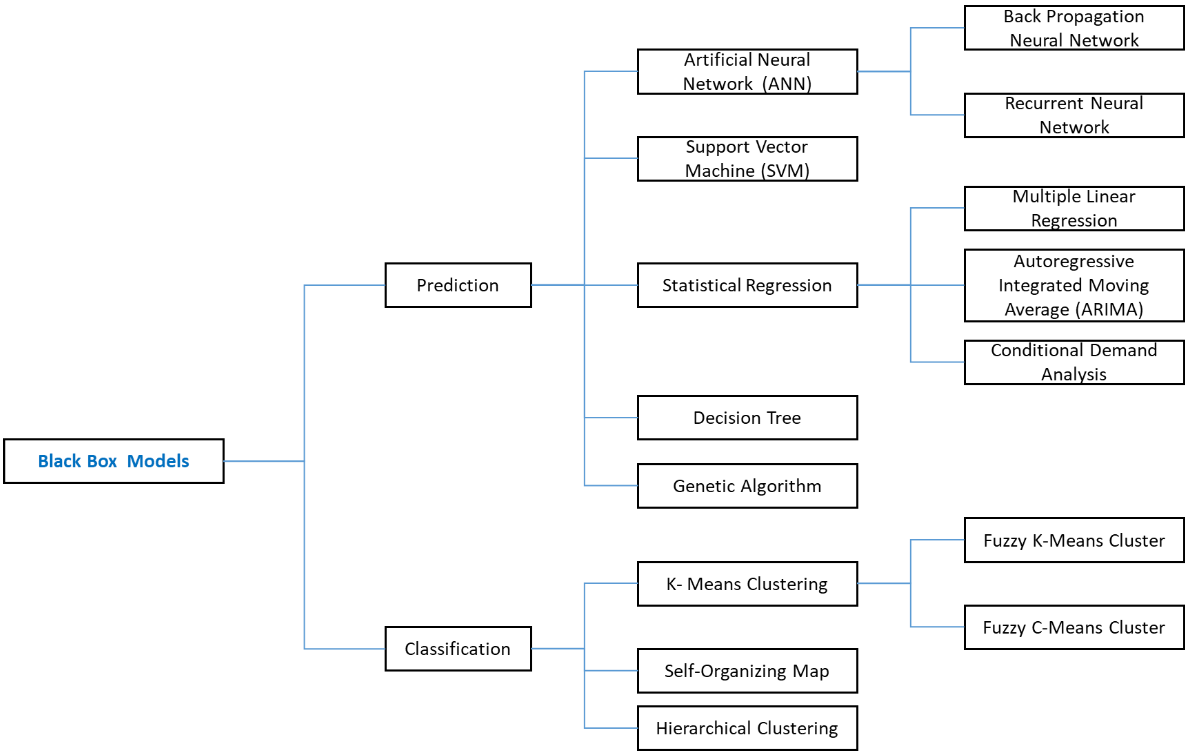
Wei, Y., Zhang, X., Shi, Y., Xia, L., Pan, S., Wu, J., . . . Zhao, X. (2018). A review of data-driven approaches for prediction and classification of building energy consumption. *Renewable and Sustainable Energy Reviews, 82*, 1027-1047.

Y.Heo, R.Choudhary, & G.A.Augenbroe. (2012). Calibration of building energy models for retrofit analysis under uncertainty. *Energy and Buildings, 47*, 550-560.

Yan, D., Hong, T., Dong, B., Mahdavi, A., D'Oca, S., Gaetani, I., & Feng, X. (2017). IEA EBC Annex 66: Definition and simulation of occupant behavior in buildings. Energy and Buildings, 156, 258-270.

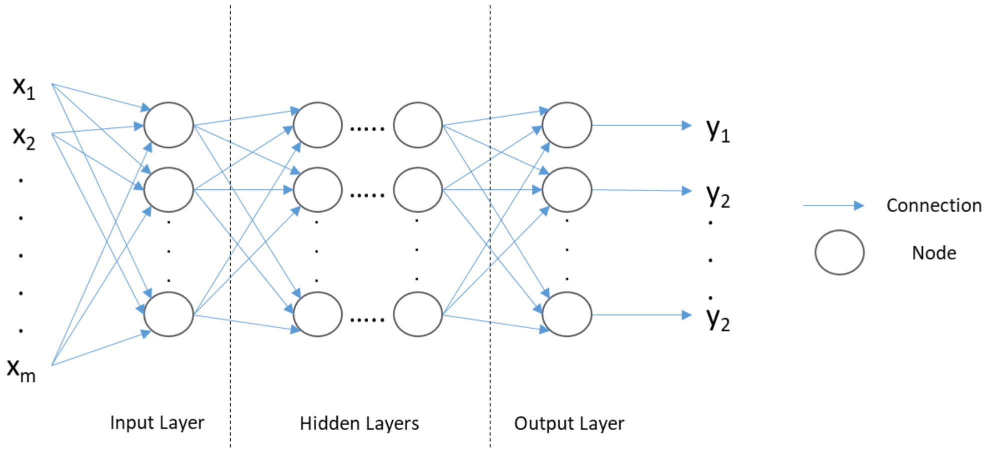
APPENDIX A

Classified black box models defined
The models are defined according to definitions obtained from (Wei, et al., 2018), (Kramer, Schijndeln, & Schellen, 2012)



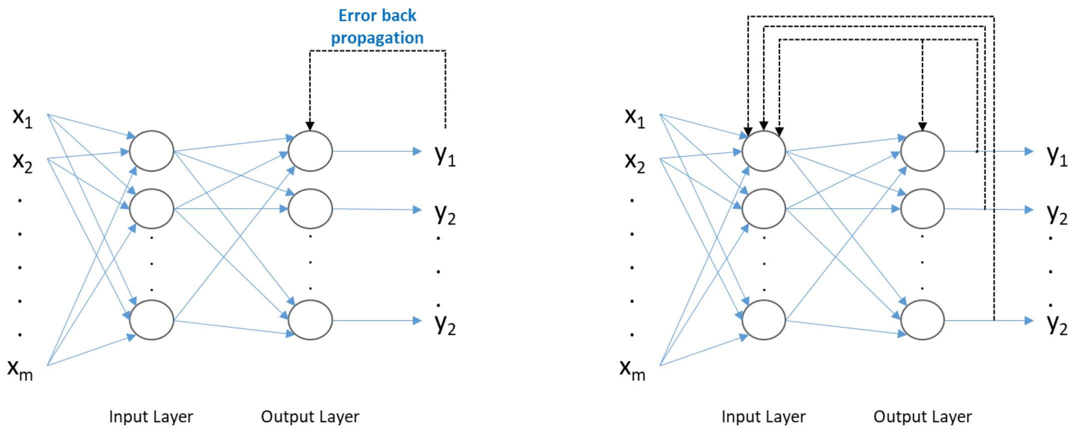
Black Box Models

1. Artificial Neural Network: The working of the ANNs is inspired from the functioning of human brains. Each node consists of inputs and a single output sent to the multiple nodes of the succeeding layer. Each input connection to a node has a weight and the output is determined by the weighted sum of the inputs. A bias is added to this sum. In general, ANN consists of three layers: the input layer, the hidden layers and the output layer. The relationship between inputs and outputs is determined by linear or nonlinear relationships defined in the neuron layers.



Artificial Neural Network

a. Back Propagation Neural Network (BPNN): In a BPNN, the error of the output is computed every time and then propagated as negative feedback to tune the incoming connection weight and bias.
b. Recurrent Neural Network (RNN): In a RNN, the output of one layer is fed as input to the former- layer or even the current layer.



Two-layer BPNN and RNN

2. Support Vector Machine (SVM): SVM can be used for both classification and regression problems. SVM used for regression is called Support Vector regression (SVR). A decision function $F(x_i)$ is first constructed using the training data. For given a input x_i, the predicted output should not deviate from the actual target Y_i by more than the predefined threshold ε.
3. Statistical Regression: A statistical regression establishes a relationship between a dependent variable and one (simple linear regression) or more (multiple linear regression) independent variable.
   a. Multiple Linear Regression: A equation representing multiple linear regression is given by

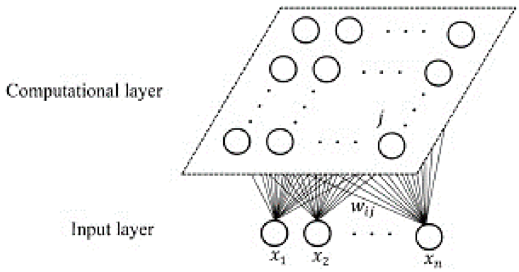
$$Y_i=\alpha_i + \beta_1 x_{i,1} + \beta_2 x_{i,2} + \ldots + \beta_m x_{i,m} + \varepsilon_i$$

ε_i is the error and α_i , β_i are parameters that are to be estimated. A cost function is usually defined to minimise the error between the predicted and actual outputs for appropriate parameter estimation.

b. Auto Regressive Integrated Moving Average (ARIMA): The ARIMA models are time series models which are simple and have a linear approach. It has two parts:
The AR component: $y_t=y_t + a_1y_{t-1} + \ldots + a_py_{t-p} + c$
p is the order of the AR, u_t is the white noise(error), the c is a constant and $a_1, \ldots, a_p$ are the AR parameters
And the MA component: $y_t=u_t + m_1u_{t-1} + \ldots + m_qy_{t-q} + \mu$
u_t, u_{t-1}, …, u_{t-q} are error terms, μ is the expectation of actual value (y_t), m_1, …, m_q are the MA parameters and q is the order of MA

c. Conditional Demand Analysis: "Conditional demand analysis is a multivariate regression technique which combines utility billing data with weather information and customer survey data to produce robust end-use energy consumption estimates." – (Using conditional demand analysis to estimate residential energy use and energy savings by K.H. Tiedemann)

4. Decision Tree: A decision tree partitions the data into groups using a tree- like flowchart. And each branch represents a possible output value.
5. Genetic Algorithm: Genetic algorithm is based on the idea of "survival of the fittest". It is particularly used in parameter estimation to obtain optimal solutions which would otherwise take a longer time. A population size and number of generations must be initially chosen. Then through the process of genetic operations: crossover and mutation, the next generation population of solution is obtained. This optimisation should run several times to procure optimal solutions, which is often combined with an objective function (Eg., RMSE)
6. K- means clustering: K- means clustering is classification algorithm. "The K-means clustering algorithm partitions a set of data into a number of non-hierarchical groups of similar data points, i.e., clusters. The similarity among data points is quantified by the Euclidean distance" (Wei, et al., 2018). This algorithm can be improved and modified into the fuzzy methods. Here, each data point belongs to multiple clusters and the degree of association or membership is defined. The fuzzy methods include:
   a. Fuzzy K means cluster
   b. Fuzzy C means cluster
7. Self- Organising Map (Wei, et al., 2018): SOM is inspired from the ANN and belongs to the unsupervised learning class. It consists of one-dimensional input layer and a two dimensional computational layer. In this computational layer, a number of process units, i.e., neurons (j=1, 2, …, m), are arranged in rows and columns, each of which connects all input signals (x_i, i = 1, 2, … n) with connection weights w_{ij}. In SOM, a squared Euclidean distance between all the input signals and connection weights pertinent to every neuron is computed. This distance is termed as the discriminant function. The neuron with the smallest discriminant function is designated as the winner for a given set of input signals.



Self-Organising Map

8. Hierarchical Clustering (Rokach & Maimon, 2005): Hierarchical clustering is another kind of clustering method. It has two approaches:
    a. The agglomerative approach or the bottom-up approach where each observation starts in its own cluster, and pairs of clusters are merged as one moves up the hierarchy.
    b. The Divisive approach or the top-down approach all observations start in one cluster, and splits are performed recursively as one moves down the hierarchy.

APPENDIX B

How a black box model becomes a grey box model?
A set of equations describing this process is given below along with a figure. The equations show how an ARMAX model with a physical interpretation is achieved. Here, Q is used as the output variable. For specific details, explanation and how parameters were estimated from the established ARMAX model, (Jiménez, Madsen, & Andersen, 2008) can be referred.

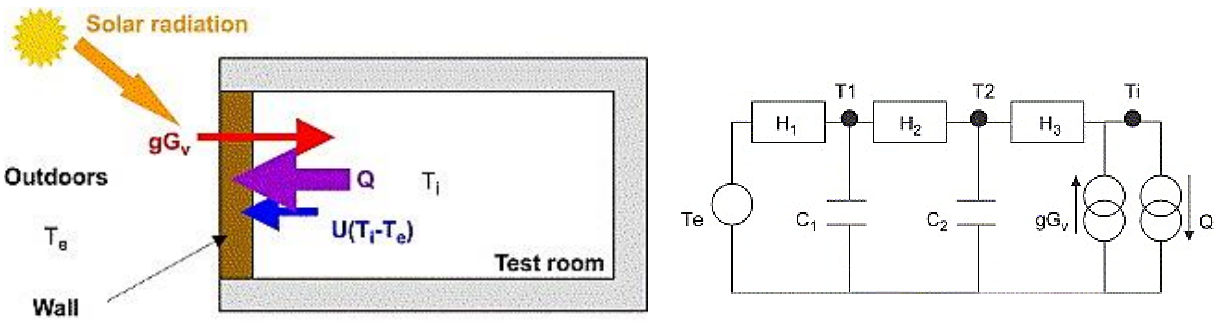


Figure 10 RC network for a wall (Jiménez, Madsen, & Andersen, 2008)

State space equations for the above figure can be written as:

$$C_1 \frac{dT_1}{dt} = H_1(T_e - T_1) + H_2(T_2 - T_1) + \frac{d\omega_1}{dt} \quad (1)$$

$$C_2 \frac{dT_2}{dt} = H_2(T_1 - T_2) + H_3(T_i - T_2) + \frac{d\omega_2}{dt} \quad (2)$$

$$Q = H_3(T_i - T_2) + e; e \in N(0, \sigma_q^2) \quad (3)$$

Where, T_e is the outside temperature, T_i is the inside temperature Q is the heat flux density through the wall, G_v is the global solar irradiance, g is the solar energy transmittance, H_1, H_2 and H_3 are the heat conductance per unit area corresponding to the outer wall, the insulation and the inner walls respectively, C_1 and C_2, T_1 and T_2 are the heat capacitance per unit area and temperature of the outer and inner wall respectively, ω_1 and ω_2 are two independent Wiener processes with incremental standard deviations σ_1 and σ_2.

Rearranging equations (1) and (2), introducing a_{ij} and b_{ij} to simplify notation and only consider the deterministic part of the state space equation, equations 1and 2 becomes,

$$\begin{bmatrix} dT_1 \\ dT_2 \end{bmatrix} = \begin{bmatrix} -a_{11} & a_{12} \\ a_{21} & -a_{22} \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} dt + \begin{bmatrix} b_{11} & 0 \\ 0 & b_{22} \end{bmatrix} \begin{bmatrix} T_e \\ T_i \end{bmatrix} dt \quad (4)$$

Taking Laplace transform and isolating T_1 and T_2, the resulting equation is given by,

$$\begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = \frac{\begin{bmatrix} b_{11}(s + a_{22}) & a_{12}b_{22} \\ a_{21}b_{11} & b_{22}(s + a_{11}) \end{bmatrix} \begin{bmatrix} T_e \\ T_i \end{bmatrix}}{\det A} \tag{5}$$

The measurement equation equivalent to (3) is

$$Q = c(T_i - T_2) + e;\ e \in N(0, \sigma_q^2) \tag{6}$$

Substituting (5) into (6),

$$Q = cT_i - c\frac{a_{21}b_{11}T_e + b_{22}(s + a_{11})T_i}{\det A} + e \tag{7}$$

Thus, Equation (7) is in the form of a an ARMAX model of the form

$$A(q)Q = B_1(q)T_e + B_2(q)T_i + C(q)e \tag{8}$$

APPENDIX C

Measurement method: The Average Method
The Average method as described by (ISO9869-1, 2014) is a stationary model and requires in-situ measurement. It is used to estimate the thermal resistance of building components from the heat flux measured at the interior surface and surface temperatures measured at both sides of the components. Thus, the resistance R_c of a component, say a wall, is calculated by averaging the measured (dynamic) data and is given by,

$$R_c = \frac{\sum_{t=0}^{m} \Delta T^t}{\sum_{t=0}^{m} \Delta \dot{q}^t}$$

ΔT is the temperature gradient, $\dot{q}^t$ the heat flux and *t* the time interval. The cumulative R_c values which also include the averages of the previous days are reported each day until the R_c value converges to a certain constant value. The entire process is carried out based on specific conditions described in detail by (ISO9869-1, 2014) and summarised in the table below.

Table 10. Average Method

Stationary Method	Data Required	Criteria for convergence of R_c values
Average Method (ISO9869-1, 2014)	1. Heat flux measured at the interior surface of the building component 2. Surface temperatures at both sides of the building component	- minimum measurement duration of 3 days. - The R_c value obtained at the end of a day should do not deviate more than ±5% than the previous day value. - The R_c values obtained at first 67% of the measured data should not vary more than ±5% to the values obtained at the last 67% of the measured data.

This averaging is done to approximate steady state values. To fulfil the criteria of ISO 9869 and obtain reliable estimates of R_c, this average should be taken over a long duration (minimum of 3 days) to cancel out the dynamic behaviour of the particular building component. Thus, limiting its applicability because short measurement period is generally preferred. Moreover, the method is valid only if the thermal properties of the building components are assumed constant over the measurement period. The method also requires the effect of heat storage to be negligible. In essence, this method cannot be used in summer when there is an increased dynamic storing of heat by the building fabric due to solar gains. And, since the average method cannot capture the dynamic behaviour of the building, it can only be used to determine stationary thermal properties. Also, VirginiaGori & Elwell (2018), Atsonios et al. (2017) showed that the reliability of the average method estimates was sensitive to the temperature gradients. Thus, the use of average method when the temperature difference is too low (less than 3°C) is not recommended.

Rasooli & Itard (2018) addressed the problem of longer measurement duration by placing heat flux sensors on both sides of the wall. It was concluded that the average R_c value obtained based on the heat flux measurements on both sides of the walls converged faster than the R_c values on each side of the homogenous walls. And for heterogeneous walls, it was concluded that if one of the R_c values (outside or inside) converged earlier than the other, the R_c value from that respective side should be considered. It was also established that by adopting this method, the obtained R_c values were closer to the actual values, hence precise. Deconinck & Roels (2016) used the average method with a correction to account for the thermal storage effects. The study was conducted to determine the R_c values in different seasons: summer, spring and winter. In general, for the summer period, the average method did not show any meaningful estimates and the correction did not improve the estimates. With the correction, the duration of measurement was considerably reduced for the winter and spring seasons, with winter requiring even lesser days for the same accuracy. It is important to note that the thermal properties required for the correction was precisely known in this particular study, in reality they are rarely known.

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