

# Surrogate Models for efficient implementation of Building Performance Analysis and Optimization

November 2025

Gonçalo Roque Matias Araújo    PhD | Sustainable Energy Systems



# Supervisors

*Surrogate Models to improve Building  
Performance Analysis and Optimization*

**Paulo Manuel Cadete Ferrão**

Instituto Superior Técnico

Supervisor

ferrao@tecnico.ulisboa.pt

**Maria da Glória Gomes**

Instituto Superior Técnico

Co-supervisor

maria.gloria.gomes@tecnico.ulisboa.pt

**Manuel de Arriaga Brito Correia Guedes**

Instituto Superior Técnico

Co-supervisor

manuel.guedes@tecnico.ulisboa.pt

# Structure

*Surrogate Models to improve Building  
Performance Analysis and Optimization*

I Motivation

---

II Context

---

III Research Question

---

IV Methodology

---

V Results

---

VI Discussion

---

[Motivation](#)[Context](#)[Research Questions](#)[Methodology](#)[Case Studies](#)[Discussion](#)



Renovate the built environment  
Optimize building design and construction



Renovate the built environment  
Optimize building design and construction

Population welfare



Economic growth



Sustainable goals





Renovate the built environment  
Optimize building design and construction

Population welfare

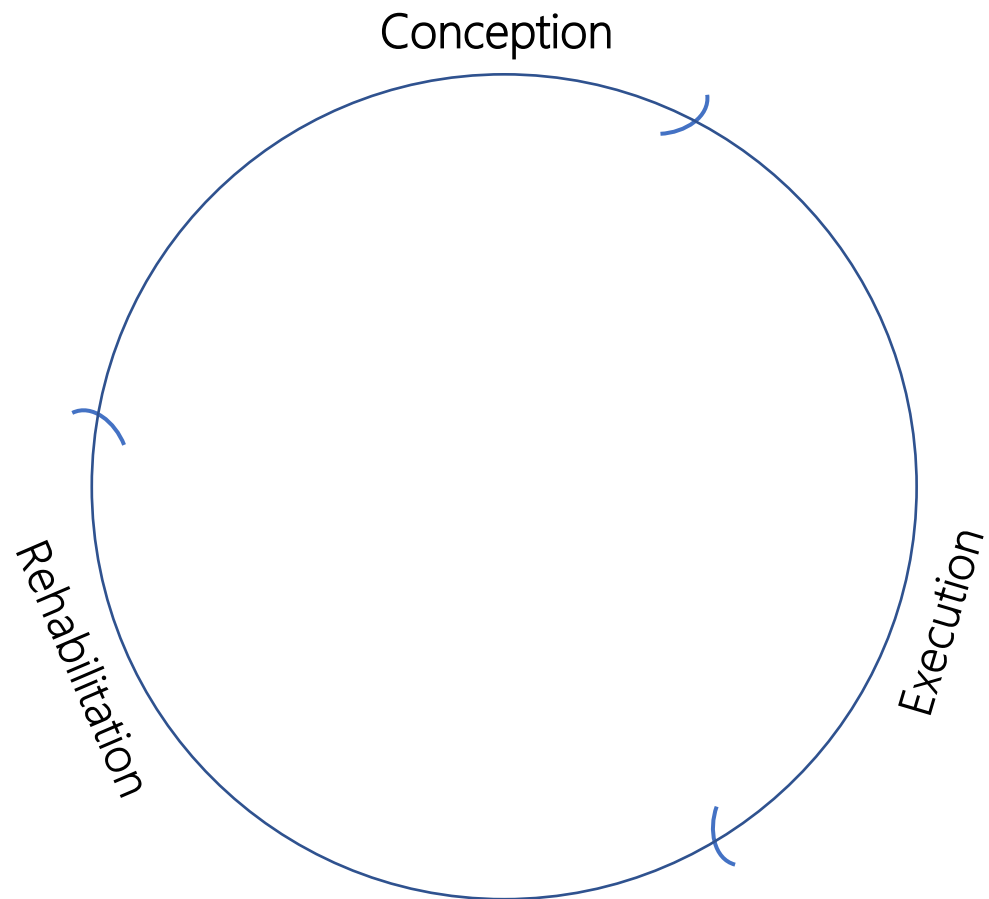


Economic growth



Sustainable goals





Renovate the built environment  
Optimize building design and construction

Population welfare



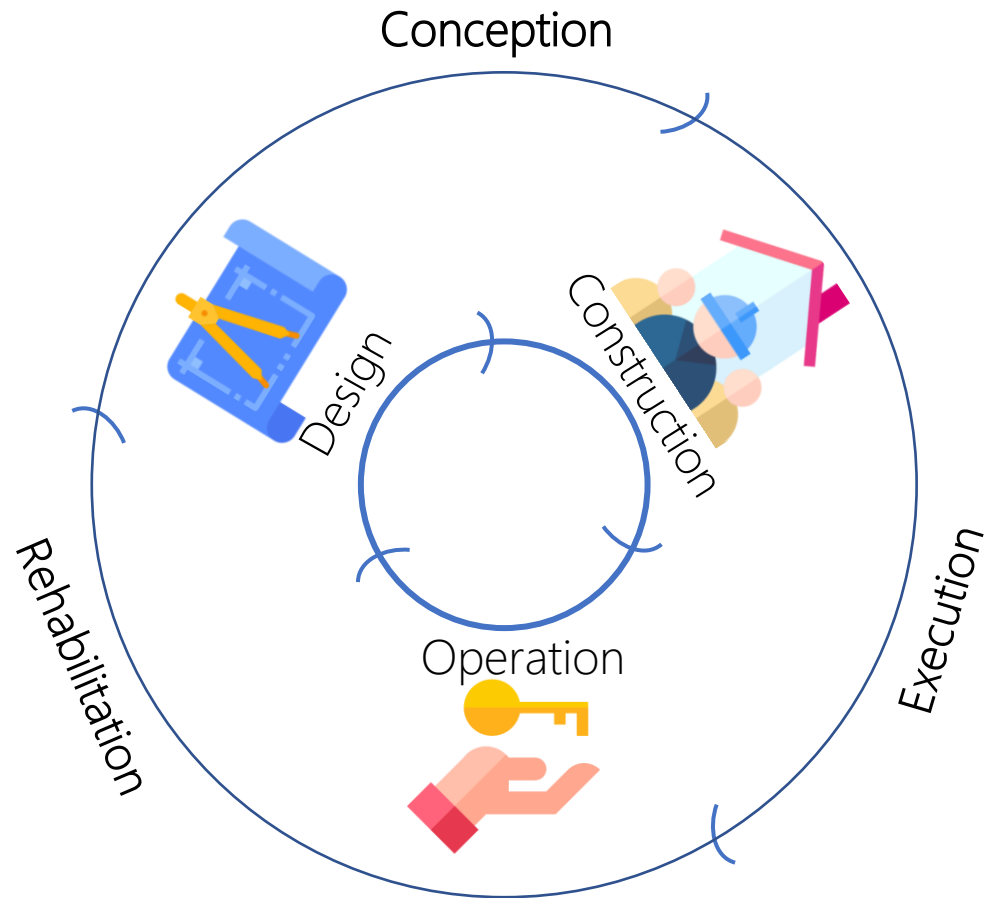
Economic growth



Sustainable goals







Renovate the built environment  
Optimize building design and construction

Population welfare

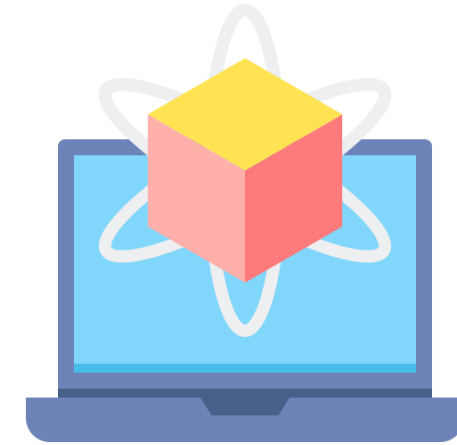
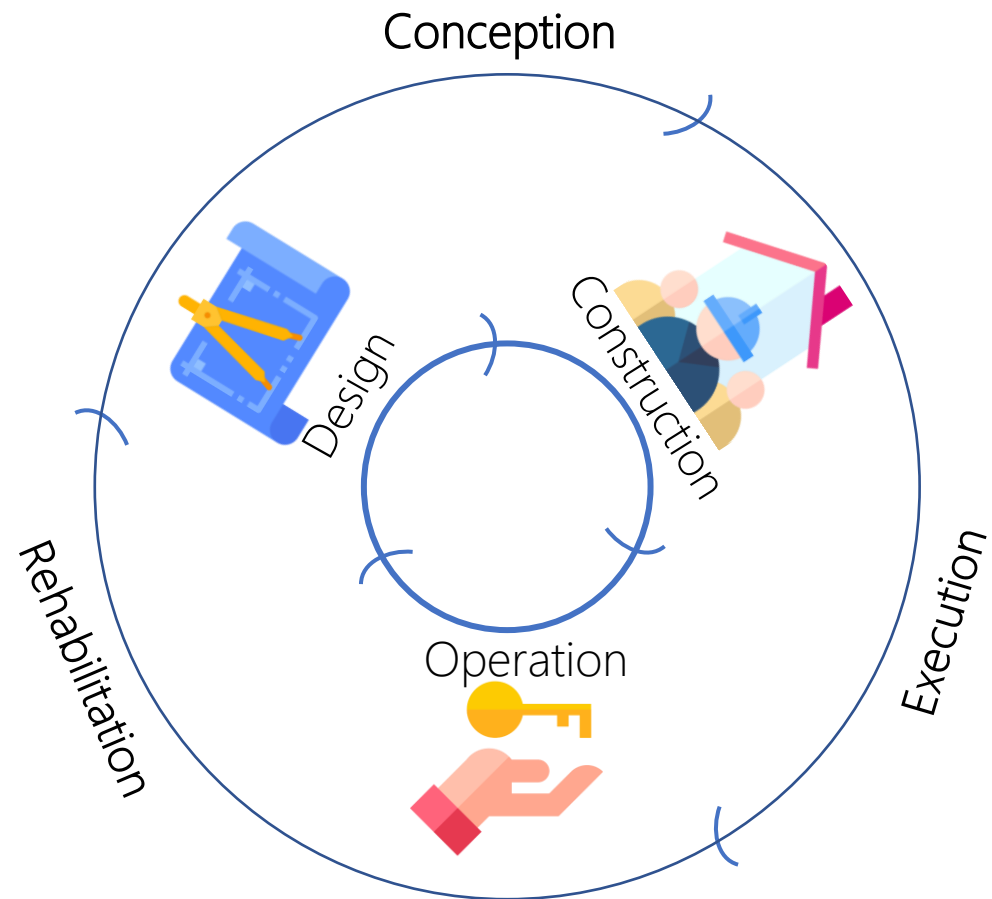


Economic growth

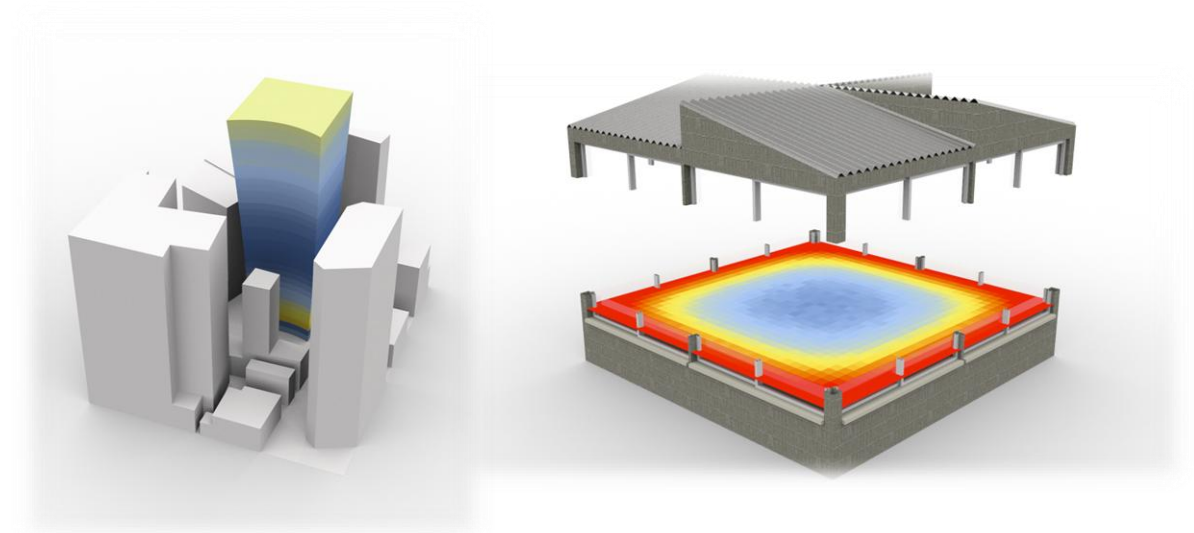


Sustainable goals



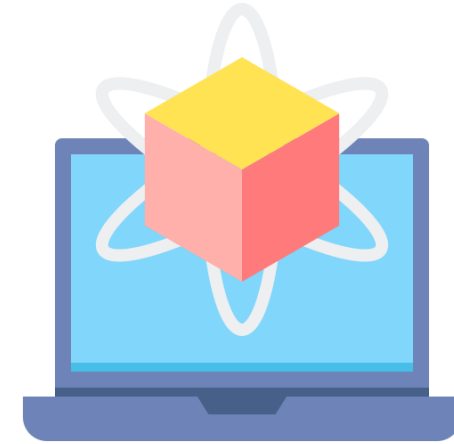
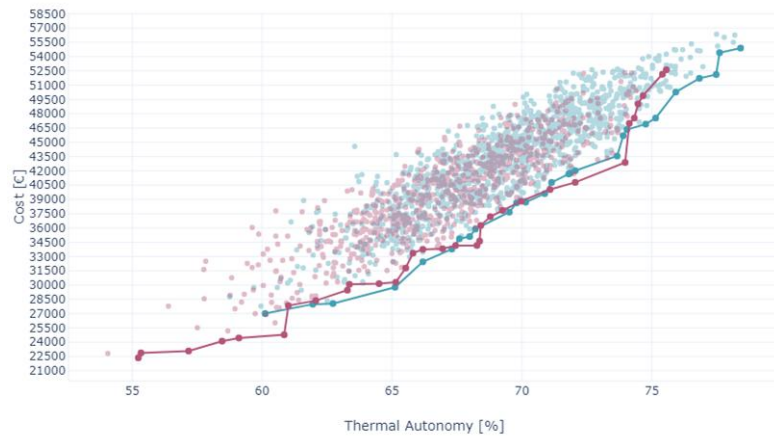


Building Performance Simulation tools

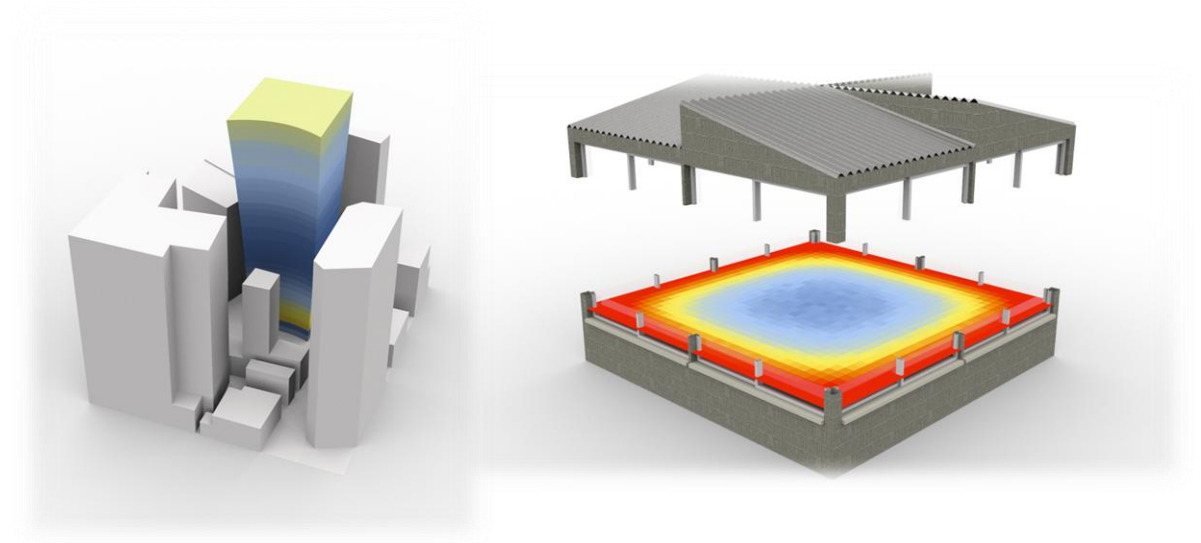




Analyses and Optimization Processes

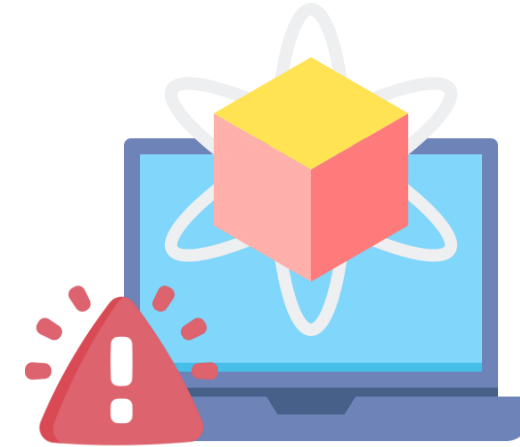


Building Performance Simulation tools





## Analyses and Optimization Processes



## Building Performance Simulation tools



Time consuming [1]



Portability [2]



Expertise [3]

[1] Wei, T. (2013). A review of sensitivity analysis methods in building energy analysis. *Renewable and Sustainable Energy Reviews*, 20, 411–419.

[2] Crawley, D. B., Hand, J. W., Kummert, M., & Griffith, B. T. (2008). Contrasting the capabilities of building energy performance simulation programs. *Building and Environment*, 43(4), 661–673.

[3] Wang, H., & Zhai, Z. (John). (2016). Advances in building simulation and computational techniques: A review between 1987 and 2014. *Energy and Buildings*, 128, 319–335.



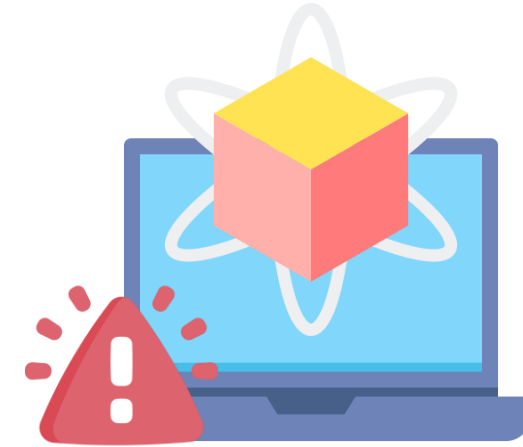
### Analyses and Optimization Processes



Multiple Objectives [4, 5]



Multiple Algorithms [5, 6]



### Building Performance Simulation tools



Time consuming [1]



Portability [2]



Expertise [3]

[4] Evins, R. (2013). A review of computational optimisation methods applied to sustainable building design. *Renewable and Sustainable Energy Reviews*, 22, 230–245.

[5] Nguyen, A., Reiter, S., & Rigo, P. (2014). A review on simulation-based optimization methods applied to building performance analysis. *Applied Energy*, 113, 1043–1058.

[6] Waibel, C., Wortmann, T., Evins, R., & Carmeliet, J. (2019). Building energy optimization: An extensive benchmark of global search algorithms. *Energy and Buildings*, 187, 218–240.

[1] Wei, T. (2013). A review of sensitivity analysis methods in building energy analysis. *Renewable and Sustainable Energy Reviews*, 20, 411–419.

[2] Crawley, D. B., Hand, J. W., Kummert, M., & Griffith, B. T. (2008). Contrasting the capabilities of building energy performance simulation programs. *Building and Environment*, 43(4), 661–673.

[3] Wang, H., & Zhai, Z. (John). (2016). Advances in building simulation and computational techniques: A review between 1987 and 2014. *Energy and Buildings*, 128, 319–335.



### Analyses and Optimization Processes



Multiple Objectives [4, 5]



Multiple Algorithms [5, 6]



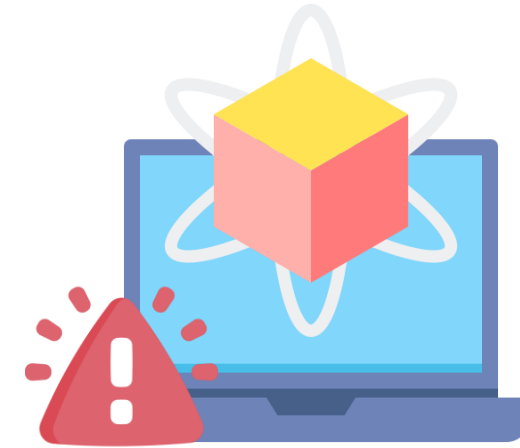
Time consuming [1]



Portability [2]



Expertise [3]



### Building Performance Simulation tools

[4] Evins, R. (2013). A review of computational optimisation methods applied to sustainable building design. *Renewable and Sustainable Energy Reviews*, 22, 230–245.

[5] Nguyen, A., Reiter, S., & Rigo, P. (2014). A review on simulation-based optimization methods applied to building performance analysis. *Applied Energy*, 113, 1043–1058.

[6] Waibel, C., Wortmann, T., Evins, R., & Carmeliet, J. (2019). Building energy optimization: An extensive benchmark of global search algorithms. *Energy and Buildings*, 187, 218–240.

[1] Wei, T. (2013). A review of sensitivity analysis methods in building energy analysis. *Renewable and Sustainable Energy Reviews*, 20, 411–419.

[2] Crawley, D. B., Hand, J. W., Kummert, M., & Griffith, B. T. (2008). Contrasting the capabilities of building energy performance simulation programs. *Building and Environment*, 43(4), 661–673.

[3] Wang, H., & Zhai, Z. (John). (2016). Advances in building simulation and computational techniques: A review between 1987 and 2014. *Energy and Buildings*, 128, 319–335.



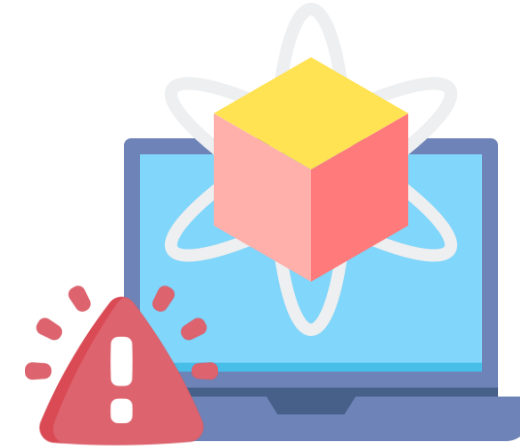
### Analyses and Optimization Processes



Multiple Objectives [4, 5]



Multiple Algorithms [5, 6]



### Building Performance Simulation tools



Time consuming [1]



Portability [2]



Expertise [3]

**How to efficiently integrate AOP with building and urban projects?**



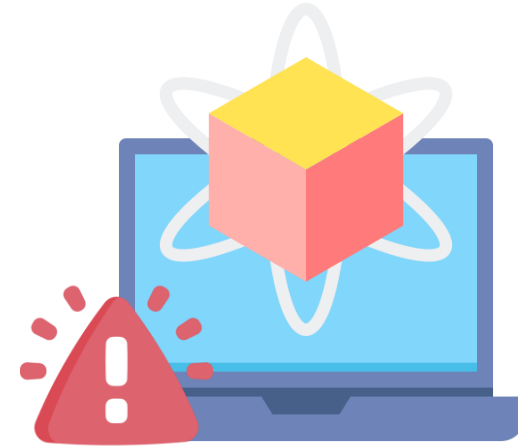
### Analyses and Optimization Processes



Multiple Objectives [4, 5]



Multiple Algorithms [5, 6]



### Building Performance Simulation tools



Time consuming [1]



Portability [2]



Expertise [3]

## How to efficiently integrate AOP with building and urban projects?

**Make it quicker**

**Make it portable**

**Make it easier**





## Algorithmic Design and Analysis



Automates Design, Analysis, and Optimization processes. [7]

[7] Aguiar, R., Cardoso, C., & Leitão, A. (2017). *Algorithmic design and analysis - fusing disciplines*. *Proceedings Catalog of the 37th Annual ACADIA 2017*, 28–37.

[9] Araújo, G., Pereira, I., Leitão, A., & Correia Guedes, M. (2021). *Conflicts in passive building performance: Retrofit and regulation of informal neighbourhoods*. *Frontiers of Architectural Research*, 10(3), 625–638.



## Algorithmic Design and Analysis



Automates Design, Analysis, and Optimization processes. [7]

BPS are still time-consuming for large models. [8]

Additional expertise to learn a programming language. [7]

[7] Aguiar, R., Cardoso, C., & Leitão, A. (2017). *Algorithmic design and analysis - fusing disciplines*. *Proceedings Catalog of the 37th Annual ACADIA 2017*, 28–37.

[9] Araújo, G., Pereira, I., Leitão, A., & Correia Guedes, M. (2021). *Conflicts in passive building performance: Retrofit and regulation of informal neighbourhoods*. *Frontiers of Architectural Research*, 10(3), 625–638.



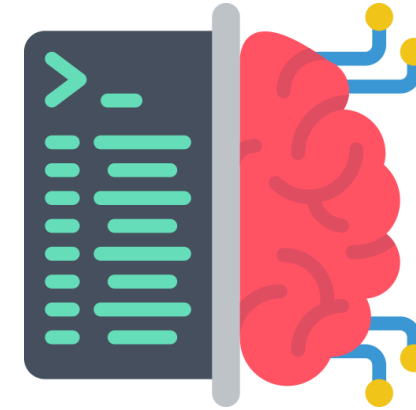
### Algorithmic Design and Analysis



Automates Design, Analysis, and Optimization processes. [7]

BPS are still time-consuming for large models. [8]

Additional expertise to learn a programming language. [7]



### Surrogate Models



Quickly predict BPS outputs with fewer inputs. [10]

[7] Aguiar, R., Cardoso, C., & Leitão, A. (2017). *Algorithmic design and analysis - fusing disciplines*. *Proceedings Catalog of the 37th Annual ACADIA 2017*, 28–37.

[9] Araújo, G., Pereira, I., Leitão, A., & Correia Guedes, M. (2021). *Conflicts in passive building performance: Retrofit and regulation of informal neighbourhoods*. *Frontiers of Architectural Research*, 10(3), 625–638.

[10] Wortmann, T., Costa, A., Nannicini, G., & Schroepfer, T. (2015). *Advantages of surrogate models for architectural design optimization*. *Artificial Intelligence for Engineering Design, Analysis and Manufacturing*, 29(4), 471–481.

[11] Alizadeh, R., Allen, J. K., & Mistree, F. (2020). *Managing computational complexity using surrogate models: a critical review*. *Research in Engineering Design*, 31(3), 275–298.



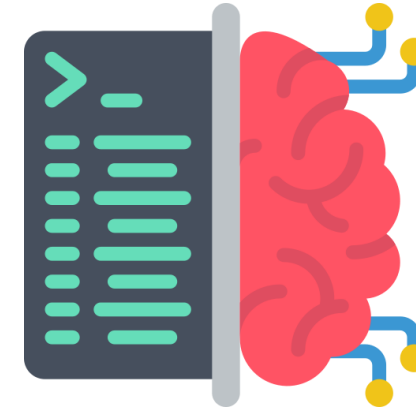
### Algorithmic Design and Analysis



Automates Design, Analysis, and Optimization processes. [7]

BPS are still time-consuming for large models. [8]

Additional expertise to learn a programming language. [7]



### Surrogate Models



Quickly predict BPS outputs with fewer inputs. [10]

Are usually case-specific and do not apply outside the study's boundaries. [11]

Reduces BPS expertise but requires expertise to develop and test the models. [10]

[7] Aguiar, R., Cardoso, C., & Leitão, A. (2017). *Algorithmic design and analysis - fusing disciplines*. *Proceedings Catalog of the 37th Annual ACADIA 2017*, 28–37.

[9] Araújo, G., Pereira, I., Leitão, A., & Correia Guedes, M. (2021). *Conflicts in passive building performance: Retrofit and regulation of informal neighbourhoods*. *Frontiers of Architectural Research*, 10(3), 625–638.

[10] Wortmann, T., Costa, A., Nannicini, G., & Schroepfer, T. (2015). *Advantages of surrogate models for architectural design optimization*. *Artificial Intelligence for Engineering Design, Analysis and Manufacturing*, 29(4), 471–481.

[11] Alizadeh, R., Allen, J. K., & Mistree, F. (2020). *Managing computational complexity using surrogate models: a critical review*. *Research in Engineering Design*, 31(3), 275–298.



Flexible framework to develop Surrogate Models and integrate them with AOP.

Motivation

Context

Research Questions

Methodology

Case Studies

Discussion



Flexible framework to develop Surrogate Models and integrate them with AOP.



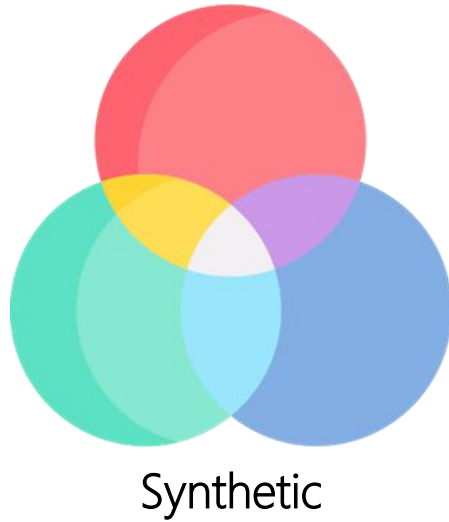
Synthetic



Iterative



Existing



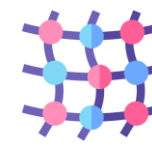
$$f(x_1, x_2, \dots, x_n) = y$$

$$f\left(\begin{bmatrix} x_{11} & \cdots & x_{1n} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mn} \end{bmatrix}\right) = \begin{bmatrix} y_1 \\ \vdots \\ y_m \end{bmatrix}$$

where  $m$  represents combinations of the features' domain



Building  
Archetypes



Features'  
domain



Simulation

We can develop multiple building models that vary along specified domains of different features, simulate them, and build a database.



Comprehensive feedback of the features impact in simulation results.

Surrogate Models for multiple analysis and optimization problems.

Highly detailed database.



Simulation and computation times exponentially increase with the number of features and simulation types, to the point of being unfeasible.



Iterative

$$f(x_1, x_2, \dots, x_i) = \min(o_1, o_2, \dots, o_j)$$

$$f\left(\begin{bmatrix} x_{11} & \cdots & x_{1i} \\ \vdots & \ddots & \vdots \\ x_{m1} & \cdots & x_{mi} \end{bmatrix}\right) = \begin{bmatrix} o_{11} & \cdots & o_{1j} \\ \vdots & \ddots & \vdots \\ o_{m1} & \cdots & o_{mj} \end{bmatrix}$$

where  $m$  represents the number of iterations in the optimization



We can develop building optimization problems and build a database from the explored solutions' variables and objectives.



Less computational time than feature domains depending on the number of iterations.

Can support a high number of features.

Can support a high number of objectives.



Specific to the optimization problem at hand.





Existing



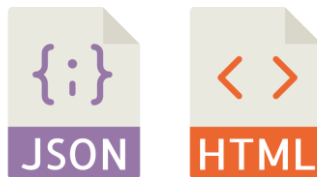
Extract



Cleaning

Analyses and  
Optimization

Extract building features from existing building databases and develop surrogate models for multiple AOP.



Database with real values.

Might not require simulations.

Surrogate Models for multiple analysis and optimization problems.



Noisy and imbalanced data.

Often does not feature many objectives.

## Surrogate Models



Model type



Model tuning



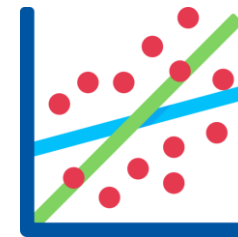
Model deployment



Model type



Classification Models



Regression Models



## Model type

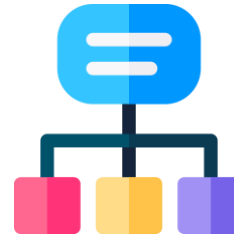
### Key Performance Indicators

Accuracy

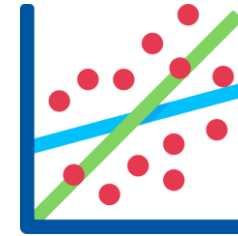
Precision

Recall

F1-score



Classification Models



Regression Models

Models that predict **discrete** target outputs.



Neural Networks



Logistic regression



Ensemble models



## Model type

### Key Performance Indicators

Accuracy

Mean Absolute Error (MAE)

Precision

Mean Squared Error (MSE)

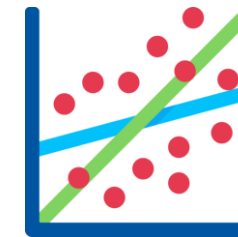
Recall

Mean Average Percent Error (MAPE)

F1-score

Coefficient of determination ( $R^2$  score)

Classification Models



Regression Models

Models that predict **discrete** target outputs.



Neural Networks



Logistic regression



Ensemble models

Models that predict **continuous** target outputs.



Neural Networks



Linear regression



Ensemble models



Interpolation



## Model tuning

### Key Performance Indicators

Accuracy

Mean Absolute Error (MAE)

Precision

Mean Squared Error (MSE)

Recall

Mean Average Percent Error (MAPE)

F1-score

Coefficient of determination ( $R^2$  score)



## Model tuning

### Key Performance Indicators

Accuracy	Mean Absolute Error (MAE)
Precision	Mean Squared Error (MSE)
Recall	Mean Average Percent Error (MAPE)
F1-score	Coefficient of determination ( $R^2$ score)



## Feature Engineering



## Hyperparameter optimization



## Model tuning

### Key Performance Indicators

Accuracy

Mean Absolute Error (MAE)

Precision

Mean Squared Error (MSE)

Recall

Mean Average Percent Error (MAPE)

F1-score

Coefficient of determination ( $R^2$  score)

### Feature Engineering

Clean, change, and develop features



Clean outliers



Create new features



Select relevant features



### Hyperparameter optimization





Model tuning

Key Performance Indicators

Accuracy	Mean Absolute Error (MAE)
Precision	Mean Squared Error (MSE)
Recall	Mean Average Percent Error (MAPE)
F1-score	Coefficient of determination ( $R^2$ score)



Feature Engineering

Clean, change, and develop features



Clean outliers



Create new features



Select relevant features



Hyperparameter optimization

Optimize the model's parameters for best suitable KPI

Neural Networks

Solver

Learning rate

Hidden layer sizes

Linear regression

Polynomial degree

Ensemble models

Number of estimators

Depth

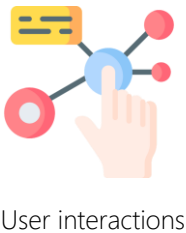
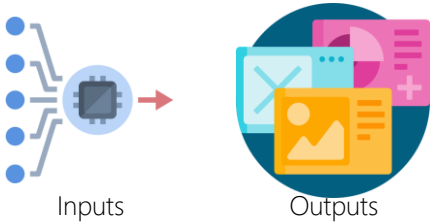
Samples split

Interpolation

Solver



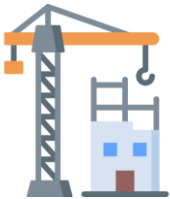
Model deployment



Case studies with different AOP and BID



Design



Construction



Retrofit



Synthetic



Optimization



Existing



Model deployment



3D Models



Programming



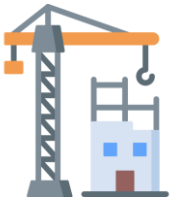
Web App



Case studies with different AOP and BID



Design



Construction



Retrofit



Synthetic



Optimization



Existing

# Case Studies

*Surrogate Models to improve Building  
Performance Analysis and Optimization*



Synthetic



Retrofit



Design

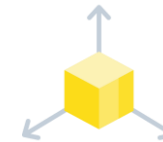


Urban area in Lisbon



Data is retrieved from GIS file by extraction of the buildings':

Construction period	Number	Wall U_Value (kWh/m <sup>2</sup> )	Roof U_Value (W/m <sup>2</sup> ·°C)	Floor U_Value (W/m <sup>2</sup> ·°C)	Window U_Value (W/m <sup>2</sup> ·°C)	Wall retrofit U-value (W/m <sup>2</sup> ·°C)	Roof retrofit U-value (W/m <sup>2</sup> ·°C)
<1919	1	2.78	1.99	1.80	2.69	0.61	0.63
1919-1945	2	2.78	1.99	1.80	2.69	0.61	0.63
1946-1960	3	1.49	1.99	1.80	2.69	0.57	0.63
1961-1970	4	1.08	1.99	3.03	2.69	0.49	0.63
1971-1980	5	1.26	1.99	3.03	2.69	0.53	0.63
1981-1990	6	0.50	1.99	3.03	2.69	0.32	0.63
1991-1995	7	0.49	1.99	3.03	2.69	0.32	0.63
1996-2000	8	0.46	1.99	2.31	2.69	0.29	0.63
2001-2005	9	0.25	1.99	2.31	2.69	0.19	0.63
>2006	10	0.25	1.99	2.31	2.69	0.19	0.63



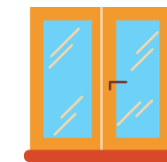
Geometry



Number of Floors



Age



Glazing ratio

## Motivation

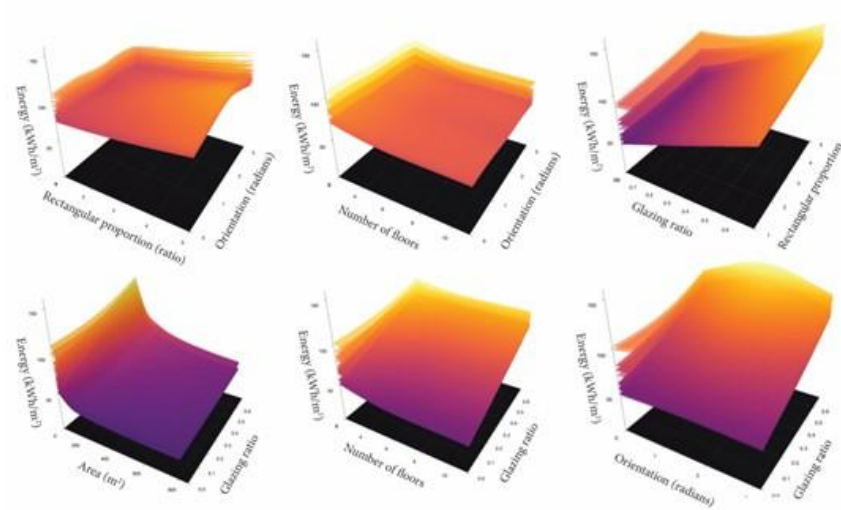
## Context

## Research Questions

## Methodology

## Case Studies

## Discussion



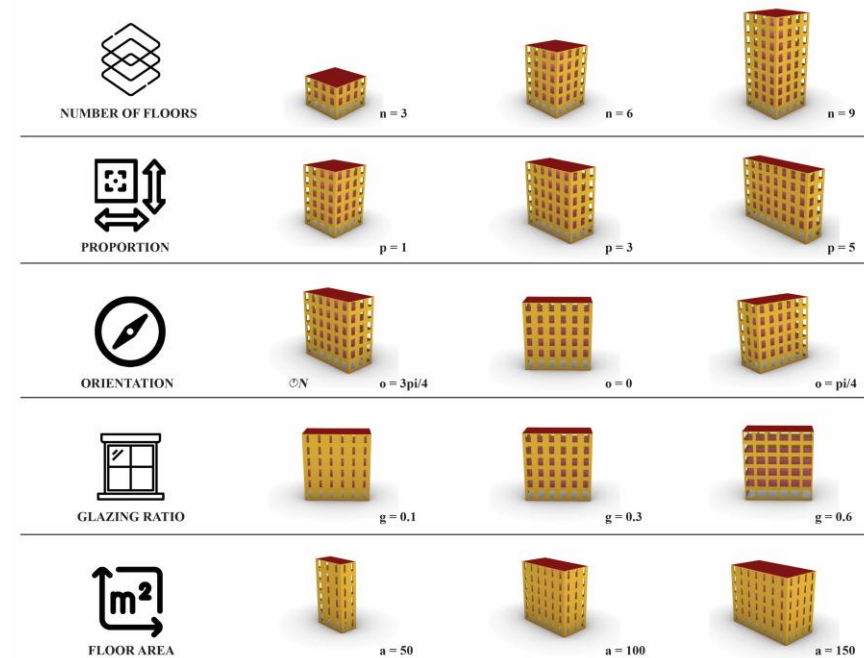
$$E(c, n, p, o, g, a) = \text{Annual Energy Loads [kWh/m}^2\text{]}$$

$$f \left( \begin{bmatrix} c_1 & n_1 & p_1 & o_1 & g_1 & a_1 \\ c_1 & n_1 & p_1 & o_1 & g_1 & a_1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c_i & n_i & p_i & o_i & g_i & a_i \end{bmatrix} \right) = \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_i \end{bmatrix}$$

Synthetic



Create a dataset that encompasses a grid-based set of feature values.





Linear regression



Interpolation



Ensemble models

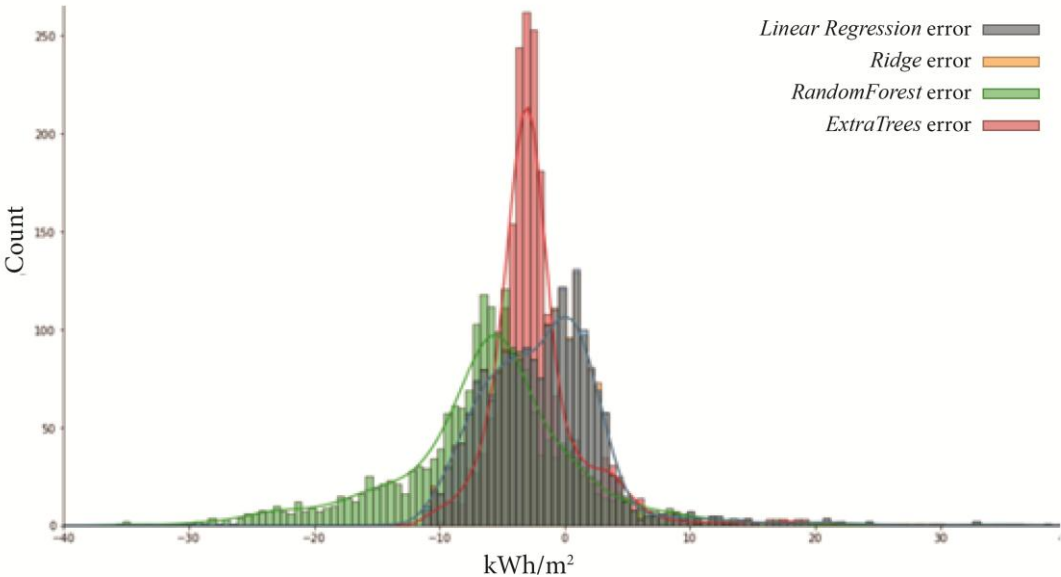
	Linear Regression	Ridge	Random Forest	Extra Trees
Mean Error (kWh/m <sup>2</sup> )	15.85	15.79	-6.06	-2.21
Root Mean Squared Error (kWh/m <sup>2</sup> )	15.40	15.40	9.88	5.44
R <sup>2</sup> score	0.64	0.64	0.85	0.95

Regression Models



Results are used to train Surrogate models.

The case study simulation results are used to validate and select the best model:





Linear regression



Interpolation



Ensemble models

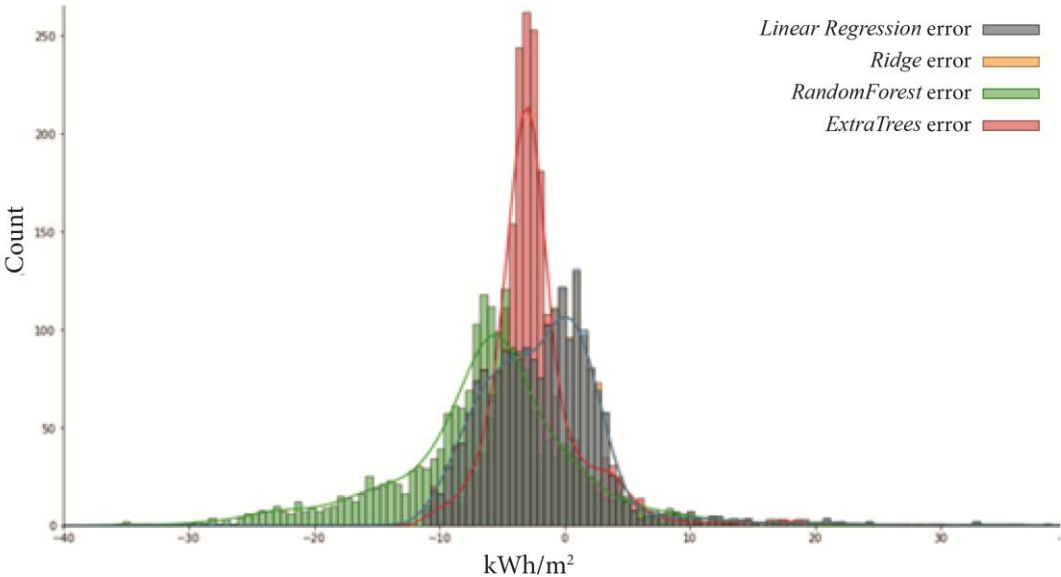
	Linear Regression	Ridge	Random Forest	Extra Trees
Mean Error (kWh/m²)	15.85	15.79	-6.06	-2.21
Root Mean Squared Error (kWh/m²)	15.40	15.40	9.88	5.44
R² score	0.64	0.64	0.85	0.95

Regression Models

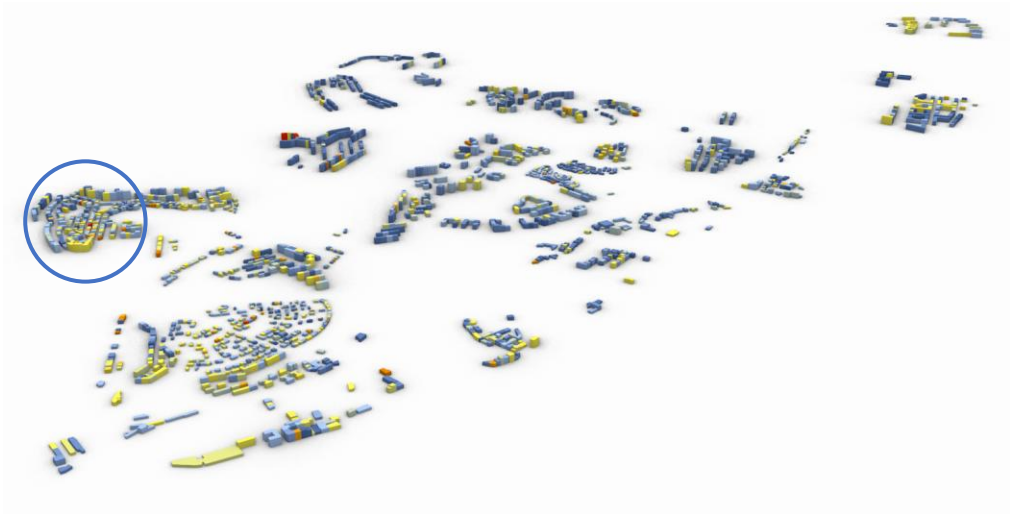


Results are used to train Surrogate models.

The case study simulation results are used to validate and select the best model:







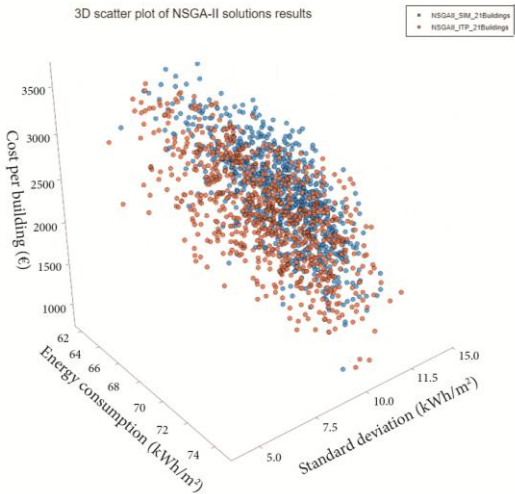
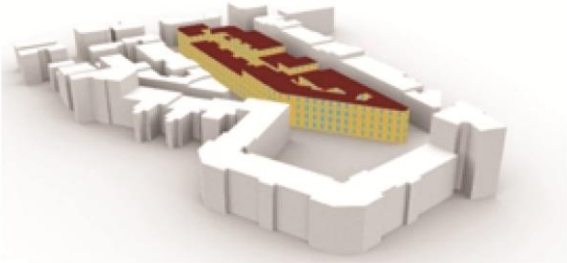
ExtraTrees regressor

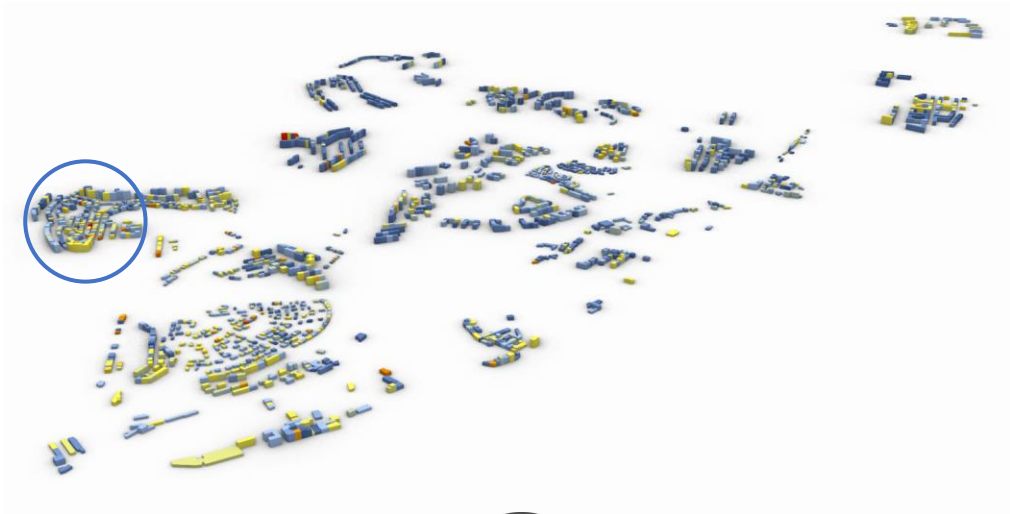


$$\frac{\sum_{i=1}^n \text{annual loads}_i}{n} [kWh/m^2]$$

$$\sigma \left( \bigcup_{i=1}^n \text{annual loads}_i \right) [kWh/m^2]$$

$$\frac{\sum_{i=1}^n \text{Cost}_i}{n} [€]$$





Speed up  
factor of 85x

	elapsed time (seconds)	
	Dataset simulation	Optimization
Surrogate model	0.08	791.99
Simulation	5820.00	67516.70

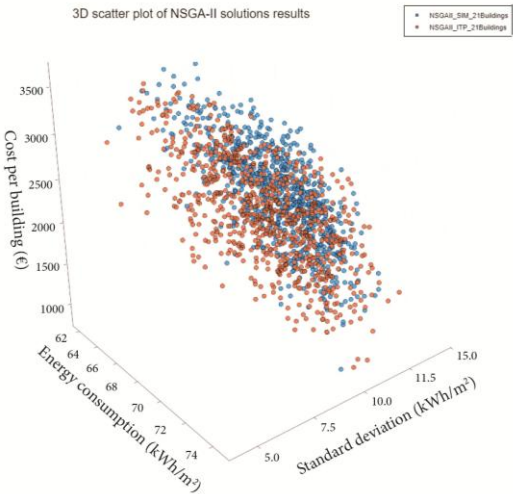
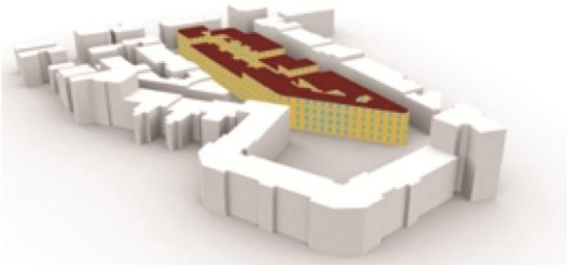
ExtraTrees regressor



$$\frac{\sum_{i=1}^n \text{annual loads}_i}{n} [kWh/m^2]$$

$$\sigma \left( \bigcup_{i=1}^n \text{annual loads}_i \right) [kWh/m^2]$$

$$\frac{\sum_{i=1}^n Cost_i}{n} [€]$$




Below you can download the Example upload file:

Download sample data as CSV

Below are the construction typologies information that you can download via csv file:

Download constructions as CSV

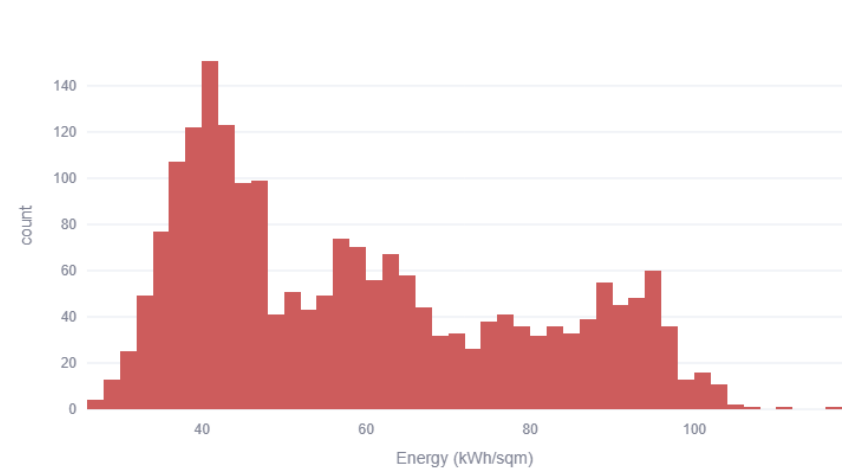
Input CSV file with all the buildings you want to test as seen in the example file above



Drag and drop file here  
Limit 200MB per file

Browse files

Predict annual energy loads



ExtraTrees regressor



Model is deployed in a web app prototype



Prediction of input buildings' energy use



Optimization of building design

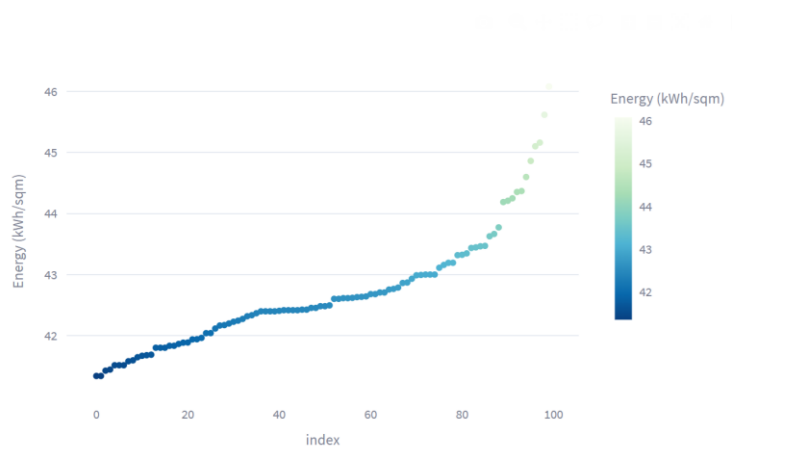
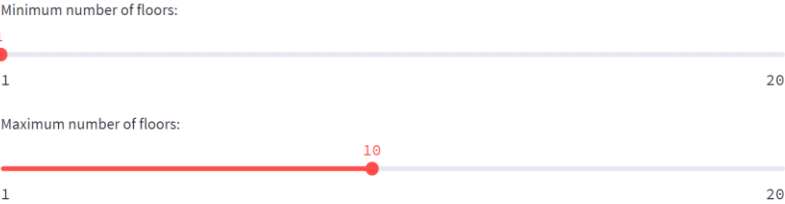
Building design Optimization

In this section you can select the design variables and their boundaries for a building and optimize its values for minimum annual energy loads

Select the design variables you wish to optimize:

Number of floors × Rectangular pro... × Orientation (Rad... × Floor area (sqm) ×

Number of floors - boundaries



ExtraTrees regressor



Model is deployed in a web app prototype



Prediction of input buildings' energy use



Optimization of building design

# Results

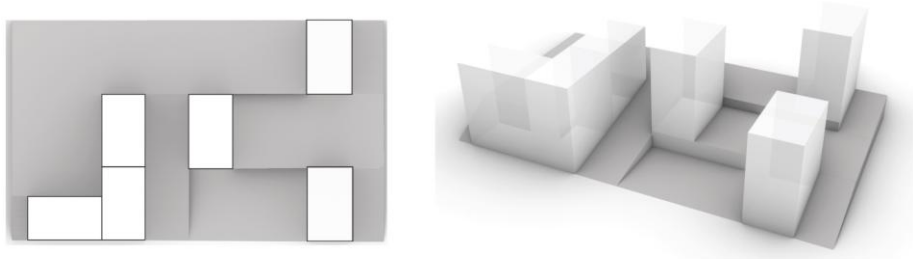
*Surrogate Models to improve Building  
Performance Analysis and Optimization*



Iterative



Construction



Optimization of construction materials for a 6 building block design



## Variables:

$$(w, r, f, w_i) \in \{0, 1, 2\}$$

$w \rightarrow$  wall possible constructions

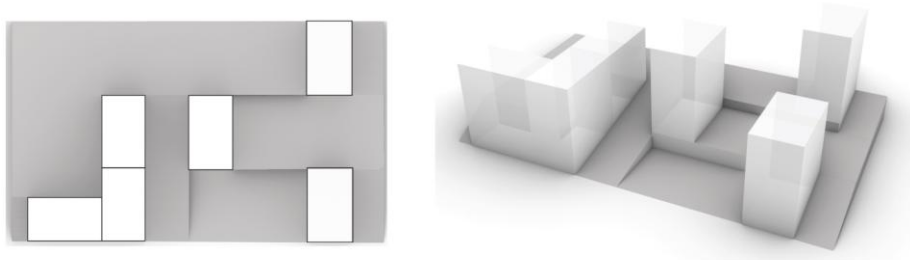
$r \rightarrow$  roof possible constructions

$f \rightarrow$  floor possible constructions

$w_i \rightarrow$  window possible constructions

Use previous iterations of a simulation-based optimization to train surrogate models capable of predicting the specified objectives

$$g \left( \begin{bmatrix} (w, r, f, w_i)_{11} & \cdots & (w, r, f, w_i)_{1n} \\ \vdots & \ddots & \vdots \\ (w, r, f, w_i)_i & \cdots & (w, r, f, w_i)_{in} \end{bmatrix} \right) = \begin{bmatrix} f_{11} & f_{21} & f_{31} \\ \vdots & \vdots & \vdots \\ f_{1i} & f_{2i} & f_{3i} \end{bmatrix}$$



Optimization of construction materials for a 6 building block design

## Objectives:

$$f_1(w, r, f, w_i) = \sum_{i=1}^n Heating_i + Cooling_i$$

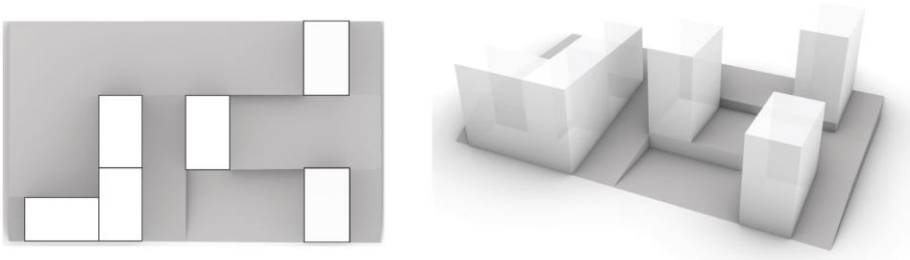
$$f_2(w, r, f, w_i) = \sigma \left( \bigcup_{i=1}^n Heating_i + Cooling_i \right)$$

$$f_3(w, r, f, w_i) = \sum_{i=1}^n Cost_i$$



Use previous iterations of a simulation-based optimization to train surrogate models capable of predicting the specified objectives

$$g \left( \begin{bmatrix} (w, r, f, w_i)_{11} & \cdots & (w, r, f, w_i)_{1n} \\ \vdots & \ddots & \vdots \\ (w, r, f, w_i)_i & \cdots & (w, r, f, w_i)_{in} \end{bmatrix} \right) = \begin{bmatrix} f_{11} & f_{21} & f_{31} \\ \vdots & \vdots & \vdots \\ f_{1i} & f_{2i} & f_{3i} \end{bmatrix}$$

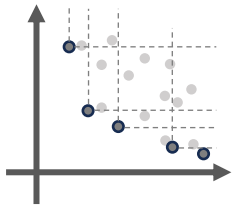


Optimization of construction materials for a 6 building block design

Objectives:

$$f_4(i_0, \dots, i_n) = R^2(\text{test}, \text{predictions})$$

$i \in [6, 300]$  —Number of filters  
 $n = \text{Number of layers}$



$H(f_1, f_2, f_3)$

- $f_1 \in [\min(f_1), \max(f_1)]$
- $f_2 \in [\min(f_2), \max(f_2)]$
- $f_3 \in [\min(f_3), \max(f_3)]$

Hyperparameter optimization



Maximize a Neural Network’s  $R^2$  score and the optimization algorithms’ Hypervolume of non-dominated solutions.



Neural Network Sequential model



Metaheuristics



Motivation

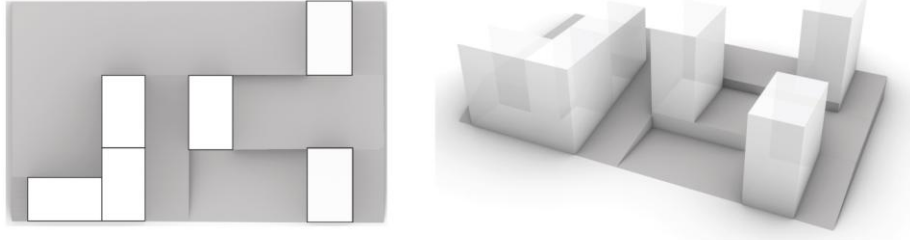
Context

Research Questions

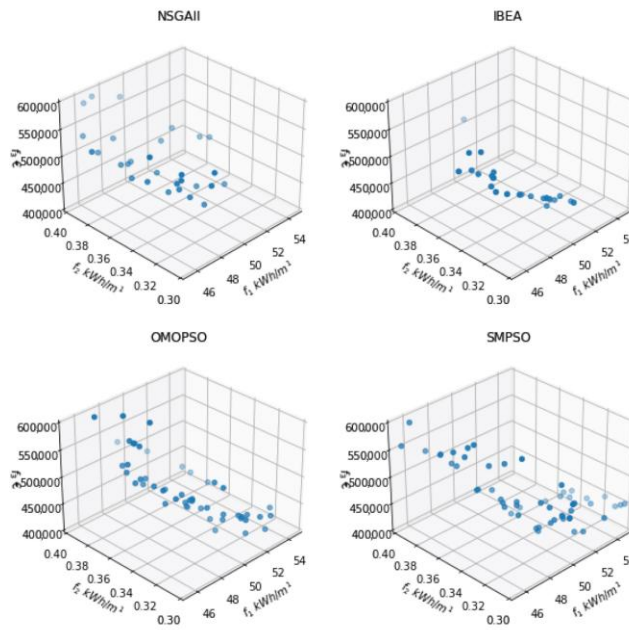
Methodology

Case Studies

Discussion



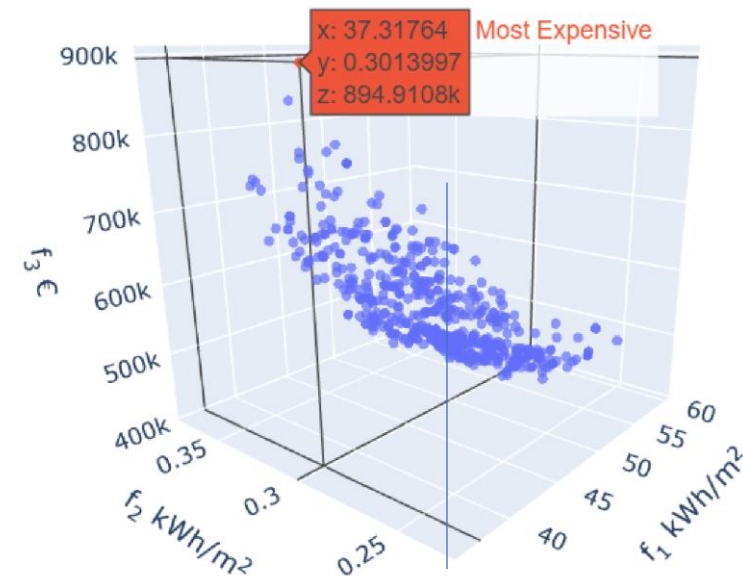
Optimization of construction materials for a 6 building block design

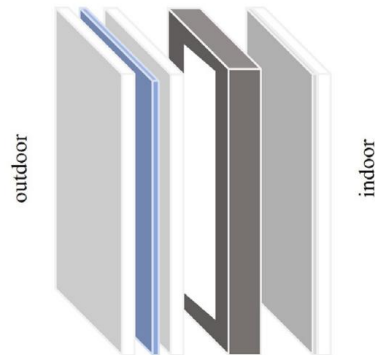
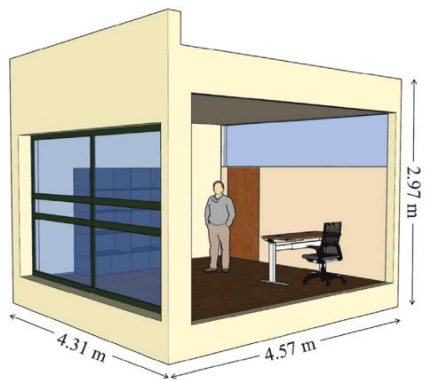


Neural Network Sequential model



Model is deployed in a programming environment where a user can upload a building design solution, specify the variables and run the optimization with different algorithms



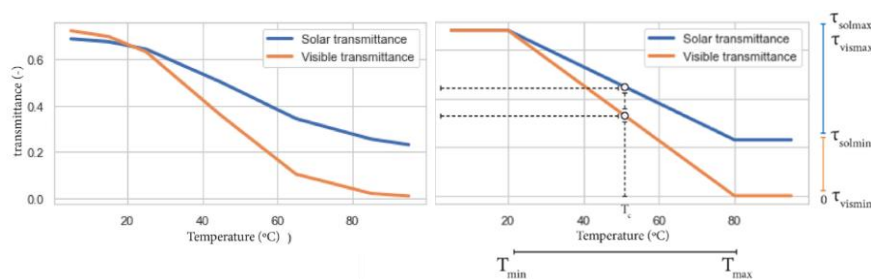


Optimization of Thermochromic glazing properties for an office space

Iterative



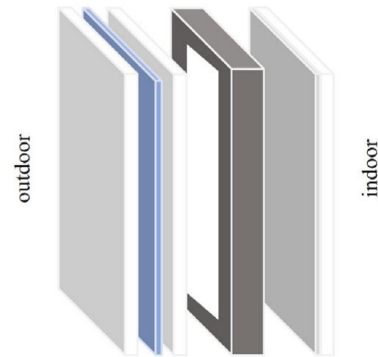
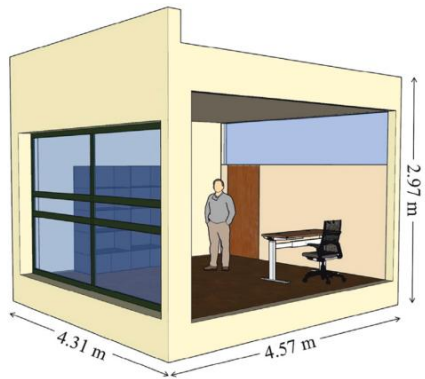
## Variables:



$$\tau_{sol}(T, T_{min}, T_{max}, \tau_{solmax}, \tau_{solmin}) = \begin{cases} \tau_{solmax} & \text{if } T \leq T_{min} \\ \tau_{solmax} - \frac{\tau_{solmax} - \tau_{solmin}}{(T_{max} - T_{min})} \times (T - T_{min}) & \text{if } T_{min} < T < T_{max} \\ \tau_{solmin} & \text{if } T \geq T_{max} \end{cases}$$

Use previous iterations of a simulation-based optimization to train surrogate models capable of predicting the specified objectives

$$g \left( \begin{bmatrix} T_{max1} & T_{min1} & \tau_{min1} & \tau_{max1} \\ T_{max2} & T_{min2} & \tau_{min2} & \tau_{max2} \\ \vdots & \vdots & \vdots & \vdots \\ T_{maxi} & T_{mini} & \tau_{mini} & \tau_{maxi} \end{bmatrix} \right) = \begin{bmatrix} f_{11} & f_{21} \\ f_{12} & f_{22} \\ \vdots & \vdots \\ f_{1i} & f_{2i} \end{bmatrix}$$



Optimization of Thermochromic glazing properties for an office space

## Objectives:

$$f_1(T_{min}T_{max}\tau_{min}\tau_{max}) = \text{Heating} + \text{Cooling} [kWh/m^2]$$

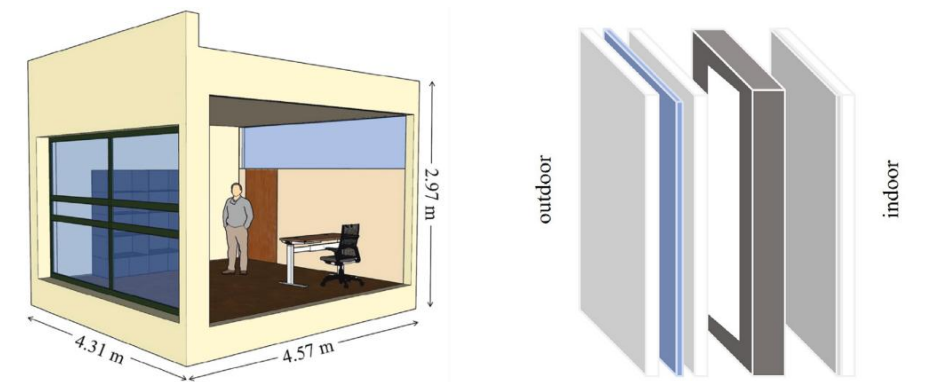
$$f_2(T_{min}T_{max}\tau_{min}\tau_{max}) = \text{Lighting} [kWh/m^2]$$

Iterative



Use previous iterations of a simulation-based optimization to train surrogate models capable of predicting the specified objectives

$$g \left( \begin{bmatrix} T_{max1} & T_{min1} & \tau_{min1} & \tau_{max1} \\ T_{max2} & T_{min2} & \tau_{min2} & \tau_{max2} \\ \vdots & \vdots & \vdots & \vdots \\ T_{maxi} & T_{mini} & \tau_{mini} & \tau_{maxi} \end{bmatrix} \right) = \begin{bmatrix} f_{11} & f_{21} \\ f_{12} & f_{22} \\ \vdots & \vdots \\ f_{1i} & f_{2i} \end{bmatrix}$$

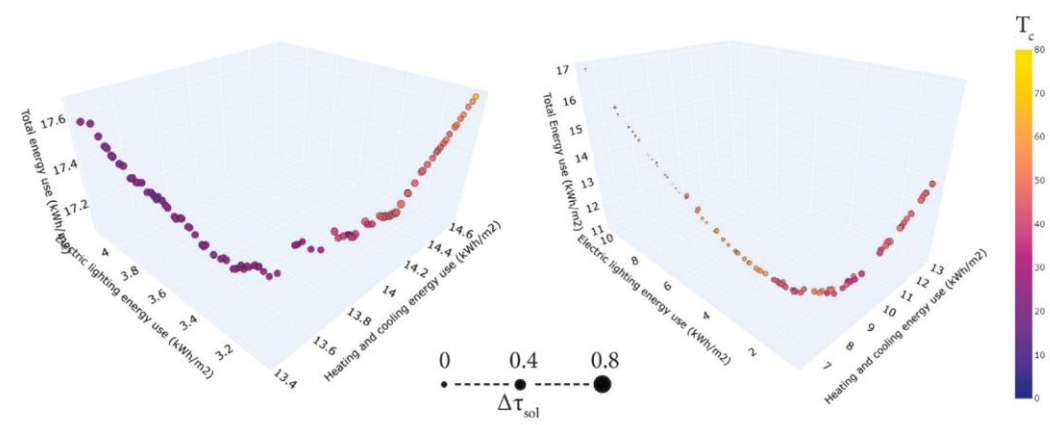


Optimization of Thermochromic glazing properties for an office space

ExtraTrees regressor



Model is deployed in a programming environment where the user can upload weather file, specify variable boundaries and run the optimizations



$$g \left( \begin{bmatrix} T_{max_1} & T_{min_1} & \tau_{min_1} & \tau_{max_1} \\ T_{max_2} & T_{min_2} & \tau_{min_2} & \tau_{max_2} \\ \vdots & \vdots & \vdots & \vdots \\ T_{max_i} & T_{min_i} & \tau_{min_i} & \tau_{max_i} \end{bmatrix} \right) = \begin{bmatrix} f_{11} & f_{21} \\ f_{12} & f_{22} \\ \vdots & \vdots \\ f_{1i} & f_{2i} \end{bmatrix}$$

# Results

*Surrogate Models to improve Building  
Performance Analysis and Optimization*



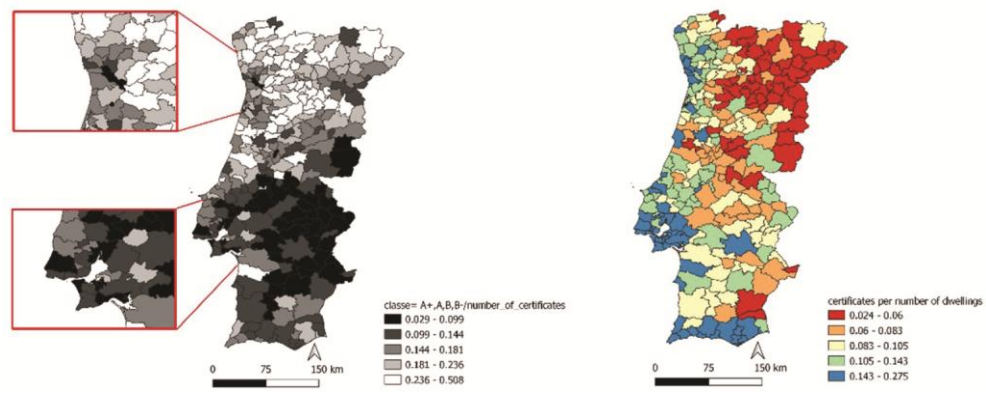
Existing



Retrofit



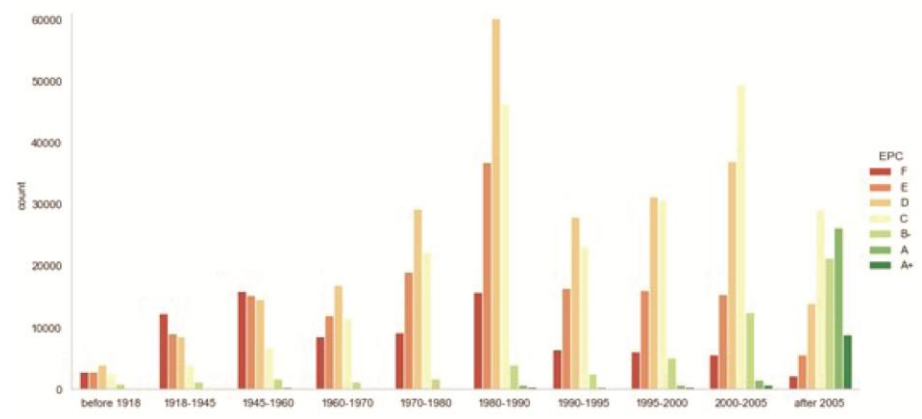
Design



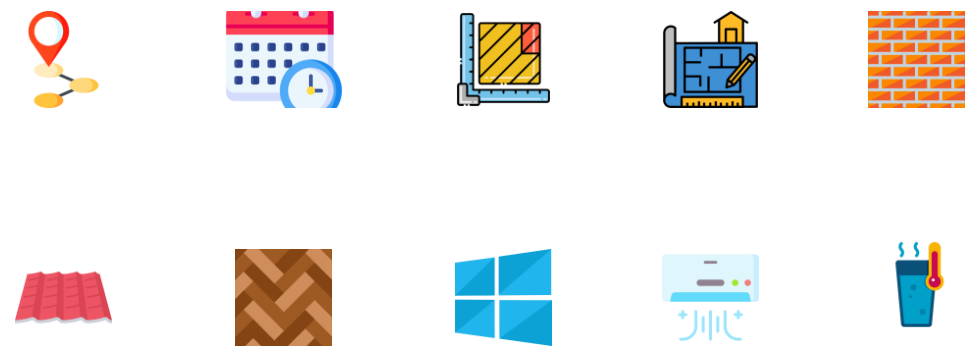
Portugal's Energy Performance Certificates (EPC)

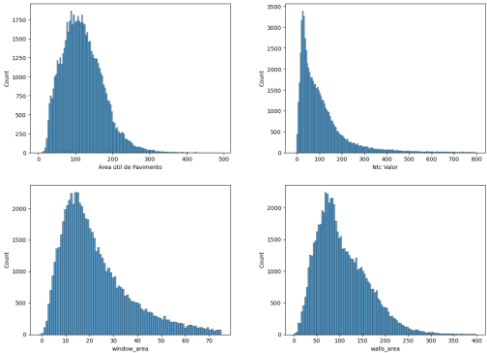


Data is retrieved from csv file by extraction of the certificates' features:



EPC labels histogram by construction period

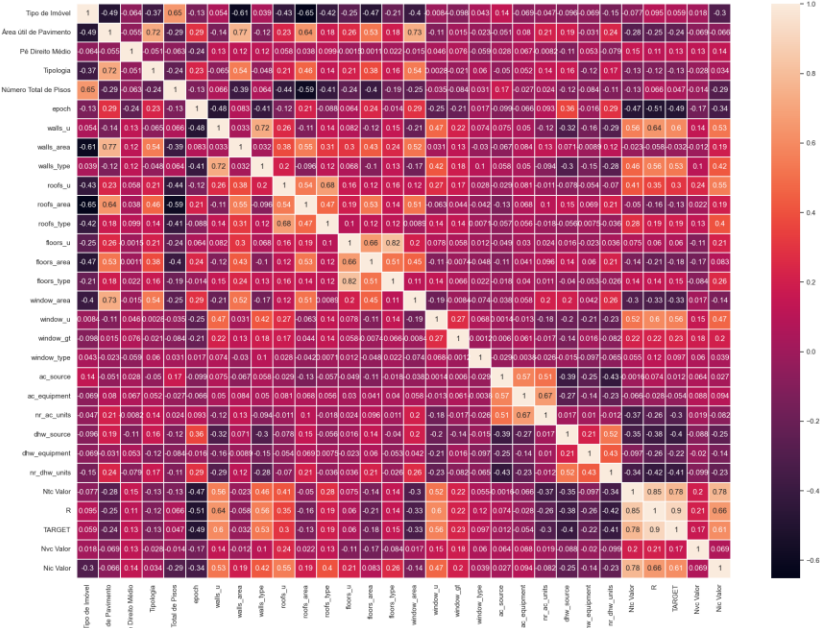




Feature Engineering



Apply feature engineering to obtain a balanced database for both features and prediction targets:



Create new features

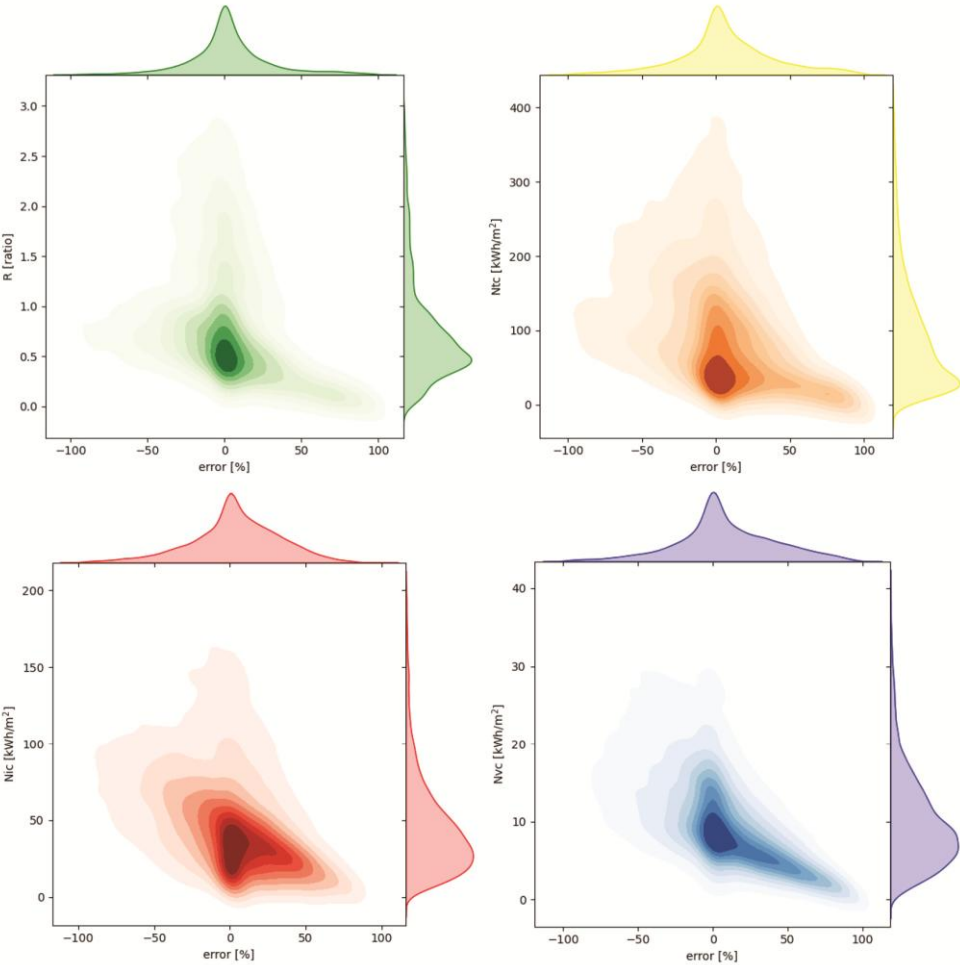


Clean outliers



Select relevant features





Regression Models



Results are used to train Surrogate models and select the best one between the lower number of features and higher  $R^2$  score.

Model training and performance indicators results.

k-best features	Model	R [ratio]		Ntc [kWh/m <sup>2</sup> ]		Nic [kWh/m <sup>2</sup> ]		Nvc [kWh/m <sup>2</sup> ]	
		$R^2$	$RMSE$	$R^2$	$RMSE$	$R^2$	$RMSE$	$R^2$	$RMSE$
10	ET	0.74	0.26	0.58	55.70	0.61	19.11	0.31	5.85
	MLP	0.71	0.27	0.51	60.22	0.55	20.46	0.16	6.43
	GB	0.69	0.28	0.50	60.98	0.53	20.89	0.14	6.51
15	ET	0.82	0.22	0.72	45.30	0.65	18.07	0.36	5.63
	MLP	0.77	0.24	0.66	49.91	0.57	20.05	0.19	6.33
	GB	0.76	0.25	0.65	51.07	0.57	20.01	0.17	6.39
20	ET	0.84	0.21	0.79	39.77	0.67	17.70	0.41	5.41
	MLP	0.78	0.24	0.72	45.29	0.58	19.77	0.23	6.15
	GB	0.78	0.24	0.73	44.87	0.57	19.96	0.24	6.14
25	ET	0.85	0.20	0.80	38.83	0.73	15.96	0.61	4.40
	MLP	0.80	0.23	0.74	44.33	0.67	17.66	0.47	5.11
	GB	0.80	0.23	0.75	43.19	0.68	17.22	0.33	5.75



General details

Location

EVORA

Type of certificate

Horizontal property

Floor location of your house

Last

Total number of floors in your building

2

Construction period

between 1996 and 2000

Area


100


Floor height

2.80

Typology


T3






Cooling energy (kWh/year)

4 k



Heating energy (kWh/year)

9 k



Total energy (kWh/year)

20 k

Predict energy indicators!

Economic details

Here you can stipulate your maximum rehabilitation budget

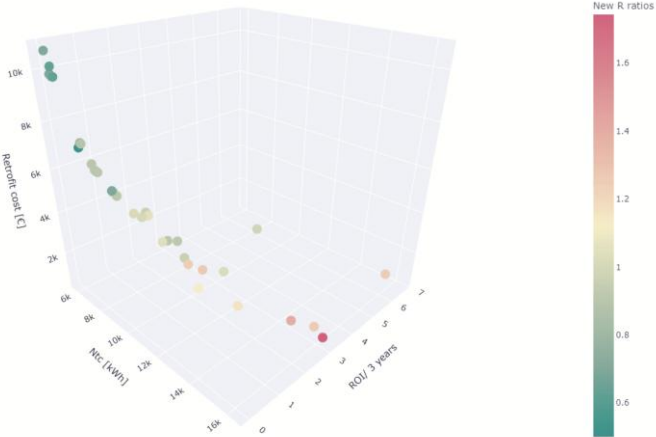
2000

Presently, how much do you pay for housing taxes?

300

☒ If you do not want to provide this information, the tool can estimate a value based on the information provided.

Click here to start



ExtraTrees Regressor with 20 features



Model is deployed in a web app prototype for the optimization of building retrofit for:



Homeowners




Policymaking

$$f\left(\begin{bmatrix} r_1 & \cdots & r_n \\ \vdots & \ddots & \vdots \\ r_i & \cdots & r_{in} \end{bmatrix}\right) = \begin{bmatrix} f_{1_1} & f_{2_1} & f_{3_1} \\ \vdots & \vdots & \vdots \\ f_{1_i} & f_{2_i} & f_{3_i} \end{bmatrix}$$

$$f_1 = Ntc \text{ [kWh/m}^2\text{]} \quad f_2 = \text{Return on investment [ratio]} \quad f_3 = \text{Retrofit cost [€]}$$

Building data upload

Here you can upload the .csv file filled in as shown in "template\_upload.csv", but with your buildings  
Input CSV file with all the buildings you want to optimize

 Drag and drop file here  
Limit 200MB per file

Browse files

Predict annual energy loads

Optimization

Here you can define the optimization problem variables, algorithm, and their parameters

Variables

Select Retrofits from government's retrofit available funding list

Wall insulation (...) x Floor insulation x Roof insulation (...) x

Window replace... x Air-to-water pump x Efficient AC units x

Solar panels for ... x Solar panels for ... x

Retrofit costs

Wall retrofit cost (€/sqm)  
70 - +

Floor retrofit cost (€/sqm)  
30 - +

Roof retrofit cost (€/sqm)  
30 - +

Window retrofit cost (€/sqm)  
300 - +

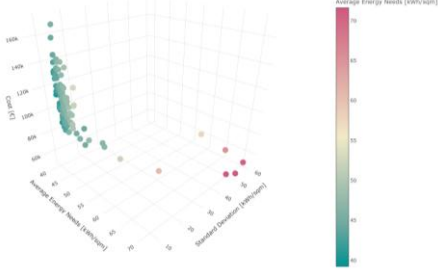
Air-to-water heat pump retrofit cost (€/unit)  
4000 - +

Efficient AC units retrofit cost (€/unit)  
700 - +

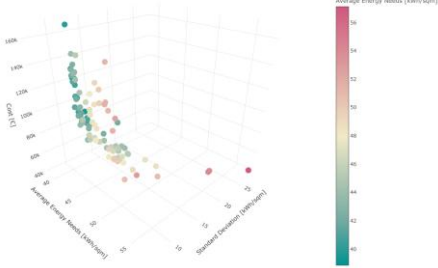
Solar panels for DHW retrofit cost (€/unit)  
2000 - +

Solar panels for energy production retrofit cost (€/unit)  
600 - +

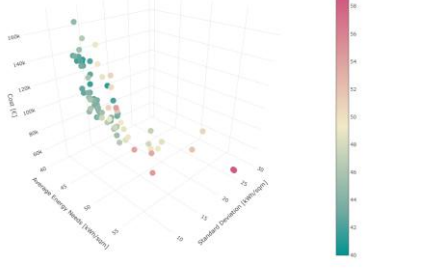
SPEA II



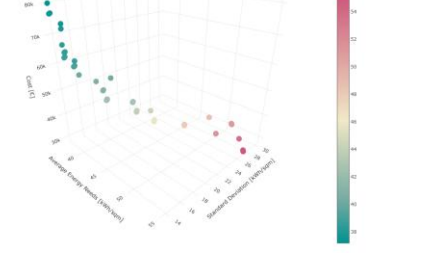
NSGAII



NSGAIII



IBEA



ExtraTrees Regressor with 20 features



Model is deployed in a web app prototype for the optimization of building retrofit for:



Homeowners



Policymaking

$$f\left(\begin{bmatrix}(r_1, \dots, r_n)_1 & \cdots & (r_1, \dots, r_n)_m \\ \vdots & \ddots & \vdots \\ (r_1, \dots, r_n)_i & \cdots & (r_1, \dots, r_n)_{im}\end{bmatrix}\right) = \begin{bmatrix}f_{11} & f_{21} & f_{31} \\ \vdots & \vdots & \vdots \\ f_{1i} & f_{2i} & f_{3i}\end{bmatrix}$$

$$f_1 = \sum_{i=1}^m Ntc_i [kWh/m^2] \quad f_2 = \sigma \left( \cup_{i=1}^m Ntc_i \right) [kWh/m^2] \quad f_3 = Retrofit\ cost\ [€]$$

# Discussion

*Surrogate Models to improve Building  
Performance Analysis and Optimization*

**How to efficiently integrate AOP with  
building and urban projects?**





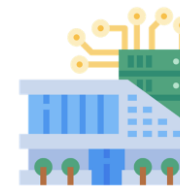
Flexible framework to develop Surrogate Models and integrate them with AOP.



Synthetic

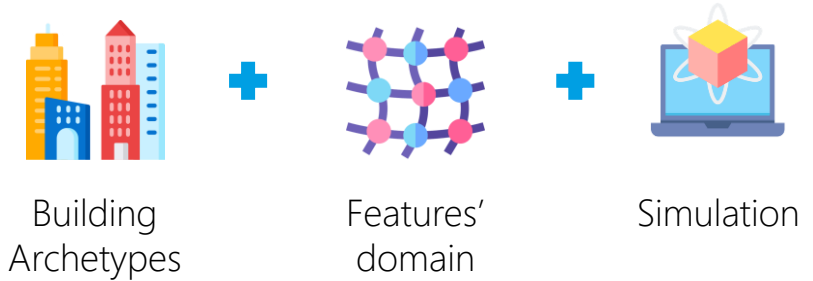


Iterative



Existing

## Model trained with a Synthetic BID.



**0.95  $R^2$  score**, suitable for early design stages.  
 Simulation **time decreased** by 2 orders of magnitude.  
 Small set of 6 inputs requires **minimum expertise**.  
**Versatile** and **adaptable** to any building or urban project.



Small set of 6 inputs **decreases building details**.

**High development time.**

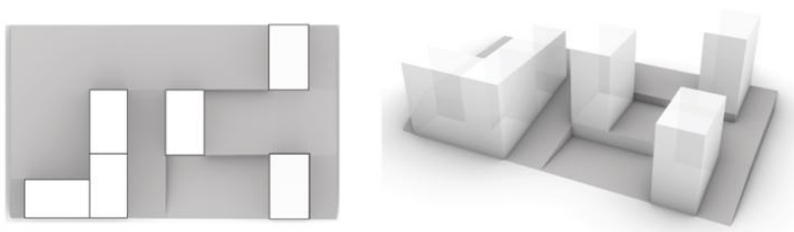
Increase in the **number of inputs exponentially increases** the model **development time**.

Process needs to be **repeated** for different simulation tools/outputs.

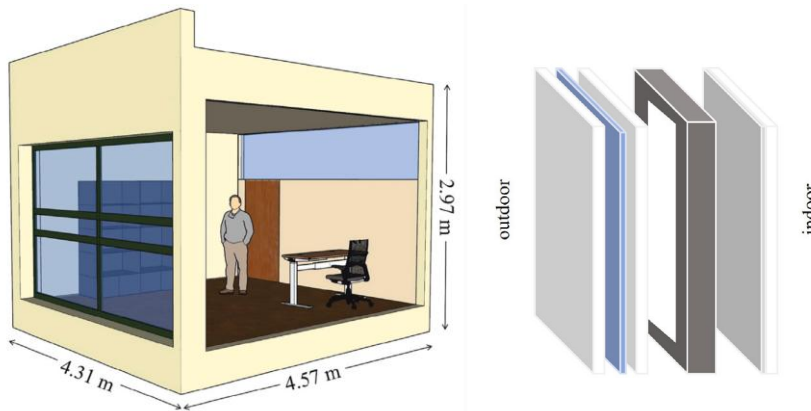


*"AD based surrogate models for simulation and optimization of large urban areas"*

## Model trained with BID obtained from optimization processes



*"Surrogate Models for Efficient Multi-Objective Optimization of Building Performance"*



*"Multi-objective optimization of thermochromic glazing properties to enhance building energy performance"*



Variables



Objectives



Simulation



0.97, 0.99  $R^2$  Score. Accuracy can be improved with hyperparameter optimization.

Lower development time than Synthetic databases.

Simulation time decreased by 2 orders of magnitude.

Supports any number of features.

Supports multiple objectives.



Model is **case-specific** and not adaptable to problems outside the realms of the optimization.

Increase in the number of inputs (variables) also increases the model development time.

**Less accurate than Synthetic databases** in predicting worse solutions.

## Model trained with BID obtained from existing databases



Extract



Cleaning



Analyses and  
Optimization

### General details

Location  
EVORA

Type of certificate  
Horizontal property

Floor location of your house  
Last

Total number of floors in your building  
2

Construction period  
between 1996 and 2000

Area  
100

Floor height  
2.80

Typology  
T3



Cooling energy (kWh/year)  
4 k



Heating energy (kWh/year)  
9 k



Total energy (kWh/year)  
20 k

Predict energy indicators!

### Economic details

Here you can stipulate your maximum rehabilitation budget

2000

Presently, how much do you pay for housing taxes?

300

☒ If you do not want to provide this information, the tool can estimate a value based on the information provided.

[Click here to start](#)



No simulations required.

Supports **any number of features**.

Supports **multiple objectives** if available in the data.

**Lower development time** than generating other BID.






Accuracy **highly dependable** on the existing **data's quality**.

**Limited outputs and prediction targets**.

**0.84 R<sup>2</sup> score**, **Less accurate** than **Synthetic** and **Optimization** (Can improve depending on the data).

*"Optimizing building retrofit through data analytics: A study of multi-objective optimization and surrogate models derived from energy performance certificates"*

Quantitative Comparison

	Problem	Scale	Objectives	Improvements	Inputs	Speed-up	R <sup>2</sup>
	Retrofit	Urban	3	16%	6	≈85x	0.95
	Design	Building	1	8%			
	Material	Room	2	17%	4	≈200x	0.99
	Construction	Urban	3	22%	24	≈200x	0.97
	Retrofit	Building	3	60%	20	-	0.84/0.79
	Retrofit	Urban	3	25%		-	



Qualitative Comparison

	R <sup>2</sup>	Development speed	Number of features	Number of objectives	Adaptability	Suitable for:
						<div><p>Early-stage project studies with a low number of features</p></div>
						<div><p>Project construction and execution stages</p></div>
						<div><p>Building operation and retrofit</p></div>

## Future projects



Explore new ways to develop a **smaller number of building samples** without losing model accuracy and, therefore, be able to **increase the number of features and complexity** of a model.



**Benchmark** optimization and machine learning **algorithms** for multiple simulation outputs and analyses



**Explore** different feature engineering and selection techniques to improve the quality of the databases. **Experimental measurement** of building use and performance for data calibration.

## Future applications



Assistance to field studies. Data feedback for field work.



Digital twin city models and databases. Enhance current data repositories.



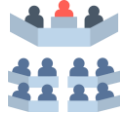
Quick and easy Policymaking tools to achieve sustainable and economic goals.



On-the-fly assistance for design and execution projects. Enhanced collaborative work.

## Research Outputs

### Core Publications



Araújo, Gonçalo; Santos, Luís; Leitão, António & Gomes, R. (2022, April). *Ad based surrogate models for simulation and optimization of large urban areas*. In Proceedings of the 27th International Conference of the Association for Computer-Aided Architectural Design Research in Asia (CAADRIA 2022), Sydney, Australia (pp. 9-15).



Araújo, G. R., Gomes, R., Gomes, M. G., Guedes, M. C., & Ferrão, P. (2023). *Surrogate Models for Efficient Multi-Objective Optimization of Building Performance*. *Energies*, 16, 4030. <https://doi.org/https://doi.org/10.3390/en16104030>



Araújo, G. R., Teixeira, H., Gomes, M. G., & Rodrigues, A. M. (2023). *Multi-objective optimization of thermochromic glazing properties to enhance building energy performance*. *Solar Energy*, 249(October 2022), 446–456. <https://doi.org/10.1016/j.solener.2022.11.043>



Araújo, G., Gomes, R., Ferrão, P., & Gomes, M. da G. (2023). *A study of multi-objective optimization with surrogate models derived from energy performance certificates*. *Energy and Built Environment*.

### Others



Araújo, Gonçalo; Teixeira, Henriqueta; Glória, G. M., & Moret, R. A (2022). *Otimização de Envidraçados Termocrômicos para um Clima Mediterrânico*. *Congresso Construção 2022*, 239.



Araújo, G., Pereira, I., Leitao, A., & Guedes, M. C. (2021). Conflicts in passive building performance: Retrofit and regulation of informal neighbourhoods. *Frontiers of Architectural Research*, 10(3), 625-638.



Aleixo, J., Araújo, G. R., & Guedes, M. C. (2021). Comparison of passive design strategies to improve living conditions: a study in Ondjiva, Southern Angola. *Renewable Energy and Environmental Sustainability*, 6, 21.



Guedes, M. C., Araújo, G., & Albuquerque, N. (2023). *Thermal Comfort in Informal Settlements: Case Studies in Sub-Saharan Africa*. In *Climate Change and Sustainable Development* (pp. 129-148). CRC Press.



Araújo, Gonçalo; Leitão, António, Inês Pereira; Gomes, Ricardo & Ferrão, Paulo (2021). *A non-linear surrogate model of building archetypes to speed up cities' adaptation to the post-carbon age*. In *Congresso MITPortugal 2021*.



Araújo, Gonçalo; Gomes, Ricardo & Ferrão, Paulo (2022). *Surrogate models for time-consuming building performance simulations and optimizations*. In *Congresso MITPortugal 2022*.



3<sup>rd</sup> place at the PhD Open Days 2021 pitch competition.



# Surrogate Models to improve Building Performance Analysis and Optimization

Thank you for listening!



Fundação  
para a Ciência  
e a Tecnologia



TÉCNICO LISBOA



CENTER for INNOVATION,  
TECHNOLOGY and POLICY RESEARCH

CERIS