Metamodelling in robust low-energy dwelling design

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ABSTRACT: Deterministic simulations are commonly used in building design to calculate for instance the energy use. Many influential parameters are however inherently uncertain. As a result, deterministic optimisation unreliably predicts the impact of design measures. In order to improve the optimisation process, uncertainties need to be taken into account through a robust design method. Such a simulation based optimisation is often extremely time-consuming and hence unrealistic. To overcome this barrier, metamodelling is of high interest as a metamodel aims to imitate the original numerical model with a simplified fast model. In this paper, metamodels are constructed for the energy demand and indoor temperature of a semi-detached dwelling. Polynomial regression and multivariate adaptive regression splines (MARS) are compared as well as the number of training samples. For the current case, MARS models show to be more accurate. Furthermore, the models appeared more reliable for some outputs than for others. To ensure the reliability of the metamodels, a cross-validation strategy is proposed to construct metamodels with as less training sets as possible.

1 INTRODUCTION

Building energy efficiency is raising concern regarding climate change and imminent fossil fuel depletion. In research and design of low-energy buildings deterministic simulations are commonly used to calculate the energy use and indoor climate and to optimise buildings by adjusting design parameters. However, many influential parameters such as user behaviour are inherently uncertain. As a result, deterministic simulations are unable to determine the optimal design measures for energy use and indoor climate, potentially resulting in solutions which are not favourable in all conditions. Accurate optimisation is however essential to investigate the most effective and robust measures as both governments and dwelling owners need confidence in optimal design solutions. In order to improve the optimisation process, uncertainties need to be taken into account through a robust design method in which for all performance criteria the target value is optimised and the impact of uncertain conditions is minimised.

In building physics, uncertainty analysis was recently introduced to reliably calculate building performances under uncertainties (MacDonald & Strachan 2001, de Wit & Augenbroe 2002, Haarhoff & Mathews 2006). Advanced sampling schemes allow reducing the amount of simulations and thus calculation time, making such an uncertainty analysis realistic (Janssen 2013). Unfortunately, due to fewer samples, several design options are unreliably compared. As an example, one can calculate the output distributions with 200 optimal-schemed simulations instead of 2000 randomly selected, but comparing the two possible U-value solutions included in the simulations, becomes though if numerous parameters are involved. Because only 100 samples remain for each potential U-value, it is non-guaranteed that the other influential parameters are equally distributed, resulting in a potentially unreliable comparison. This example indicates the need for more samples in a robust design method.

Coupling such a robust design method to dynamic energy simulation models is generally very time-consuming, which makes metamodelling extremely interesting since a metamodel aims at mimicking the original model, but with a strongly reduced calculation time. In building physics, metamodels were recently used as predictive models based on simulations (Caldera et al. 2008) and measurements (Catalina et al. 2013) and in building optimisation (Eisenhower et al. 2012).

In this paper, metamodels are constructed for the energy demand and indoor temperature of a semi-detached dwelling to exemplify the benefits and drawbacks. Section 2 clarifies the robust design method; section 3 explains the metamodelling techniques used. The case study is described in section 4. In section 5, used techniques are compared as well as the number of training samples. The reliability of the best model is investigated and a strategy to construct reliable metamodels is proposed.

2 ROBUST DESIGN METHOD

Both occupants in particular and society in general need confidence in selected measures in optimisation as dwelling owners require guaranteed returns on their investments in energy efficiency and indoor climate, while governments must ensure that their subsidy programs have the desired impact. The de-
development and promotion of effective and robust building envelope and service solutions is thus an important step to optimise the performances while limiting the spread, and thus to minimise the impact of uncertain conditions. In robust design, effectiveness and robustness of design options are evaluated at the same time for all performance criteria and all uncertain conditions and design options.

The effectiveness $e$ and robustness $R_p$ of a design option $x_n$ for performance $y$ are illustrated in Figure 1 and defined as (Van Gelder et al. 2013): 

\begin{align}
e(x_n) &= 1 - \frac{y_{50}(x_n) - y_{\min}}{y_{50} - y_{\min}} \quad (1) \\
R_p(x_n) &= 1 - \frac{y_{50+p/2}(x_n) - y_{50-p/2}(x_n)}{y_{50+p/2} - y_{50-p/2}} \quad (2)
\end{align}

with $P$ the user specified percentile of included sample points, $y_k$ the $k^{th}$ percentile under full uncertainty and $y_k(x_n)$ the $k^{th}$ percentile after selecting design option $x_n$. $y_{\min}$ corresponds to the simulated minimal value which is not an outlier, whereby an outlier is defined as a sample point smaller than $y_{25}.1.5(y_{75} - y_{25})$. In this definition the performance indicator $y$ is defined in such a way that it is greater or equal to zero and to be minimised. Effectiveness is thus defined as the improvement the median performance of a design option makes in proportion to the best possible reduction. The robustness is analogously determined as the improvement the performance spread of a design option makes in proportion to the spread under full uncertainty. According to this definition a measure with an effectiveness and robustness of one is the best possible, while negative values are to be avoided. Figure 1 shows as an example that design option $x_i$ is more robust, while $x_j$ is more effective.

In robust design, effectiveness and robustness are included in the optimisation of design variables according to the performance criteria. The sampling scheme used in a robustness study is a crossed array scheme with the same sampling scheme for the uncertain parameters of all design options, allowing the user to calculate the effectiveness and robustness of every design option (Sanchez et al. 1996). A full factorial scheme, in which all chosen values of design options are combined with all considered values of uncertain parameter, can be used, but more optimal schemes are available as well (Dehendorff et al. 2011). Weight factors might be introduced to give priorities to several performance criteria and e.g. to effectiveness over robustness.

Optimisation by a crossed array scheme can become time consuming if several uncertain and design parameters are taken into account, which is generally true for robust design problems in building physics. Even if the two layers in the design are constructed with an optimal scheme, still many combinations need to be taken into account. As metamodelling can enormously reduce calculation time, the next section will introduce some simple metamodels applicable for the current problem.

3 METAMODELLING

Metamodels, also known as surrogate models, have the intention to stand in for the original model. The major advantage is theirs highly reduced calculation time. While for extreme cases, the original model might take days for one simulation, the metamodel only takes about a second.

A metamodel is constructed for every output parameter with training data and validated on validation data coming from the original model as we want to design a metamodel which obtains good performance on unseen data. In general, all input and output data is standardised (zero mean, unit variance) to overcome influences from parameter units.

One of the most important steps in metamodelling is to select validation criteria (Kleijnen & Sargent 2000) as the accuracy required for a predictive metamodel is usually very high.

Polynomial regression and multivariate adaptive regression splines (MARS) are selected for this case study due to their simplicity. Both techniques quickly build models with short execution time.

3.1 Polynomial regression

Polynomial regression is one of the most known metamodelling techniques and fits a relation between the sampled input and output data using the method of least squares. In general, the model is a function of the form

$$y = b_0 + \sum_{m=1}^{m} \sum_{j=1}^{k} b_m x_m^p + \sum_{m=1}^{m} \sum_{j=1}^{k} \sum_{j=1}^{k} b_{mnp} x_m^p x_j^q$$ (3)
with \( y \) the estimated output parameter, \( x \) the input parameters, \( k \) the amount of input parameters, \( m \) the order of the polynomial and \( b \) the regression coefficients (Jin et al. 2001, Wikipedia 2013a). First, second and third order polynomials are studied in this paper using Matlab tool polyfitn (D’Errico 2012).

An additional advantage of first order polynomial regression is that the significance of the parameters can be identified from the coefficients.

3.2 MARS

Multivariate adaptive regression splines (MARS) is a regression method that takes stepwise nonlinearities into account. The models are constructed through a forward/backward iterative approach and are of the form

\[
y = \sum_{i=1}^{k} c_i B_i(x)
\]

(4)

with \( y \) the estimated output parameter, \( x \) the input parameters, \( k \) the amount of basis functions \( B_i \) and \( c_i \) the weight factors (Friedman 1991, Jin et al. 2001). A basis function is a constant, a hinge function or a product of hinge functions to take interactions into account (Wikipedia 2013b). A hinge function has the form \( \max(0, x - \text{constant}) \) or \( \max(0, \text{constant} - x) \). In the backward stage the least effective model terms are deleted to improve its generalization ability.

The MARS models in this paper are piecewise-cubic regression models created with the Matlab tool ARESLab (Jekabsons 2011).

4 CASE STUDY

4.1 Simulation model

A semi-detached dwelling is modelled with two thermal zones and simulated in a transient simulation tool developed in Modelica (Baetens et al. 2012) for the reference climate year of Uccle, Belgium. This dwelling has a volume of 450 m³ and sun shading sheds, while the indoor temperature of the adjacent dwelling is assumed constant at 19 °C (Van Gelder et al. 2013). The hourly heat demand and indoor temperatures are calculated in these simulations under stochastic boundary conditions taking several design options into account. The resulting total annual heat demand, maximal temperature and amount of hours with temperatures exceeding 25 °C for the day zone are successively computed based on the simulation output.

4.2 Probabilistic approach

Many parameters influencing heat demand and indoor temperature are either inherently uncertain, such as user behaviour and workmanship, or design variables to be optimised. Both design and uncertain

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Options*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type of ventilation system</td>
<td>natural ventilation</td>
</tr>
<tr>
<td>Infiltration rate</td>
<td>( U(0.45,12.5) ) m³/min</td>
</tr>
<tr>
<td>Construction type</td>
<td>massive</td>
</tr>
<tr>
<td>U-value roof</td>
<td>( U(0,1,0.3) ) W/m²K</td>
</tr>
<tr>
<td>U-value floor</td>
<td>( U(0,1,0.3) ) W/m²K</td>
</tr>
<tr>
<td>U-value wall</td>
<td>( U(0,1,0.3) ) W/m²K</td>
</tr>
<tr>
<td>U-value door</td>
<td>( U(0,8,0.2) ) W/m²K</td>
</tr>
<tr>
<td>Type of window</td>
<td>( U ) 2.07 W/m²K – g 0.631</td>
</tr>
<tr>
<td>Type of sunscreen control</td>
<td>none</td>
</tr>
<tr>
<td>Type of sunscreen control</td>
<td>automatic on solar irradiance</td>
</tr>
</tbody>
</table>

*Explanation of the symbols used:
\( U(a,b) \): uniform distribution between \( a \) and \( b \)
\( \mathcal{N}(\mu, \sigma) \): normal distribution with mean value \( \mu \) and standard deviation \( \sigma \)
\( \mathcal{L}(a,b) \): lognormal distribution with mean value \( a \) and standard deviation \( b \)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Distribution*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Occupancy profile day zone</td>
<td>4 discrete profiles</td>
</tr>
<tr>
<td>Occupancy profile night zone</td>
<td>3 discrete profiles</td>
</tr>
<tr>
<td>Set temperature occupancy day zone</td>
<td>( \mathcal{N}(21,1.35) ) °C</td>
</tr>
<tr>
<td>Set temperature absence day zone</td>
<td>( \mathcal{D}(15,\text{no reduction}) ) °C</td>
</tr>
<tr>
<td>Set temperature occupancy night zone</td>
<td>( \mathcal{N}(19,2) ) °C</td>
</tr>
<tr>
<td>Recovery efficiency ventilation system (only for balanced ventilation)</td>
<td>( U(0,7,0.95) )</td>
</tr>
<tr>
<td>Air change rate day zone</td>
<td>Natural ventilation</td>
</tr>
<tr>
<td></td>
<td>Other</td>
</tr>
<tr>
<td>Air change rate night zone</td>
<td>Natural ventilation</td>
</tr>
<tr>
<td></td>
<td>Other</td>
</tr>
<tr>
<td>Internal heat gains persons</td>
<td>( \mathcal{U}(35,175) ) W</td>
</tr>
<tr>
<td>Basis internal gains appliances</td>
<td>( \mathcal{U}(20,180) ) W</td>
</tr>
<tr>
<td>Summer internal gains appliances</td>
<td>( \mathcal{U}(130,1000) ) W</td>
</tr>
<tr>
<td>Winter internal gains appliances</td>
<td>( \mathcal{U}(180,1300) ) W</td>
</tr>
<tr>
<td>Spring and autumn internal gains appliances</td>
<td>( \mathcal{U}(140,1150) ) W</td>
</tr>
</tbody>
</table>

*Explanation of the symbols used:
\( \mathcal{N}(\mu, \sigma) \): normal distribution with mean value \( \mu \) and standard deviation \( \sigma \)
\( \mathcal{D}(a,b) \): discrete uniform distribution between \( a \) and \( b \)
\( \mathcal{U}(a,b) \): uniform distribution between \( a \) and \( b \)
\( \mathcal{L}(a,b) \): lognormal distribution with mean value \( a \) and standard deviation \( b \)
parameters are considered stochastic. The former are uniformly distributed (Table 1), while the latter are assigned a probability distribution inspired by a measurement campaign (Table 2) (Staepels et al. 2013, Van Gelder et al. 2013).

A Monte Carlo simulation in Matlab is coupled to the dynamic simulation tool to process all uncertainties and design variables. The maximin Latin Hypercube advanced sampling technique was applied to reduce calculation time (Janssen 2013), when ten sets of 60 samples are created to enable bootstrapping.
5 RESULTS

5.1 Polynomial regression versus MARS

Because ten simulation sets are available, we can compare both the metamodelling techniques and the number of training sets. One to nine sets are used to train the metamodels, while the tenth set is used for validation. As mentioned before, the simulation outputs heat demand, maximal temperature and amount of hours with temperatures above 25 °C (TE25°C) are modelled for the day zone based on the input parameters.

Figure 2 shows the coefficients of determination \( r^2 \) for the outputs of both techniques in function of the number of training sets. The coefficient of determination \( r^2 \) indicates how accurate the original model is approximated by the metamodel as shown in Figure 3. A perfect correlation is given by an \( r^2 \)-value of 1 and trend line \( y=x \). Figure 4 also shows the maximal relative error (MRE), which is the deviation between simulation and metamodel divided by the average simulation value, as both the overall fit and the maximal error are important in robust design.

Comparing the validation indicators for the different outputs learns that MARS models have a better approximating ability than the polynomial regression models as higher-order polynomials tend to overfit the training data. As can be seen in Figures 2 and 4, the heat demand and maximal temperature are much easier to mimic than the temperature exceedings of 25 °C, even for few training sets. Furthermore, more training sets do not guarantee a better fit. For each output parameter, the MARS model based on six training sets shows good generalisation ability and is chosen as investigation object for the next subsection.

5.2 Reliability of metamodels

The selected MARS models are now tested on the four remaining sets. The cumulative distribution function of the considered outputs of both original simulation and metamodel are compared in Figure 5. The coefficient of determination \( r^2 \) and the maximal relative error of the metamodel are given as well. One can conclude that the overall agreement is sufficient for the heat demand model. This model can be perfectly used in robust design. If one wants to include indoor comfort in the optimisation as well, one preferably opts for the maximal temperature model instead of temperature exceeding model because of its better similarity.

In the previous subsection, several training sets were available and different models were built to select the best performing model. When making a metamodel in robust design optimisation, one wants to judge the constructed model independently of other potential models. Due to time constraints, one wants to create as less simulation sets as possible.

Therefore the next paragraph investigates the reliability of a constructed model and thus the influence of training and validation sets on the goodness of the fit.

Seven training set combinations with six out of nine available sets are used to construct metamodels as shown in Table 3. One can see that the metamodels based on some training set combinations perform better than on other sets. On the other hand, the validation set used also has its influence on the validation indicators, as presented in Table 4. The metamodels selected in the previous subsection, are validated on each of the four remaining sets. As it is important that the validation indicators do not differ in function of the used training and validation sets, it is recommended to test the metamodel for as many samples as possible. Because of calculation time, this is unfortunately impossible.
The previous section shows that metamodels should be constructed and validated with care. Nevertheless, one wants to limit calculation time. To judge the metamodel accuracy, validation criteria, which are dependent on the goal of the model, are therefore needed. As stated before, the accuracy of predictive models is preferably very high. The required metamodel reliability has to be studied in further research to know which accuracy is sufficient to obtain the same robust design as with the original simulation tool. Based on that research, validation criteria will be determined. Both the overall fit and maximal errors are considered, of which the overall fit is probably most important.

Once validation criteria are determined, metamodels can be constructed based on the proposed strategy. The first step is to simulate two sampling sets. One of these sets is selected as training set, the other as validation set. A metamodel is constructed and \( r^2 \)-value and maximal relative error of all models after cross-validation are calculated for the validation set. To control the reliability of this model, an f-fold cross-validation is performed (Wikipedia 2013c). This implies that each set is once used as validation set, while the other set is a training set. In this way, as many metamodels are constructed and validated as simulation sets are available. Both \( r^2 \)-values and maximal relative errors of these metamodels are averaged. The minimal, maximal and average validation indicators are then compared with the validation criteria. If these criteria are met, the constructed metamodel can be used for robust design optimisation; otherwise, an additional training set is generated. Again, metamodels are constructed and a cross-validation is performed. The validation indicators are recalculated and again compared with the criteria. These steps are repeated until a metamodel is constructed which meets the validation criteria as exemplified in Table 5. The validation indicators of the metamodels after cross-validation are presented. A comparison with validation criteria will be possible in further research, allowing the judgement of the constructed metamodels. As can be seen in Table 5, the metamodels for heat demand and maximal temperature models will meet these criteria with less simulations than the metamodel for temperature exceedings.

### 6 CONCLUSION

This paper focussed on metamodeling in the context of robust design for low-energy dwellings. Although
deterministic simulations are commonly used in building optimisation, many influential parameters are inherently uncertain, with the result that deterministic simulations are unable to determine the optimal design measures. Taking the uncertainties into account through a robust design, which was explained in this paper, results in an improvement, but with the disadvantage of longer calculation time. To strongly improve the time efficiency, metamodelling was proposed.

Metamodels were constructed for the energy demand and indoor temperature of a semi-detached dwelling. Comparison of polynomial regression and multivariate adaptive regression splines (MARS) learned that the fitting agreement of the latter was significantly better. The metamodels of heat demand and indoor temperature of a semi-detached dwelling were significantly better. The metamodels of heat demand and indoor temperature of a semi-detached dwelling was strongly improve the time efficiency, metamodelling with the explained in this paper, results in an improvement.

To construct a reliable metamodel with as less simulation sets as needed, this paper proposed a metamodelling strategy. Because training and validation sets may be of influence for the validation of the model, cross-validation is preferred. Sample sets are added to construct a metamodel meeting the validation criteria. However, more research is needed to define what accuracy is needed for a metamodel in robust design and to determine the validation criteria. These criteria handle the overall fit and maximal error of validation and cross-validation.

ACKNOWLEDGEMENTS

The authors are very thankful for the fundings of the Flemish government for the IWT TETRA BEP2020-project. They would like to thank Bart Husslage and Gijs Rennen from the Tilburg University as well for sharing their Matlab code for calculation of ‘maximin’ designs (Husslage et al. 2008).

REFERENCES


