A comparison of six metamodeling techniques applied to building performance simulations

Torben Østergård\textsuperscript{b,a},*, Rasmus Lund Jensen\textsuperscript{b}, Steffen Enersen Maagaard\textsuperscript{a}

\textsuperscript{a} Aalborg University, Department of Civil Engineering, Thomas Manns Vej 23, DK-9220 Aalborg Ø, Denmark
\textsuperscript{b} MOE Consulting Engineers, Mariane Thommens Gade 1C, DK-8000 Aarhus, Denmark

HIGHLIGHTS

- Linear regression (OLS), support vector regression (SVR), regression splines (MARS).
- Random forest (RF), Gaussian processes (GPR), neural network (NN).
- Accuracy, time, interpretability, ease-of-use, model selection, and robustness.
- 13 problems modelled for 9 training set sizes spanning from 32 to 8192 simulations.
- Methodology for comparison using exhaustive grid searches and sensitivity analysis.

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ABSTRACT

Building performance simulations (BPS) are used to test different designs and systems with the intention of reducing building costs and energy demand while ensuring a comfortable indoor climate. Unfortunately, software for BPS is computationally intensive. This makes it impractical to run thousands of simulations for sensitivity analysis and optimization. Worse yet, millions of simulations may be necessary for a thorough exploration of the high-dimensional design space formed by the many design parameters. This computational issue may be overcome by the creation of fast metamodels. In this paper, we aim to find suitable metamodeling techniques for diverse outputs from BPS. We consider five indicators of building performance and eight test problems for the comparison six popular metamodeling techniques – linear regression with ordinary least squares (OLS), random forest (RF), support vector regression (SVR), multivariate adaptive regression splines, Gaussian process regression (GPR), and neural network (NN). The methods are compared with respect to accuracy, efficiency, ease-of-use, robustness, and interpretability. To conduct a fair and in-depth comparison, a methodological approach is pursued using exhaustive grid searches for model selection assisted by sensitivity analysis. The comparison shows that GPR produces the most accurate metamodels, followed by NN and MARS. GPR is robust and easy to implement but becomes inefficient for large training sets compared to NN and MARS. A coefficient of determination, $R^2$, larger than 0.9 have been obtained for the BPS outputs using between 128 and 1024 training points. In contrast, accurate metamodels with $R^2$ values larger than 0.99 can be achieved for all eight test problems using only 32–256 training points.

1. Introduction

1.1. Motivation for metamodeling

The building sector accounts for roughly 40% of the total energy consumption and 38% of the CO$_2$ emissions in the European Union \cite{[1]}. On a global scale, the energy savings potential is estimated to 53 exajoules each year by 2050 \cite{[2]}. Building designers play a vital role in realizing this enormous energy savings potential. Architects and engineers use building performance simulations (BPS) to assess and reduce the environmental impact of buildings and, at the same time, meet strict requirements related to indoor climate. Examples of performance objectives are energy demand, CO$_2$ footprint, thermal comfort, daylight availability, and construction costs. To find possible solutions, the design team may vary a large number of design parameters such as building geometry, insulation thickness, glazing properties, and HVAC systems. The variations of these parameters constitute an enormous multi-dimensional “design space”. The many design parameters

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(model inputs) and requirements (model outputs) makes it difficult and
time-consuming to explore the design space efficiently and find favorable
solutions that meet all requirements. To address this multivariate
problem, it is becoming increasingly popular to perform a large number of
simulations using Monte Carlo methods or optimization routines
[3–7]. Unfortunately, most BPS software are computational demanding.
A single simulation often takes minutes to compute or even hours in the
case of CFD simulations. For real-life applications, the task of running
thousands or millions of simulations is an obstacle for widespread
adoption of design space exploration, uncertainty analysis, sensitivity
analysis, and optimization.

The computational obstacle of BPS may be overcome by super-
computers, cloud computing, or metamodeling. Supercomputers are
expensive if not managed efficiently to avoid downtime. Cloud comput-
ing is presumably a cheaper alternative, and several popular BPS
tools provide this feature for optimization or uncertainty analysis [3].
Still, if the design team wish to perform sensitivity analysis to identify
important inputs or interaction effects, such analysis easily requires
thousands of simulations. This is likely to take hours or days—even with
access to cloud computers [8,9]. An extensive set of Monte Carlo si-
mulations allows the design team to explore a high-dimensional design
space under various constraints and immediately observe the con-
sequences of different design choices [10]. A useful tool for such ana-
ysis is the interactive parallel coordinate plot, which enables rapid and
visual exploration of multivariate data (see Fig. 5) [11]. In terms of
computational effort, Østergård et al. [10] demonstrated that 5000 si-
mulations were insufficient when applying five constraints representing
building legislation and architects’ ambitions. Similarly, in the devel-
opment of a design tool for thermal comfort evaluation, it was neces-
sary to run millions of simulations to cover the design space sufficiently,
even though the model only contained nine design parameters and two
objectives [12]. Conclusively, this “curse of dimensionality” advocates
the use of fast metamodels to overcome the computational challenges.

1.2. Performance requirements of metamodels

Above, we have argued for a potential of using metamodeling in the
context of BPS. The type of metamodeling, addressed in this paper, is
also referred to as supervised learning, which overlap with regression
analysis. Hence, the metamodels are constructed from a set of input and
output data to enable predictions of future outputs. That means we need
to run a number of building simulations from which we construct the
metamodel to be used for faster predictions of building performance.
The metamodels may be constructed in a wide variety of ways using
many different techniques. These may differ substantially with respect
to predictive accuracy, computational efficiency, ease-of-use, trans-
parency, and robustness (see Section 4.1). Unfortunately, there is no
“perfect” and one-fits-all method. Thus, in searching for the most sui-
table metamodel for BPS, we have to describe the characteristics of our
building simulations and define requirements, and optionally desirable
features, of the metamodels. Emphasis is on applicability for novel users
and the applied algorithms are all available with Matlab.

Building simulations are typically performed with complex “black
box” models with many variable design parameters. Therefore, the
users normally have no clear knowledge of the underlying equations
and how the inputs interact with each other. In addition, the design
team need to assess quite different building performance indicators,
such as energy, thermal comfort, and daylight. These vary sub-
stantially in complexity and in the shape of the output distribution (see
Section 4.2). Thus, the metamodeling technique must be robust to the
number of inputs and the type of output. We have identified three se-
parate cases for which metamodeling can be applied to enable design
space exploration, optimization, and sensitivity analysis. The three
cases denoted A, B, and C can be distinguished by their diverse re-
quirements, which may be characteristic for many other applications
across scientific disciplines:

A. Expert with considerable time (~days) and emphasis on accuracy.
The task is to develop a generic, reusable tool for early design
support based on a predefined room types that often occur in
buildings, e.g. open-Offices and meeting rooms. Time for training
and construction of the metamodel is not critical.
B. Non-expert with limited time (~hours) and need for ease-of-use and
robustness
For each building project, an engineer (or architect) with pre-
sumably limited knowledge of metamodeling needs to construct
metamodels, which represent the particular building and its desired
performance. The applied technique must be robust towards dif-
ferent objectives and easy to use.
C. Automated metamodeling requiring a minimum of training points
(obtained in minutes) and high robustness
These conditions apply to the development of a joint CAD and BPS
framework, in which the design team selects specific rooms in a CAD
environment. For the selected room, BPS and metamodels are au-
tomatically performed with no user interaction and within a limited
time frame.

For all cases, a large number of new predictions must be performed
rapidly for real-time design-space exploration during meetings with
multiple stakeholders [10].

The purpose of this study is to perform a comprehensive comparison
of metamodeling techniques and thereby identify the techniques most
suitable to accommodate the requirements listed above. We have
strived for an extensive comparison by considering diverse building
performance metrics and well-known mathematical test functions.
The number of training data points has been varied substantially, i.e. from
$2^5$ to $2^{13}$ (32–8192). To improve transparency and reproducibility, we
show all hyperparameter variations and data online [13]. In addition,
we use the unit-less $R^2$ values to report accuracies, which makes it
easier to compare the accuracies for diverse problems encountered in
different disciplines. With these intensions, we strongly believe that this
study is relevant to all research areas and industries, which apply me-
tamodeling in the form of supervised learning.

2. Literature review

First, we investigate earlier uses of metamodeling in the context of
building simulations. Afterwards, we look for promising metamodeling
techniques based on comparisons made across scientific disciplines.
Emphasis is on accurate, rapid techniques that can be applied by a
practitioner of building performance simulations with limited knowl-
edge of metamodeling. Moreover, non-Gaussian distributions of ag-
gregated outputs (see Section 4.2) and interaction effects must be
captured without knowing the underlying equations, which are mostly
hidden in the commercial “black box” software.

2.1. Metamodeling in the field of building performance simulations

Metamodeling has been applied to building simulations for a variety
of reasons, which include early design decision-making [14–17], un-
certainty and sensitivity analysis [15,17–22], design optimization
[16,18,19], and model calibration [21,23,24]. Most research addresses
energy consumption, though metamodels have also been used to
emulate thermal comfort [18,25,22], daylight [16,22], and financials
costs [19]. A wide range of metamodeling techniques have been applied in
the reviewed studies: linear regression (OLS) [14,5,22,24], poly-
nomial regression (PR) [16,17,24], multivariate adaptive regression
splines (MARS) [22], support vector regression (SVR) [18], neural
network (NN) [20], and Gaussian processes regression (GPR) [21,25].
Additional methods, such as step-wise linear regression, decision trees
(CART) and random forests (RF), have been found in works that com-
pare metamodel methods in relation to BPS [26–28]. To sum up, a wide
variety of metamodeling methods have been applied for diverse