Comparison of Bayesian Parameter Estimation and Least Squares Minimization for Inverse Grey-Box Building Model Identification

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Abstract

Bayesian parameter estimation and nonlinear least squares minimization are used for Inverse Grey-Box model identification of a retail and large commercial office model. Detailed simulation engine EnergyPlus is used to generate surrogate data for estimation of parameters, and optimal parameters are compared through annual simulation of building zone temperature and thermal loads. A brief overview of Bayesian estimation techniques is provided, along with ideas for improvements and future work.
Acknowledgements

I would like to acknowledge my colleague Anthony Florita for generously providing a MATLAB Bayesian parameter estimation routine and kindly offering his knowledge of Bayesian statistics.
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1 Introduction

Advanced building control and fault detection methods utilize building energy models to predict or estimate expected building performance. Online implementation of such methods requires light-weight, computationally efficient models that capture the critical system dynamics. Inverse Grey-Box models have shown the potential for blending the benefits of building physics knowledge with measured performance data. Inverse Grey-Box building models have been successfully used to predict cooling loads and energy consumption for optimal control strategy evaluation, as well as online next-day load predictions [1],[2], [8]. Extended Kalman Filters (EKF) have also been incorporated with similar model structures to improve real-time load estimates using available BAS data [5]. Various model identification techniques have been demonstrated that typically involve time or frequency domain least squares minimization via traditional (e.g. Gauss-Newton) or metaheuristic (e.g. genetic) algorithms. Lauret et al. demonstrated the use of Bayesian parameter estimation in determining better estimates of the inputs for roof-mounted radiant barrier system forward model [4]. This paper applies Bayesian parameter estimation methods to Inverse Grey-Box models and provides comparison with least squares model identification.

2 Detailed Building Models

Detailed simulation engine EnergyPlus was used generate surrogate data for two building models: 1) a 5 zone retail building and 2) a 15 zone office building. The load calculations from these detailed simulations is used as "measured" training data for the reduced order models. Figures 1 and 2 illustrate model geometry, and Table 1 highlights selected model details.

![Figure 1: 5 Zone Retail Building Model](image1)

![Figure 2: 15 Zone Office Building Model](image2)
Table 1: Selected EnergyPlus Model Details

<table>
<thead>
<tr>
<th>Property</th>
<th>Retail</th>
<th>Office</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Floors</td>
<td>1</td>
<td>32</td>
<td>floors</td>
</tr>
<tr>
<td>Total Floor Area</td>
<td>2300</td>
<td>77000</td>
<td>m²</td>
</tr>
<tr>
<td>Occupancy</td>
<td>7.11</td>
<td>51.8</td>
<td>m²/person</td>
</tr>
<tr>
<td>Lighting</td>
<td>32.3</td>
<td>9.8</td>
<td>W/m²</td>
</tr>
<tr>
<td>Appliance</td>
<td>5.23</td>
<td>4.63</td>
<td>W/m²</td>
</tr>
</tbody>
</table>

3 Reduced Order Model Structure

Inverse Grey-Box models are based on the approximation of heat transfer mechanisms with an analogous electrical lumped resistance-capacitance network. This approximation creates a flexible structure that allows the modeler to choose an appropriate level of abstraction. Model complexity can range from representing entire systems with a few parameters, to modeling each heat transfer surface with numerous parameters. Depending on the model structure and complexity, model parameters can approximate physical characteristics of the system. Model parameters are then identified through a training period with measured data. For this work, a 5 parameter model, shown in Figure 3, based on ISO13790 was used to predict summer cooling loads for a small retail and large office building [3]. Heat transfer through the opaque building shell materials is represented by $R_1$, $R_2$, and $C$. These elements link the ambient temperature node to a pseudo surface temperature node ($T_s$), accounting for potential heat storage of the mass materials. Glazing heat transfer is represented by a single resistance $R_{gw}$ connecting the ambient temperature node to the surface temperature node, as thermal storage of glazing is typically neglected. $R_3$ represents a lumped convection/radiation coefficient between the surface temperature node and zone air temperature node $T_z$. The convective portion of internal gains (lighting, occupants, and equipment) are applied as a direct heat source to the zone temperature node, shown as $\dot{Q}_{gc}$, and the radiant fraction along with glazing transmitted solar gains ($\dot{Q}_{g,r+sol,w}$) are applied to the surface node. Although, convective and radiative splits are made, radiative heat transfer mechanisms are lumped together.
An energy balance can be written on the mass temperature node \( T_m \), as
\[
C \frac{dT_m}{dt} = \frac{T_a - T_m}{R_1} + \frac{T_s - T_m}{R_2}
\]  
(1)

Since no storage occurs at the surface node, flows entering and leaving the node sum to zero.
\[
\frac{T_a - T_s}{R_w} + \frac{T_z - T_s}{R_3} + \frac{T_m - T_s}{R_2} + \dot{Q}_{g,r+sol,w} = 0
\]  
(2)

The heat gain to the space is then represented by the total heat flow to the zone air node.
\[
\dot{Q}_{sh} = \frac{T_s - T_z}{R_3} + \dot{Q}_{gc}
\]  
(3)

Equations 1 - 4 form a first order differential equation that can be rewritten in state space form
\[
\dot{x} = Ax + Bu
\]
\[
y = cx + du
\]

with non-zero matrix elements

\[
A(1,1) = \frac{1}{C} \left( \frac{-1}{R_1} + \frac{-1}{R_2} + \frac{R_w R_3}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]
\[
B(1,1) = \frac{1}{C} \left( \frac{R_w}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]
\[
B(1,2) = \frac{1}{C} \left( \frac{R_3}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]
\[
B(1,3) = \frac{1}{R_1 C}
\]
\[
B(1,6) = \frac{1}{C} \left( \frac{R_w R_3}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]
\[
B(1,7) = \frac{1}{C} \left( \frac{R_2 R_3}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]
\[
B(1,8) = \frac{1}{C} \left( \frac{R_2 R_3}{R_2 R_3 + R_w R_2 + R_w R_3} \right)
\]

\[
C(1) = \frac{R_w}{R_2 R_3 + R_w R_2 + R_w R_3}
\]
\[
D(1) = -\frac{1}{R_3} + \frac{R_w R_2}{R_3 (R_2 R_3 + R_w R_2 + R_w R_3)}
\]
\[
D(2) = \frac{R_2}{R_2 R_3 + R_w R_2 + R_w R_3}
\]
\[
D(6) = \frac{R_w R_2}{R_2 R_3 + R_w R_2 + R_w R_3}
\]
\[
D(7) = \frac{R_w R_2}{R_2 R_3 + R_w R_2 + R_w R_3}
\]
\[
D(8) = \frac{R_w R_2}{R_2 R_3 + R_w R_2 + R_w R_3}
\]
\[
D(9) = 1
\]

and state and input vectors described as
\[
x^T = [T_m]
\]
\[
u^T = [T_z \ T_a \ T_g \ \dot{Q}_{sol,c} \ \dot{Q}_{sol,e} \ \dot{Q}_{g,r,c} \ \dot{Q}_{g,r,e} \ \dot{Q}_{sol,w} \ \dot{Q}_{g,c}]
\]
$T_z$ is the zone temperature setpoint, $T_a$ is the ambient external temperature, $\dot{Q}_{sol,c}$ is the external solar gains incident on the roof, $\dot{Q}_{sol,e}$ is the solar radiation incident on exterior walls, $\dot{Q}_{g,r,c}$ is the radiative portion of internal gains applied to the ceiling surface node, $\dot{Q}_{g,r,e}$ is the radiative portion of internal gains applied to the wall surface node, $\dot{Q}_{sol,w}$ is the solar radiation transmitted through glazing, and $\dot{Q}_{g,c}$ is the total convective internal gains.

The state space equations are then converted to the following heat transfer function presented by Braun [1], and the conversion process is described by Seem [6].

$$\dot{Q}_{sh,t} = \sum_{k=0}^{n} S_k T_k u_t - \sum_{k=1}^{m} e_k \dot{Q}_{sh,t-k\Delta \tau}$$

(4)

The transfer function method is an efficient calculation method as it relates the sensible heat gains to the space ($\dot{Q}_{sh}$) at time $t$ to the inputs of $n$ and heat gains of $m$ previous timesteps. Equation 4 is used to perform load calculations for the zone that include the effects of dual temperature setpoints with deadbands and system capacity limitations.

Zone temperature predictions are also made using an inverse form of Equation 4.

$$\bar{T}_z = \frac{9 \sum_{l=2}^8 S_0(l) u_t(l) + \sum_{j=1}^8 S_j u_t-j\Delta \tau - \sum_{j=1}^8 e_k \dot{Q}_{sh,t-j\Delta \tau} + 2 \frac{C_z}{\Delta \tau} T_{z,t-\Delta \tau} + \dot{m}_{inf} C_p u_t(2) + \dot{Q}_{zs,t}}{2 \frac{C_z}{\Delta \tau} - S_0(1) + \dot{m}_{inf} C_p}$$

(5)

$$T_{z,t} = 2 \bar{T}_{z,t} - T_{z,t-\Delta \tau}$$

4 Least Squares Parameter Estimation

As a first approach to model identification, least squares minimization was used to identify model parameters that minimize the root-mean-squared error (RMSE), defined by Equation 6, between the reduced order model and EnergyPlus load calculations. A two stage optimization was implemented that first performs a direct search over the parameter space to identify a starting point for local refinement. The direct search is performed on $p$ uniform random points located within the bounds of the parameter space. The local refinement, subject to the same parameter constraints, is performed via nonlinear least squares minimization implemented using a built-in MATLAB optimizer based on trust-region methods [7].

$$J = \sqrt{\frac{\sum_{i=1}^{N} (\dot{Q}_{d,i} - \dot{Q}_{zs,i})^2}{N}}$$

(6)

For this study, 500 direct search points were used within the bounds listed in Table 2. The parameter estimation was repeated 1000 times, beginning each iteration with a new set of randomly generated direct search points.
Table 2: Reduced Order Model Parameter Bounds

<table>
<thead>
<tr>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>Rw</th>
<th>C1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>0</td>
<td>0</td>
<td>0.03030303</td>
<td>0.05</td>
</tr>
<tr>
<td>Max</td>
<td>4.988662132</td>
<td>4.988662132</td>
<td>33.33366667</td>
<td>3</td>
</tr>
<tr>
<td>Units</td>
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<td>$m^2$-K/W</td>
<td>$m^2$-K/W</td>
<td>$m^2$-K/W</td>
</tr>
</tbody>
</table>

5 Bayesian Parameter Estimation

Bayesian methods benefit over traditional methods in that an entire distribution of parameter probabilities is developed and prior knowledge of the system can be incorporated into the estimation task. Specifically, the individual probabilities of events $A$ and $B$

$$p(A), p(B)$$

are related to their conditional probabilities

$$p(A|B), p(B|A)$$

by Bayes’ Theorem (Eq. 7).

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}$$ (7)

From a parameter estimation perspective, the probability of parameters $\Theta$ given measured data $D$ and a knowledge base of the system $K$ can be written as posterior probability $p(\Theta|DK)$. Bayes’ Theorem then allows the conditional probability $p(\Theta|DK)$ to be computed from $p(\Theta|K)$, $p(D|\Theta K)$, and $p(D|K)$ as in Equation 8,

$$p(\Theta|DK) = p(\Theta|K) \frac{p(D|\Theta K)}{p(D|K)}$$ (8)

where $p(\Theta|K)$ represents prior knowledge about parameter values, $p(D|\Theta K)$ represents the likelihood of observing the measured dataset $D$ given a particular parameter set and knowledge of the system, and $p(D|K)$ is the probability of randomly observing the dataset. The relation can be written in alternate form where the numerator remains the product of likelihood and prior, and denominator is a normalization factor so that posterior probabilities sum to unity.

$$p(\Theta|D) = \frac{p(\Theta)p(D|\Theta)}{\sum_i p(\Theta_i)p(D|\Theta_i)}$$ (9)

Assuming random Gaussian noise about the measured data, the probability of an observation can be determined from its location under the normal distribution centered at $\mu$ equal to the measured value, with standard deviation $\sigma_\varepsilon$.

$$p(O_i|\Theta) = \frac{1}{\sigma_\varepsilon \sqrt{2\pi}} \exp\left(-\frac{(O_i - M_i)^2}{2\sigma_\varepsilon^2}\right)$$ (10)
Assuming independent errors, the likelihood of the entire dataset is simply the product of likelihoods of all individual points.

\[ p(O|\Theta) = p(O_1, O_2, ..., O_n|\Theta) = p(O_1|\Theta) * p(O_2|\Theta) * ... * p(O_n|\Theta) \] (11)

Computing the likelihood requires having generated a sufficient knowledge base so that the probability of combinations within the parameter space can adequately be determined. To generate the knowledge base for this study, 100,000 simulations were performed by randomly sampling a parameter set from uniform prior distributions. This results in 100,000 datasets, generated from known parameters, to which our measured data can be compared. The uniform priors represent the belief that any parameter within the bounds is equally likely.

6 Results

To compare results between least squares parameter estimation and the Bayesian methods. The 1,000 solutions from the least squares training Monte Carlo were plotted on against 2-D contour slices of the posterior distribution. This allows for comparison of the probability of a least squares solution from the Bayesian perspective. Results are provided for the retail and large office model in the following sections.

Retail Model Parameter Estimation

Figures 4 and 5 show that the least squares algorithm generally finds R1 values that are fairly probable. However, for R2, the optimizer sticks to the lower bound every time. (As a side note: If the local optimizer is unbounded it finds the optimal R2 value in the negative region.) The optimizer also seems to pick values very near the probable region for R3.

![Figure 4: Retail: R1R2 Posterior Contour](image1)

![Figure 5: Retail: R1R3 Posterior Contour](image2)
Figures 6 and 7 show that several solutions are found within the probable region of Rw, however there does not appear to be great consistency. Capacitance values appear cluster between regions of lower probability.

Figure 6: Retail: R1Rw Posterior Contour

Figure 7: Retail: R1C Posterior Contour

Figure 8 again shows the lower boundary local optimizer choice for R2, and that R3 values are within the probable range. Figure 9 again shows the range of window resistances in and outside of probable ranges.

Figure 8: Retail: R2R3 Posterior Contour

Figure 9: Retail: R2Rw Posterior Contour

Figure 10 - 13 highlights the above results in a different manner by plotting the remaining combinations of posterior slices. Table 3 compares the median estimate from the 1000 nonlinear least squares trainings to the most probable Bayesian estimate.
The best parameter set from each method were used to perform an annual simulation of the building heating and cooling loads. The predicted thermal loads and zone temperatures are shown in Figures
14 and 15, respectively. Overall, the performance is virtually the same for the period shown. The annual RMSE of the load profiles increased by 4% with the Bayesian solution.

Figure 14: Retail: Cooling Load Comparison

Figure 15: Retail: Zone Mean Air Temperature Comparison
Large Office Model Parameter Estimation

The same analysis was repeated, training the 5 parameter model to data from a large 32 story office building. It should be noted that some level of mismatch inherently exists between the simple 5 parameter model and complex office building. It seems that the 5 parameter model may be overly simple for this type of building, regardless of parameter estimation technique. Values for $R_2$ and $R_3$ are chosen near Bayesian probable locations, however the remaining parameter selection end up quite different. Figures 16 - 25 plot combinations of parameter slices for visualizing the estimation results.

**Figure 16:** Office: $R_1R_2$ Posterior Contour

**Figure 17:** Office: $R_1R_3$ Posterior Contour

**Figure 18:** Office: $R_1R_w$ Posterior Contour

**Figure 19:** Office: $R_1C$ Posterior Contour
Bayesian vs. Least Squares Parameter Estimation

Figure 20: Office: R2R3 Posterior Contour

Figure 21: Office: R2Rw Posterior Contour

Figure 22: Office: R2C Posterior Contour

Figure 23: Office: R3Rw Posterior Contour

Figure 24: Office: R3C Posterior Contour

Figure 25: Office: RwC Posterior Contour
Table 4 shows the median values from the nonlinear least squares optimizations and the expected value of the Bayesian estimation. These best parameter sets were used for an annual simulation of building cooling loads and zone air temperatures. The results in Figures 26 and 27 show that despite several large differences in parameter selections, the performance is very similar for cooling load estimation. The temperature predictions are quite different for the models, the Bayesian tending to over predict floating temperatures, and the least squares tending to under predict.

Table 4: Office Model Parameter Estimates

<table>
<thead>
<tr>
<th></th>
<th>R1</th>
<th>R2</th>
<th>R3</th>
<th>Rw</th>
<th>C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upper Bound</td>
<td>4.989</td>
<td>4.989</td>
<td>33.334</td>
<td>3.000</td>
<td>536659</td>
</tr>
<tr>
<td>NLSQ</td>
<td>4.988</td>
<td>0.083</td>
<td>0.030</td>
<td>0.536</td>
<td>503638</td>
</tr>
<tr>
<td>Bayes</td>
<td>0.776</td>
<td>0.126</td>
<td>0.050</td>
<td>1.554</td>
<td>447401</td>
</tr>
<tr>
<td>Lower Bound</td>
<td>0.000</td>
<td>0.000</td>
<td>0.030</td>
<td>0.050</td>
<td>78</td>
</tr>
<tr>
<td>Units</td>
<td>m²·K/W</td>
<td>m²·K/W</td>
<td>m²·K/W</td>
<td>m²·K/W</td>
<td>J/(m²·K)</td>
</tr>
</tbody>
</table>

Figure 26: Office: Cooling Load Comparison
7 Conclusion

Overall, the Bayesian parameter estimation selected parameter values that performed similarly to the least squares optimization for both models. The fact that similar performance was observed despite several differences in parameter selection may suggest that the model is relatively insensitive to parameter values in the range of interest. This is somewhat intuitive due to the fact that commercial buildings tend to be driven by internal gains (lights, occupants, equipment, etc.), rather than external influences (ambient temperature, ground temperature, etc.). Also, the training was performed for a three week summer period. During the cooling season, average ambient temperatures tend to be nearer to the desired internal zone temperature than in the heating season. This further reduces the influence of building shell parameters since heat transfer is driven by this temperature gradient. In both models, the R3 resistance that participates in transferring the radiative fraction of internal gains to the zone node seemed to be estimated the best, while the window resistance showed some of the largest variations. This suggests that the best training data set to identify building shell parameters may be from winter night-time operation.

Posterior contours were very useful for gaining further insight to the solution space and observing patterns in the least squares solutions. Computationally the Bayesian methods are much more demanding, however the above results should be useful in improving the least squares minimization.
8 Future Work

Similar analysis could be repeated for models of higher complexity. Currently six Inverse Grey-Box models exist ranging from 5 to 21 parameters. As model complexity increase, several parameters can model similar characteristics. It would be interesting to see if parameter tradeoffs are observed in the posterior distributions by areas of equally high probability. The estimation could also be extended to incorporate hierarchical models to investigate parameter covariance quantitatively.

The results are also sensitive to the measurement error $\sigma_\epsilon$. Lauret et al. provide some insight into dealing with this by incorporating it as a free parameter in the estimation [4]. This technique could be implemented as the current environment requires trial and error to find an appropriate value. (If $\sigma_\epsilon$ is too large, then everything is similarly likely and the posterior is useless. If $\sigma_\epsilon$ is too small, nothing is likely and the posterior is zero everywhere.)

Improvements in the least squares training method are also planned. The total least squares could be minimized between the temperature and load profiles, and the effects of various training period durations and seasons could be explored as well. State correction as a function of past deviations may also be explored.
References


