Experiment Designs for Model Calibration

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Outline

- Background: Computer Experiments
- Motivating Example
- Proposed Approach
- Wrap-up

Computer Experiments

- Rapid growth in computer power has made it possible to study costly physical phenomena
- To understand how inputs to the computer code impact the system, scientists adjust the inputs observe the response
- That is, they run a *computer experiment*

Computer Experiments

- Computer code exists to model the physical system
- The computer codes frequently:
  - require solutions to PDEs
  - use finite element analyses
  - have high dimensional inputs
  - have outputs which are complex functions of the input factors
  - require a large amounts of computing time
  - have features from some of the above

Computer Experiments - Research Problems

- Inverse problems
- Numerical integration
- Optimization
- Integration of multiple codes into predictive model
- Integration of physical and computer model
- Experiment design

View computer experiments as numerical analysis on a budget

Motivating Example

- Coating of a chocolate bar (i.e., chocolate)
- Field Data: 15 runs
  - Experiment factor (X) related to fluid temperature
  - Response Variable (Y) is the thermodynamic operating point
- Computer model: 10 runs
  $Y = 37 + 2 * \exp(\theta * X)$
- Initial Design: Random LHS Design.

Motivating Example

- Have both field data and computer model data
- Both sources contain information about the physical process
- Combine both sources of data to build a predictive model
- Use model proposed by Kennedy and OHagan (2001)
- Experiment Goal: To perform new trials (computer or field) to improve prediction of physical process

Modelling Approach - Kennedy and O'Hagan, 2001

- Have two sources of data - field and computer data
- $y_{f_i} = \eta(x_i, \theta) + \delta(x_i) + \varepsilon_i, \quad i = 1, \cdots, n$
- $y_{c_j} = \eta(x_j^*, t_j), \quad j = 1, \cdots, m$
- Use a **Ga**ussian **S**patial **P**rocess (GASP) model for both the computer code and the discrepancy

Goals and Criteria

- Goal: Improved prediction for field experiments
- Criterion: Integrated Mean Square Error
- Goal: Make computer model better surrogate by correcting appropriately through more precise estimation of θ
- Criterion: Gain in Shannon Information, D-Optimality

Data

1. Field observations:

$$y_f = (y_{f_1}, \cdots, y_{f_n})'$$

2. Computer code output:

$$y_c = (y_{c_1}, \cdots, y_{c_m})'$$

3. Full set of data:

$$d^T = (y_c^T, y_f^T) = (y_{c_1}, \cdots, y_{c_m}, y_{f_1}, \cdots, y_{f_n})$$

Model and Parameter Structure

1. Model:

   (a) $\eta(\cdot,\cdot) \sim N(\mu_\eta, c_1\{(\cdot,\cdot),(\cdot,\cdot)\})$ with

   $$c_1((x,t),(x',t')) = \sigma_\eta^2 \cdot exp\left\{-\sum_{k=1}^{p}\beta_k(x_k - x_k{}')^2 - \sum_{k'=1}^{q}\beta_{p+k'}(t_k - t_k')^2\right\}$$

   (b) $\delta(\cdot) \sim N(\mu_\delta, c_2(\cdot,\cdot))$ with

   $$c_2(x,x') = \sigma_\delta^2 \cdot exp\left\{-\sum_{k=1}^{p}\gamma_k(x_k - x_k')^2\right\}$$

   (c) $\varepsilon_i \sim N(0,\sigma_\varepsilon^2)$.

2. Parameters:

   (a) $\Omega = \{\mu,\theta,\phi,\sigma_\varepsilon^2\}$

   (b) $\mu = (\mu_\eta,\mu_\delta)^T$

   (c) $\phi = \{\sigma_\eta^2,\sigma_\delta^2,\beta,\gamma\}$

More Formulae

- Full set of data:

$$d^T = (y_c^T, y_f^T) = (y_{c_1}, \cdots, y_{c_m}, y_{f_1}, \cdots, y_{f_n})$$

- Variance of response:
- In summary,

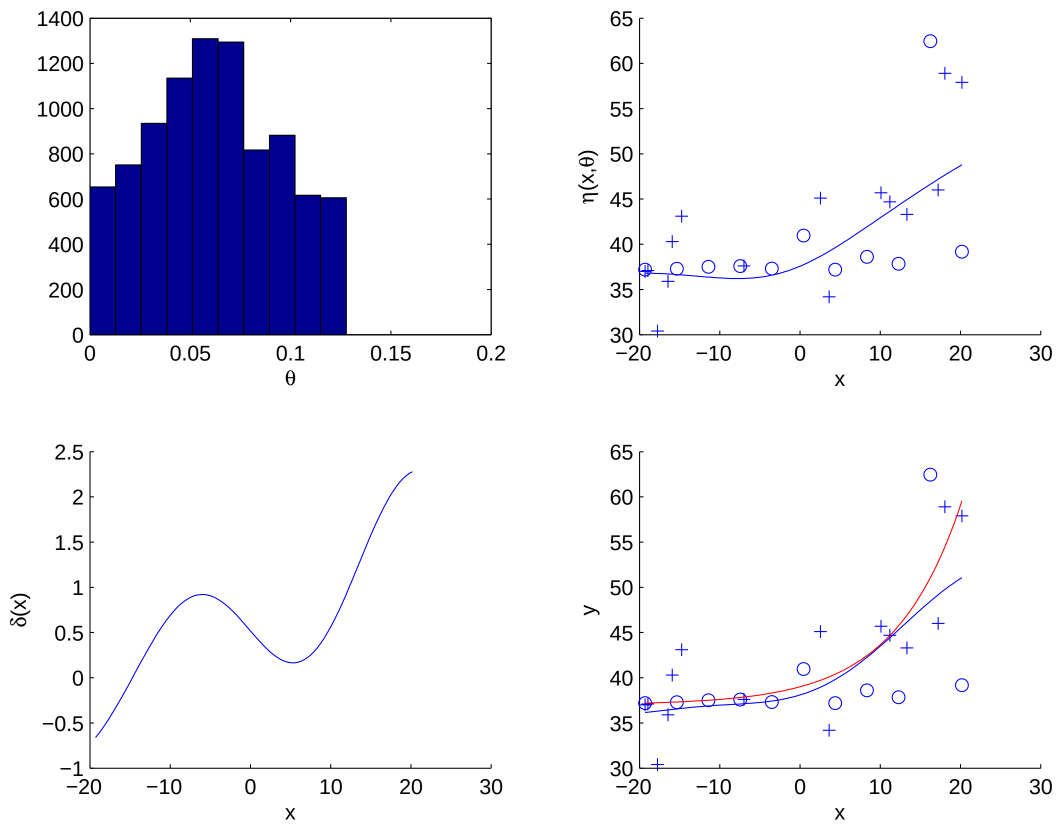
$$d|\Omega \sim N(H\mu, V_d(\theta))$$

where

$$H = \begin{pmatrix} \mathbf{1}_m & \mathbf{0} \\ \mathbf{1}_n & \mathbf{1}_n \end{pmatrix},$$

$$V_d(\theta) = \begin{pmatrix} V_1(D_1) & C_1(D_1, D_2(\theta)) \\ C_1(D_1, D_2(\theta)) & V_1(D_2(\theta)) + V_2(D_2) + \sigma_\varepsilon^2 I_n \end{pmatrix}.$$

Motivating Example



- Predicted field response (Kennedy and O'Hagan, 2001):

$$\hat{y}_f(x_0) = E\{z(x_0)|\phi = \hat{\phi}, d\} = \int E\{z(x_0)|\theta, \hat{\phi}, d\}\pi(\theta|\hat{\phi}, d)d\theta$$

- MSE of prediction:

$$\begin{aligned}
&\mathrm{MSE}[\hat{y}_f(x_0|\theta)] \\
&\quad = E[\hat{y}_f(x_0|\theta) - y_f(x_0|\theta)]^2 \\
&\quad = \sigma_\eta^2 + \sigma_\delta^2 + \sigma_\varepsilon^2 + \\
&\quad + C_f(x_0, \theta)^T V_d(\theta) C_f(x_0, \theta) - 2C_f(x_0, \theta)^T t_f(x_0, \theta),
\end{aligned}$$

and

$$\mathrm{MSE}[\hat{y}_f(x_0)] = \int \mathrm{MSE}[\hat{y}_f(x_0|\Omega)]\pi(\Omega|d)d\Omega$$

- Integrated MSE of prediction over design space $\mathcal{D} \subset R^p$:

$$\mathrm{IMSE}(\theta) = \int_{\mathcal{D}} \mathrm{MSE}[\hat{y}_f(x_0|\Omega)]dx_0,$$

and

$$\text{IMSE} = \int \text{IMSE}(\Omega)\pi(\Omega|d)d\Omega = \int\int_{\mathcal{D}} \text{MSE}[\hat{y}_f(x_0|\Omega)]\pi(\Omega|d)dx_0 d\Omega,$$

- Modified IMSE after adding candidate design points:

$$\text{IMSE}(X_{\text{new}}) = \int\int_{\mathcal{D}} \text{MSE}[\hat{y}_f(x_0|\Omega, X_{\text{new}})]\pi(\Omega|d)dx_0 d\Omega,$$

where $\hat{y}_f(x_0|\Omega, X_{\text{new}})$ and $\text{MSE}[\hat{y}_f(x_0|\Omega, X_{\text{new}})]$ will be calculated based on the same parameter estimates but with the augmented D_1 and D_2.

Design Searching Algorithm (Exchange Algorithm)

1. Randomly generate a set of new design points, X_{new}, to form the initial augmented design;
2. Determine the worst design point $x_{i_0} \in X_{\text{new}}$ at current stage:
   1) Exclude one of the design points x_i from X_{new} to form X_{new}^{i-};
   2) Compute $\text{IMSE}(X_{\text{new}}^{i-})$ for each $x_i \in X_{\text{new}}$;
   3) Decide $x_{i_0} = arg \min_{x_i \in X_{\text{new}}} \text{IMSE}(X_{\text{new}}^{i-})$.
3. Search for a replacement for x_{i_0}:
   1) Select x_k from a candidate set X_{can}, presumably a grid of design space, to form $X_k^+ = (X_{\text{new}}^{i-}, x_k)$;
   2) Computer $\text{IMSE}(X_k^+)$ for each $x_k \in X_{\text{can}}$;
   3) Decide $x_{k_0} = arg \min_{x_k \in X_{\text{can}}} \text{IMSE}(X_k^+)$ as the current replacement.

4. Repeat steps 2 and 3 until some stopping criterion met.

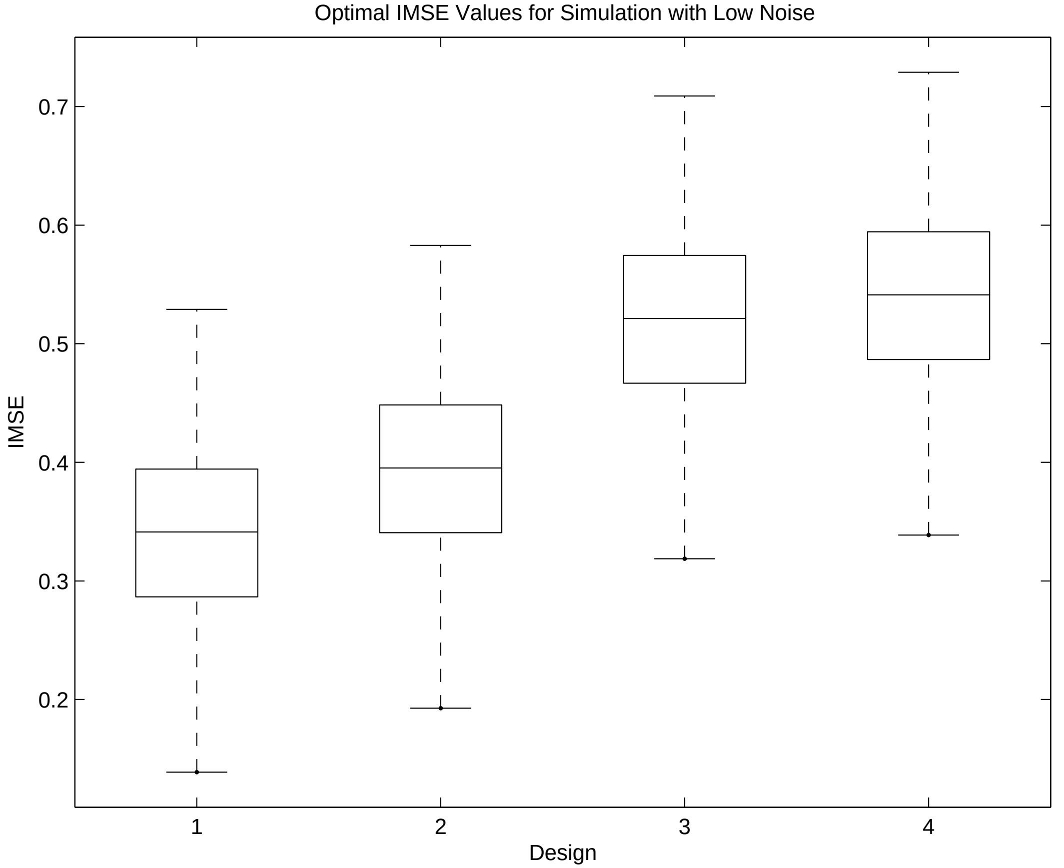
5. Restart from step 1 for a number of times.

Simulation Comparisons

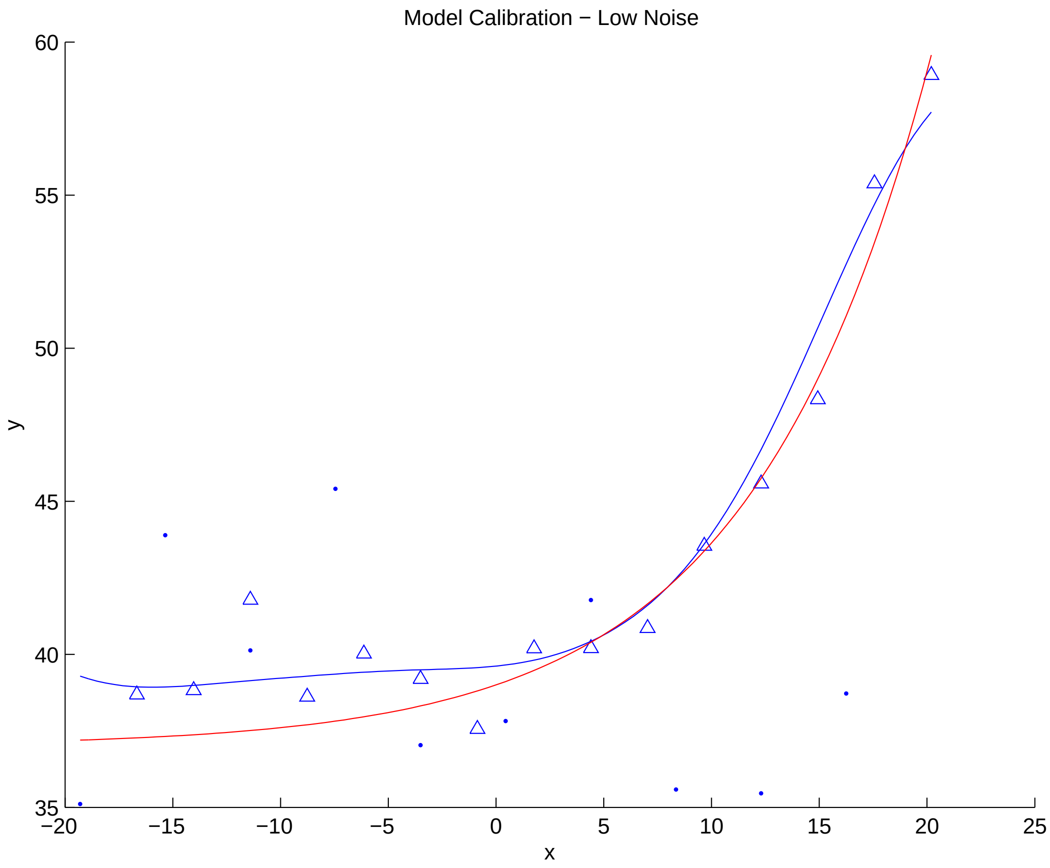
4 classes of designs

1. Optimal Designs
2. One point Replication
3. Half Replication
4. Full Replication

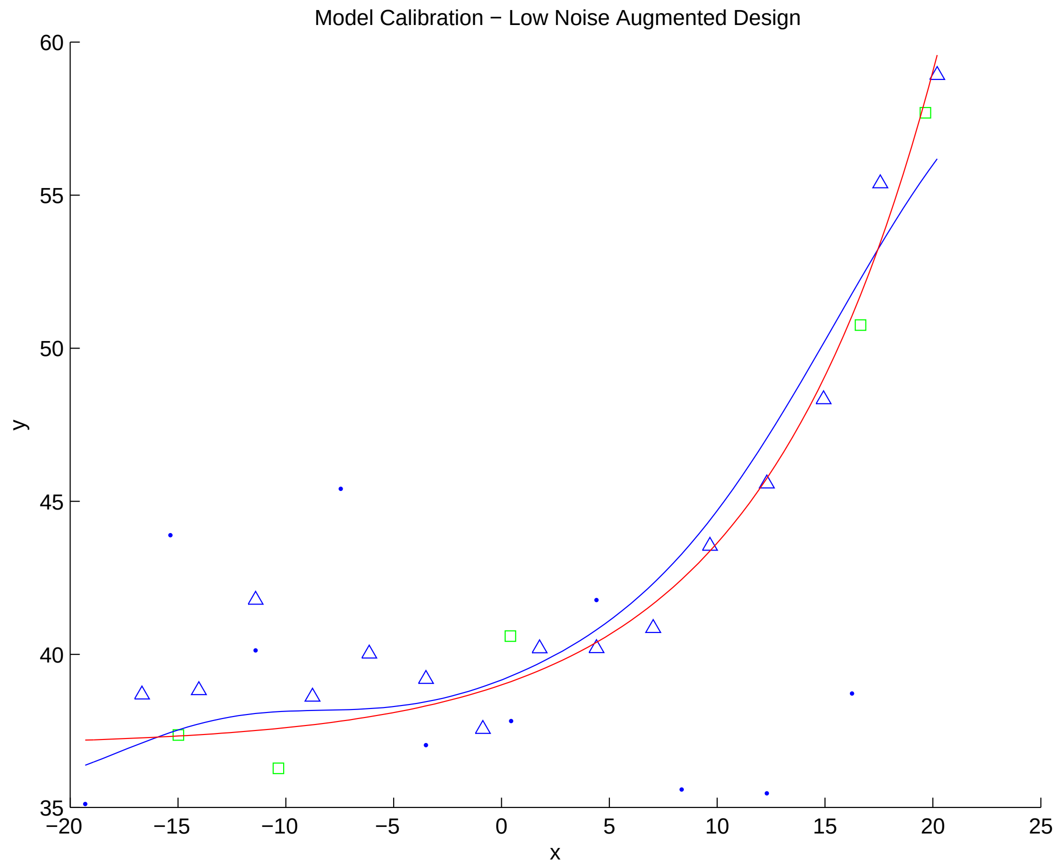
Simulation Results: σ_ε^2 small



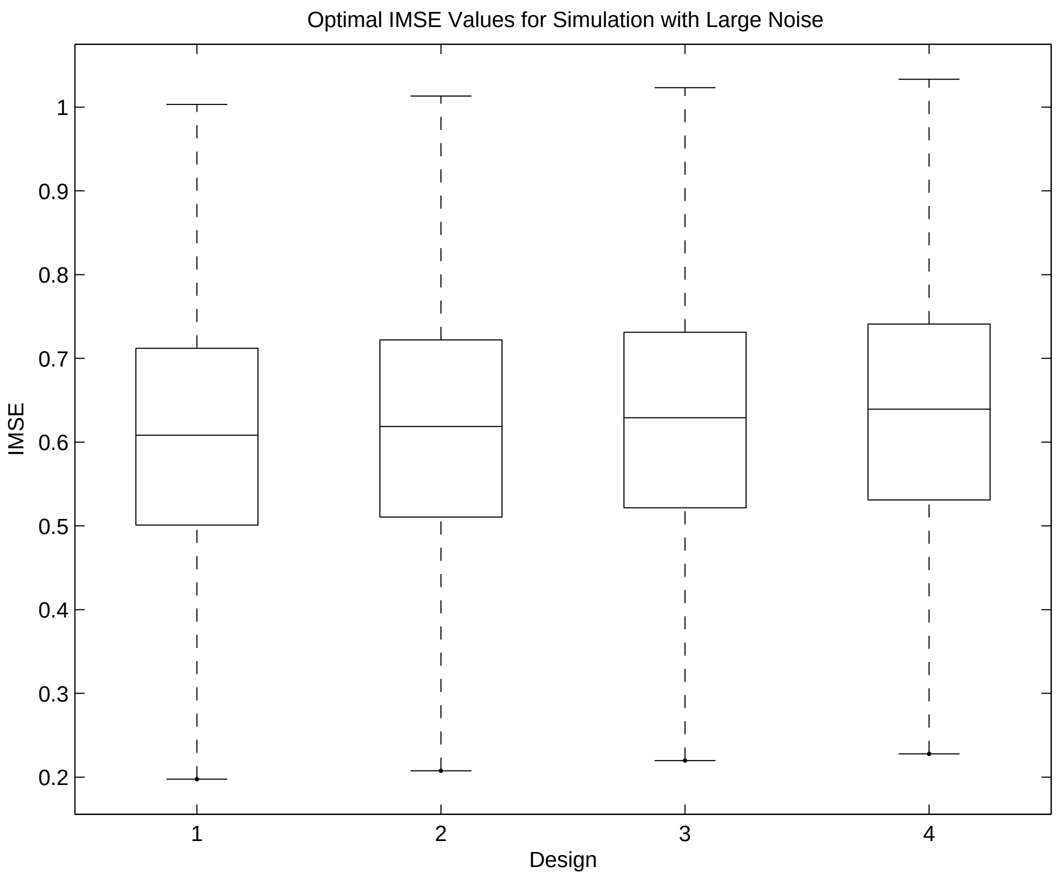
Calibration Plots



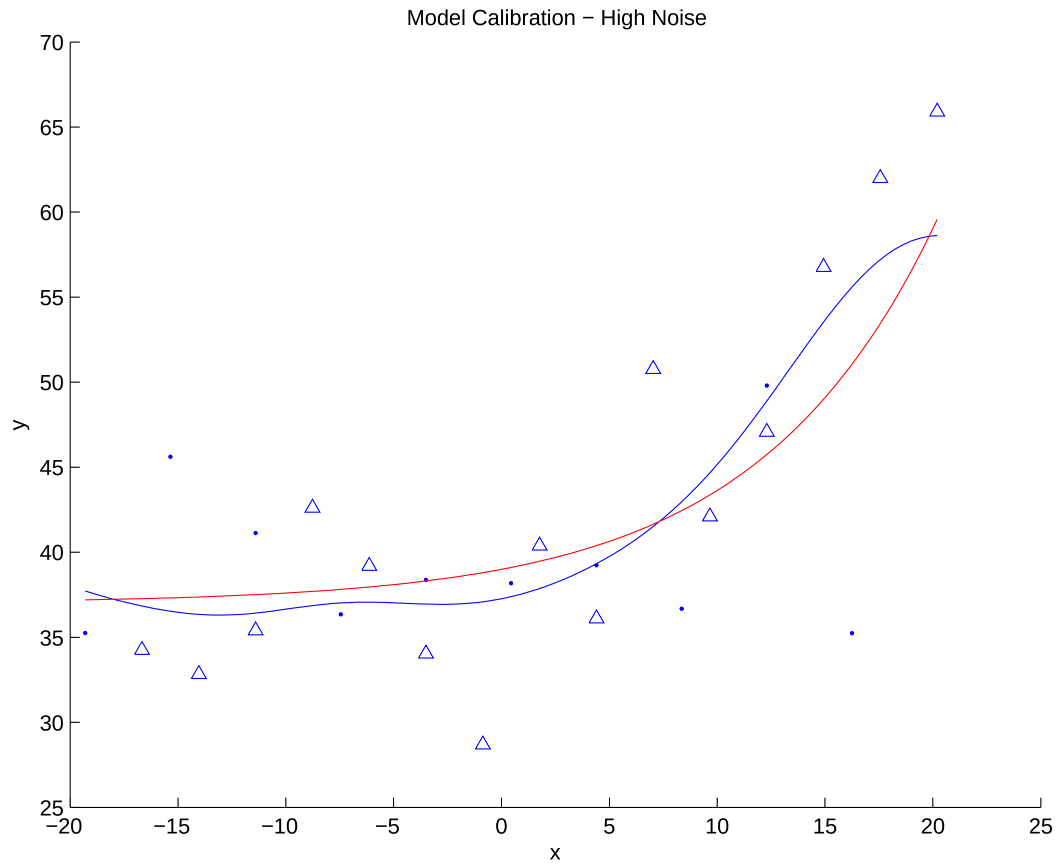
Calibration Plots



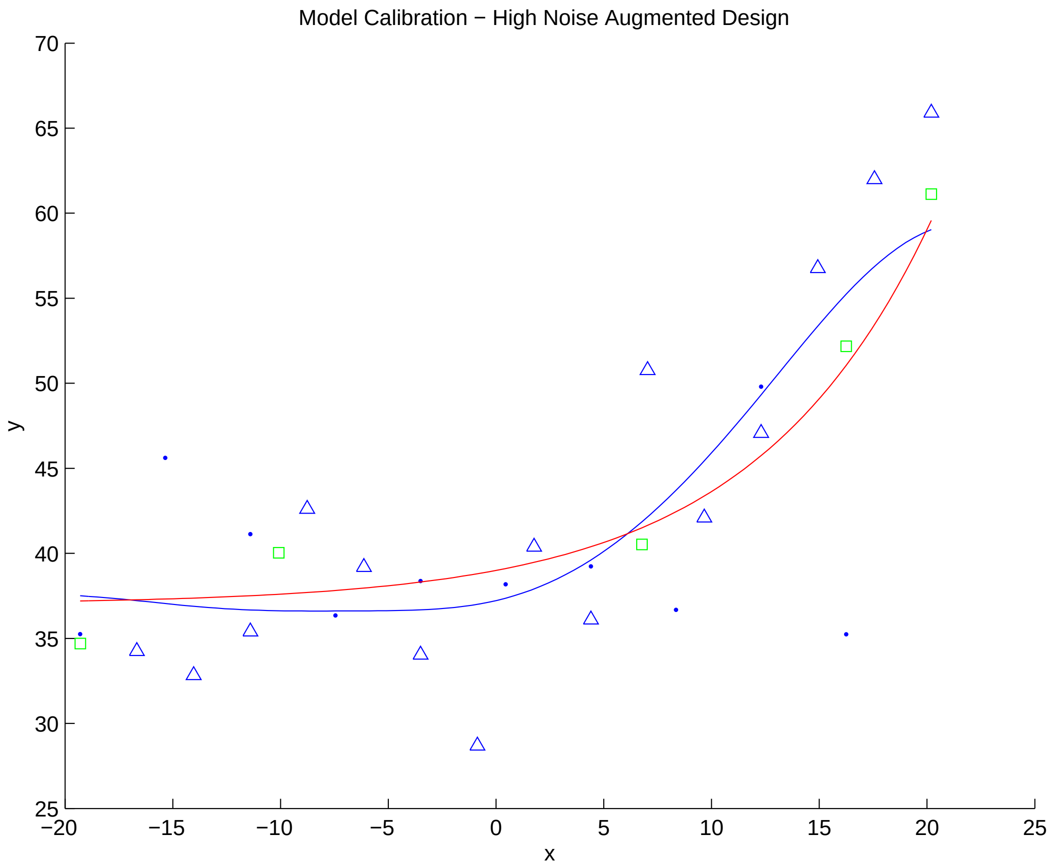
Simulation Results: σ_ε^2 large



Calibration Plots



Calibration Plots



Computer Only Runs Available

- Computer model prefers alignment with field observations
  1. Prediction of discrepancy surface ($\delta(\cdot)$)
  2. Noise estimation
- Note: Field observation prediction still goal.
- Noise appears to have little effect on results.
- Other criteria will yield substantially different results.

Comments

1. Question: What is value of replication?
   - Seems that replication is helpful, especially in presence of larger variability
2. Question: What is value of alignment of computer and physical trials?
   - Optimal design rarely (never?) aligns the computer and physical trials as a starting design, but efficiency is comparable...may wish to do so

Further research

1. Cost function to account for balance between costs:

$$C = c_1 \cdot m_{\text{new}} + c_2 \cdot n_{\text{new}}.$$

   With a fixed total cost C, the best combination of m_{new} and n_{new}.

2. Combined Physical/Computer Trials...measuring value of computer model.

Conclusions

- Value of replication
- Criteria
- Joint nature of θ and $\delta(\cdot)$.
- Knowledge of computational models is essential to solve joint nature problem....not a black box.

Simulation Results: σ_ε^2 moderate