# Diagnostics for Gaussian Process Emulators

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Managing Uncertainty in Complex Models

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# Outline

1. Introduction
   - Motivation
   - Notation
   - Gaussian Process Emulator
2. Diagnostics
   - Individual prediction errors
   - Mahalanobis distance
   - Uncorrelated prediction errors
3. Conclusion and work in progress

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# Motivation

- Emulators are stochastic approximations of computer models
- Non-valid emulators can induce wrong conclusions
- There is little research into validating emulators
- Validation often means little more than:
  "*We compared some predictions with some observations and look, they fit quite well*"
- Present some diagnostics checking whether an emulator is valid or not, taking account all the associated uncertainty.

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# Notation

- **Simulator** is a complex deterministic mathematical function

$$\eta(\cdot) \qquad \eta : \mathcal{X} \in \Re^p \to \Re$$

- **Gaussian process emulator**

$$\eta(\cdot)|\beta, \sigma^2, \psi \sim GP\left(m_0(\cdot), V_0(\cdot, \cdot)\right),$$

where

$$\begin{aligned} m_0(\mathbf{x}) &= h(\mathbf{x})^T \beta \\ V_0(\mathbf{x}, \mathbf{x}') &= \sigma^2 C(\mathbf{x}, \mathbf{x}'; \psi) \end{aligned}$$

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# Gaussian Process Emulators

- **Training data** $(\mathbf{y}, \mathbf{X}) \quad : \quad y_i = \eta(\mathbf{x}_i), \quad i = 1, \ldots, n$
- **Predictive Gaussian Process Emulator**

$$\eta(\cdot)|\mathbf{y}, \mathbf{X}, \psi = \hat{\psi} \sim \text{Student-Process}\left(n - q, m_1(\cdot), V_1(\cdot, \cdot)\right),$$

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$$\begin{aligned} m_1(x) &= h(x)^T\widehat{\beta} + t(x)^T\mathbf{A}^{-1}(\mathbf{y} - H\widehat{\beta}), \\ V_1(x, x') &= \hat{\sigma}^2\Big[C(x, x'; \psi) - t(x)^T\mathbf{A}^{-1}t(x') + \left(h(x) - t(x)^T\mathbf{A}^{-1}H\right) \\ &\times \left(H^T\mathbf{A}^{-1}H\right)^{-1}\left(h(x') - t(x')^T\mathbf{A}^{-1}H\right)^T\Big]. \end{aligned}$$

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- Our diagnostics are based on a set of new simulator runs
  **Validation data** $(\mathbf{y}^*, \mathbf{X}^*) \quad : \quad y_i^* = \eta(\mathbf{x}_i^*), \quad i = 1, \ldots, m$
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- Proposal diagnostics:
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# Toy example

- $\eta(\mathbf{x})$ is a Gaussian process $\left(\mathbf{x}^T\beta,\ \sigma^2 \exp\{\sum_k (\frac{x_k - x'_k}{\psi_k})^2\}\right)$
- 100 training data points (Maximin LHS design)
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- 3 scenarios: (Varying the plug-in correlation parameters)

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# Diagnostics

## Individual standardized prediction errors

$$D_i(\mathbf{y}^*) = \frac{(y_i^* - E[\eta(\mathbf{x}_i^*)])}{\sqrt{V[\eta(\mathbf{x}_i^*, \mathbf{x}_i^*)]}}, i = 1, \ldots, n$$

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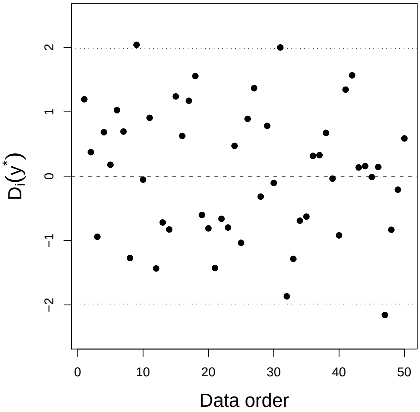


- The dotted lines indicate the 95% credible limits
- A large number of extreme errors might indicate a stationarity problem
- Too many **large errors** suggest **under-estimation** of the uncertainty
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However, these errors are not independent!

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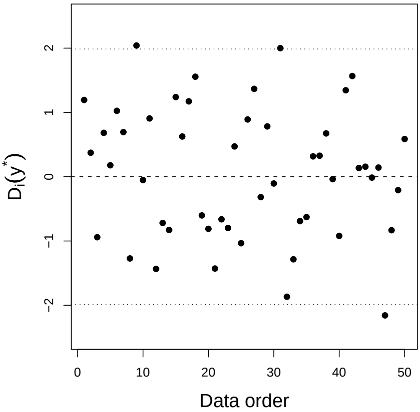


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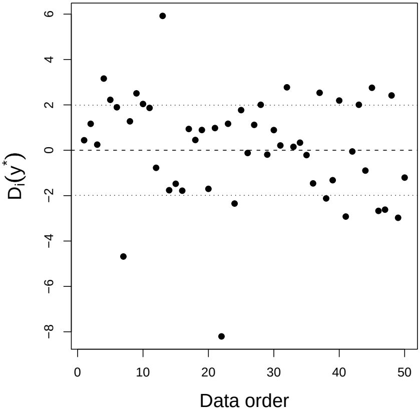


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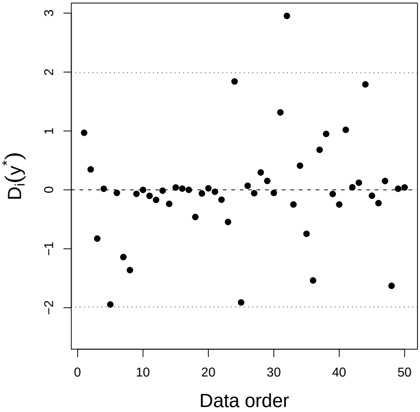


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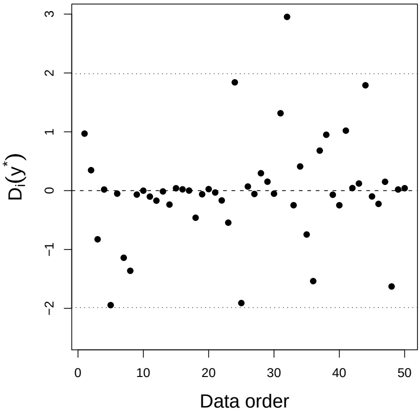


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## Mahalanobis distance

$$D_{MD}(\mathbf{y}^*) = (\mathbf{y}^* - m_1(\mathbf{X}^*))^T \, V_1(\mathbf{X}^*)^{-1} \, (\mathbf{y}^* - m_1(\mathbf{X}^*))$$

- Large values for $D_{MD}(\mathbf{y}^*)$ are associated with
  - Large individual errors
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$$\frac{(n-q)}{m(n-q-2)} D_{MD}(\eta(\mathbf{X}^*)) \sim F_{m,n-q}$$

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# Numerical diagnostics

## Uncorrelated prediction errors

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where $V_1(\mathbf{X}^*) = \mathbf{G}^{\mathbf{T}}\mathbf{G}$.

- Cholesky decomposition: $\mathbf{G}$ is a triangular matrix
- Eigen decomposition: $\mathbf{G} = \Lambda^{1/2} E^T$
- Pivoted Cholesky decomposition: $\mathbf{G} = \mathbf{P}\mathbf{R}^T$, $\mathbf{P}$ is a permutation matrix

$$D^G(\mathbf{y}^*) \sim \text{Student-t}_m(n-q, \mathbf{0}, \mathcal{I}_m)$$

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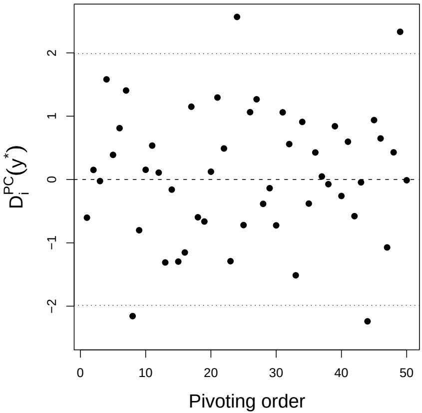
# Uncorrelated prediction errors against pivoting order




$$D_{MD}(\mathbf{y}^*) = 51.727$$

- Mahalanobis distance close to its expected value (50.0)
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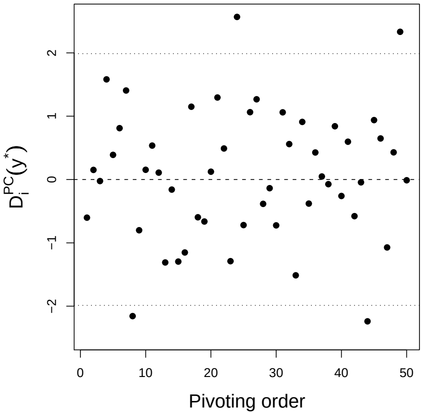


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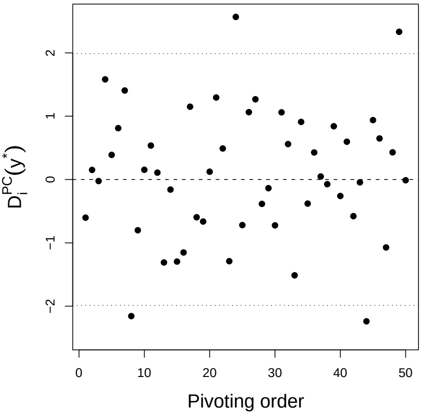


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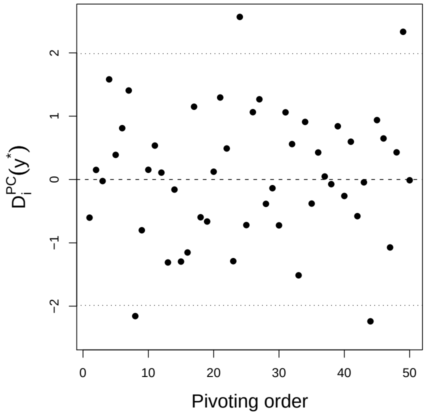


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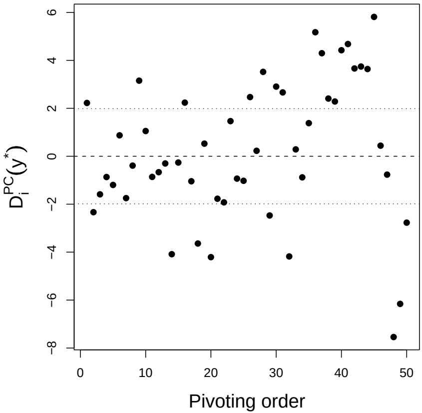


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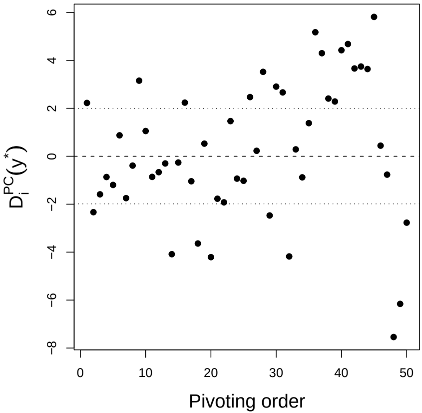


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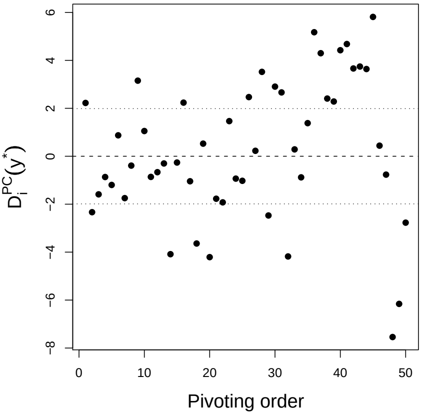


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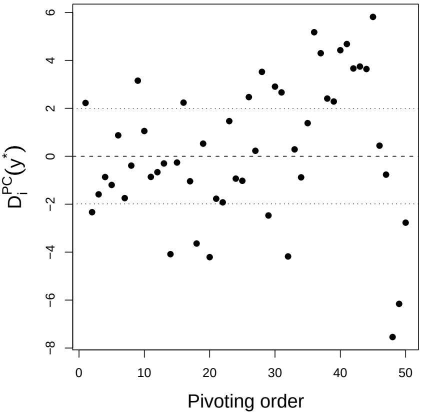


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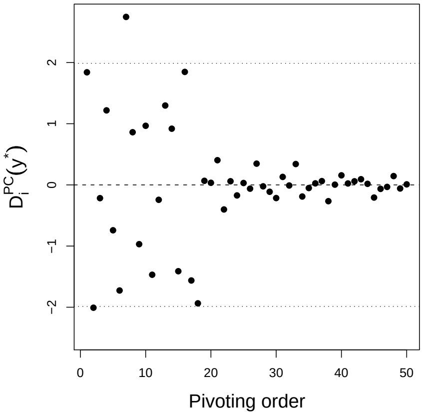


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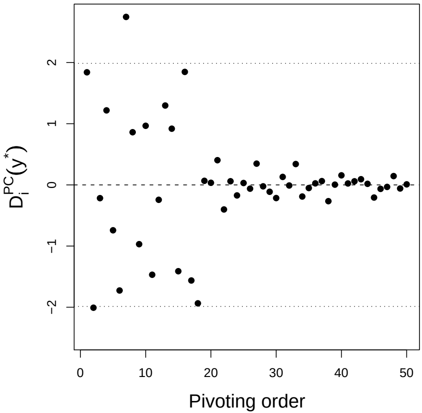


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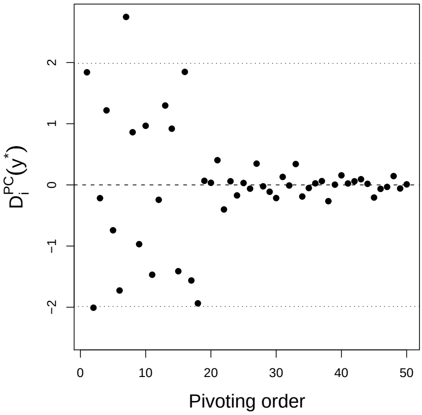


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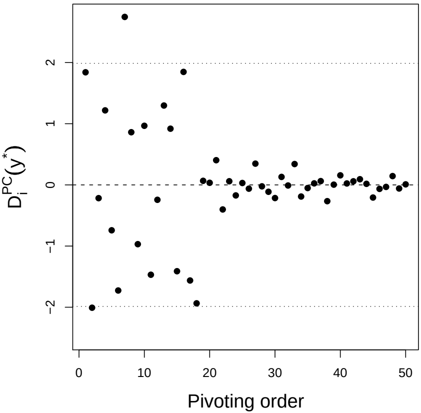


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# More graphical methods

- Individual errors against emulator's predictions
- QQ-plots of the uncorrelated standardized errors
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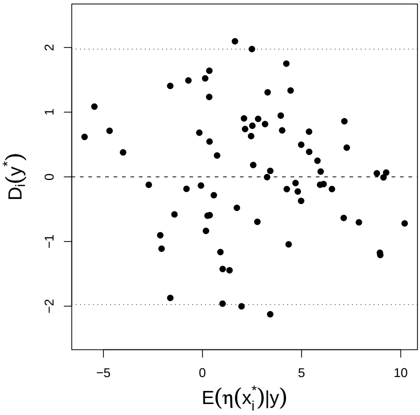


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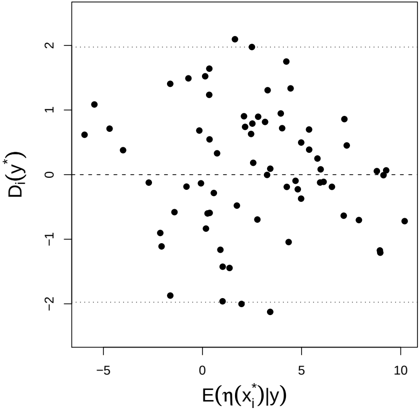


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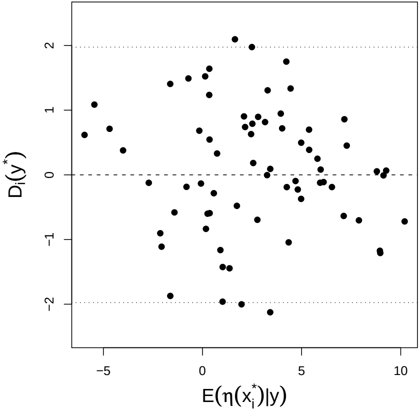


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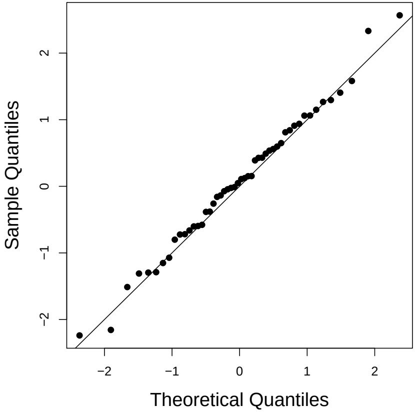


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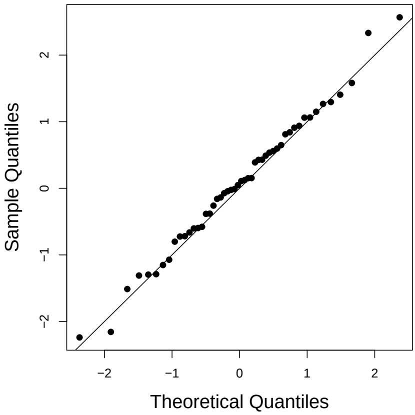


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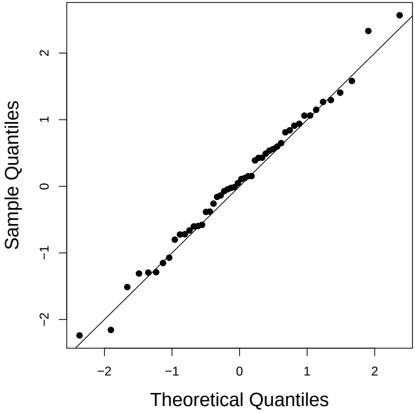


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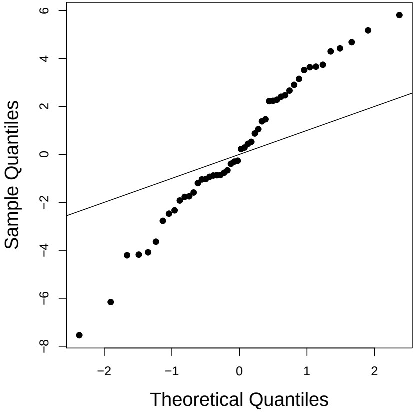


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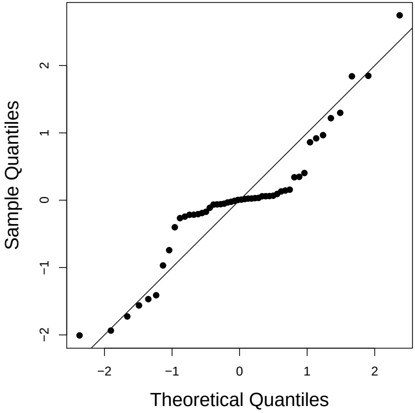


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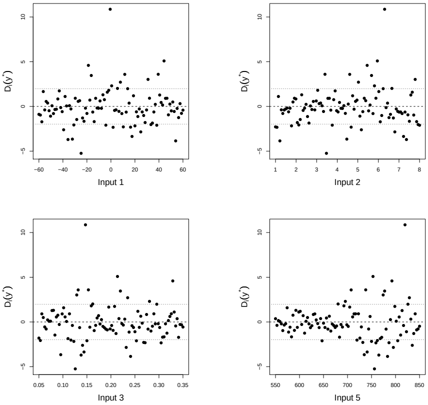


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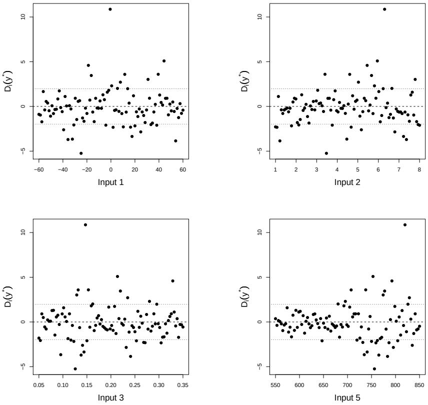


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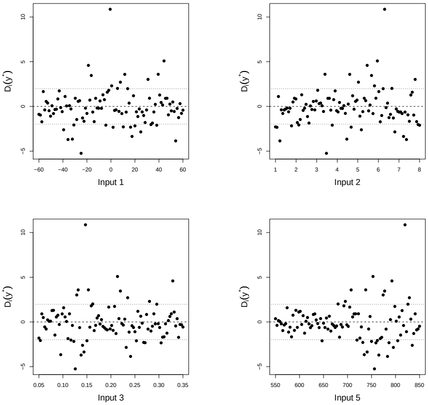


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- Our diagnostics are useful tools in the process of validating an emulator
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  - Design for validation
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