Bayesian Functional Data Analysis for Computer Model Validation

Fei Liu

Institute of Statistics and Decision Sciences
Duke University

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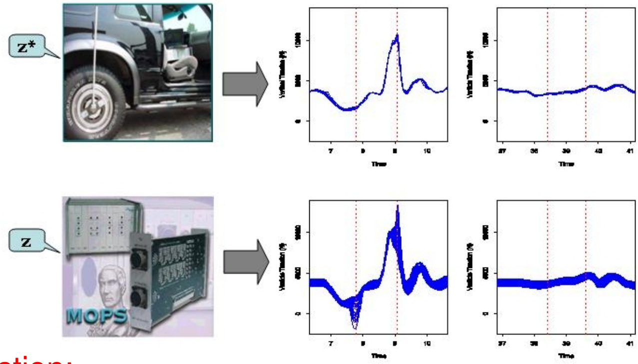
Joint work with J. O. Berger et al.

Outline

Outline

Computer model validation



Question:

Does the computer model adequately represent the reality?

Challenge 1 - Expensive-to-run

- Simulator $y^M(\boldsymbol{z})$ is exercised only at

$$y^M(\boldsymbol{z}_1), \ldots, y^M(\boldsymbol{z}_n) \,.$$

- *GaSP* (Sacks *et al.*, 1989) uses statistical models as fast surrogates,

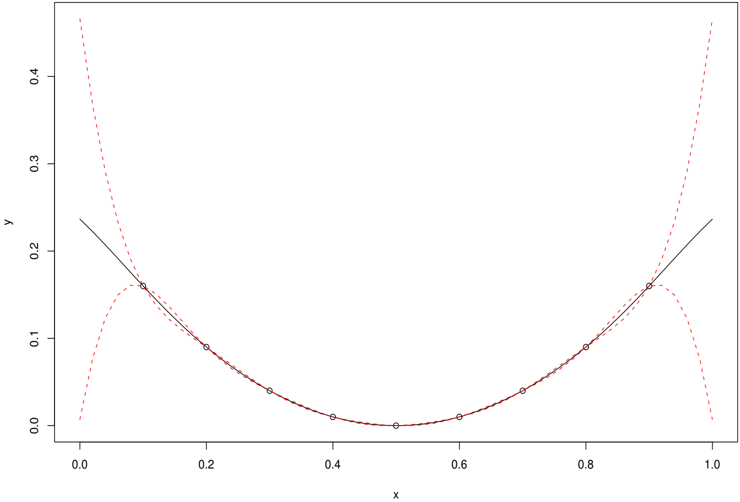
  - Prior:

$$y^M(\cdot) \sim \mathrm{GP}\left(\boldsymbol{\Psi}'(\cdot)\theta^L, \frac{1}{\lambda^M} c^M(\cdot,\cdot)\right) \,.$$

  - Emulator:

$$y^M(\boldsymbol{z}) \mid \mathrm{Data} \sim \mathrm{N}\left(\widehat{m}(\boldsymbol{z}), \widehat{V}(\boldsymbol{z})\right) \,.$$

Interpolator



Challenge 2 - Multiple sources of uncertainty

- Kennedy and O'Hagan (2001) give a broad discussion.
- Three major ones are:
  - Code uncertainty.
  - Calibration input $\boldsymbol{u}^*$.
  - Bias $b_{\boldsymbol{u}^*}$.
- *SAVE* (Bayarri *et al.*, 2005) models scalar outputs as

$$y_r^F(\boldsymbol{v}) = y^M(\boldsymbol{u}^*, \boldsymbol{v}) + b_{\boldsymbol{u}^*}(\boldsymbol{v}) + e_r(\boldsymbol{v}) \, .$$

  - Confounding between $\boldsymbol{u}^*$ and b.
  - Need informative priors.

More challenges

- Uncertain (field) inputs.

$$\boldsymbol{z} = (\boldsymbol{v}, \boldsymbol{u}, \delta) \,.$$

  - $\boldsymbol{v}$: configuration inputs.
  - $\boldsymbol{u}$: calibration inputs (true $\boldsymbol{u}^*$).
  - δ: unknown field inputs (true δ^*).
  - Let $(\boldsymbol{v}_i, \delta^*_{ij})$ denote those for the j^{th} field run in the i^{th} configuration.

- Functional outputs (over time).

  SAVE (Bayarri *et al.*, 2005) treats time t as another input.

Bias structure

$$
\begin{aligned}
y_r^F(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*; t) &= y^M(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*; t) + b(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*; t) + e_{ijr}(t)\,, \\
b(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*; t) &= b_{\boldsymbol{u}^*}(\boldsymbol{v}_i, t) + \epsilon_{ij}^b(t)\,.
\end{aligned}
$$

$$
\begin{aligned}
y^M &: \text{known}\,, \\
b(\cdot,\cdot) &\sim \mathrm{GP}\left(\mu_b, \tau^2 \mathbb{C}\mathrm{orr}_v(\cdot,\cdot)\mathbb{C}\mathrm{orr}_t(\cdot,\cdot)\right)\,, \\
\epsilon_{ij}^b(\cdot) &\sim \mathrm{GP}\left(0, \sigma_b^2 \mathbb{C}\mathrm{orr}_t(\cdot,\cdot)\right)\,, \\
e_{ijr}(\cdot) &\sim \mathrm{GP}\left(0, \sigma^2 \mathbb{C}\mathrm{orr}_t(\cdot,\cdot)\right)\,.
\end{aligned}
$$

Limitations

- Treating t as another input,
  - is only applicable to low dimensional problem.
  - need smoothness assumption.
- Need new methodology to deal with:
  - Complex computer models.
  - High dimensional irregular functional output.
  - Uncertain (field) inputs.

Outline

Notation

$$y_r^F(\boldsymbol{v}_i, \delta_{ij}^*; t) = y^M(\boldsymbol{v}_i, \delta_{ij}^*, \boldsymbol{u}^*; t) + y_{\boldsymbol{u}^*}^B(\boldsymbol{v}_i, \delta_{ij}^*; t) + e_{ijr}(t)$$

Notation

$$y^F_r(\boldsymbol{v}_i, \delta^*_{ij}; t) = y^M(\boldsymbol{v}_i, \delta^*_{ij}, \boldsymbol{u}^*; t) + y^B_{\boldsymbol{u}^*}(\boldsymbol{v}_i, \delta^*_{ij}; t) + e_{ijr}(t)$$

- Inputs to the code.
  - $\boldsymbol{v}_i$: configuration.
  - δ^*_{ij}: unknown inputs.
  - $\boldsymbol{u}^*$: calibration parameters.
- Simulator.
- Bias function.
- Reality y^R.
- Field runs.
- Measurement errors.

Notation

$$y_r^F(\boldsymbol{v}_i, \delta_{ij}^*; t) = y^M(\boldsymbol{v}_i, \delta_{ij}^*, \boldsymbol{u}^*; t) + y_{\boldsymbol{u}^*}^B(\boldsymbol{v}_i, \delta_{ij}^*; t) + e_{ijr}(t)$$

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- Measurement errors.

Basis expansion

Represent the functions as:

$$
\begin{aligned}
y^M(\boldsymbol{z}_j; t) &= \textstyle\sum_{k=1}^W w_k^M(\boldsymbol{z}_j)\psi_k(t), && j = 1, \ldots, n^M; \\
y^B_{\boldsymbol{u}^*}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}; t) &= \textstyle\sum_{k=1}^W w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\psi_k(t), && i = (1, \ldots, m), \\
& && j = (1, \ldots, n_i^f); \\
y^F_r(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}; t) &= \textstyle\sum_{k=1}^W w_{kr}^F(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\psi_k(t), && r = 1, \ldots, r_{ij}.
\end{aligned}
$$

Thresholding

Reduce computational expense,

$$
\begin{aligned}
y^M(\boldsymbol{z}_j;t) &\approx \textstyle\sum_{k=1}^{W_0} w_k^M(\boldsymbol{z}_j)\psi_k(t), && j=1,\ldots,n^M;\\
y^B_{\boldsymbol{u}^*}(\boldsymbol{v}_i,\boldsymbol{\delta}^*_{ij};t) &\approx \textstyle\sum_{k=1}^{W_0} w_k^B(\boldsymbol{v}_i,\boldsymbol{\delta}^*_{ij})\psi_k(t), && i=(1,\ldots,m)\,,\\
& && j=(1,\ldots,n_i^f)\,;\\
y^F_r(\boldsymbol{v}_i,\boldsymbol{\delta}^*_{ij};t) &\approx \textstyle\sum_{k=1}^{W_0} w_{kr}^F(\boldsymbol{v}_i,\boldsymbol{\delta}^*_{ij})\psi_k(t), && r=1,\ldots,r_{ij}\,.
\end{aligned}
$$

Emulators

For each $k = 1, \ldots, W_0$,

$$w_k^M(\cdot) \sim \text{GP}\left(\mu^{M_k}, \sigma^{2M_k}\mathbb{C}\text{orr}_k(\cdot,\cdot)\right) .$$

- $\mathbb{C}\text{orr}_k(\cdot,\cdot)$: power exponential family,

$$\mathbb{C}\text{orr}_k(\boldsymbol{z},\boldsymbol{z}') = \exp\left(-\sum_{d=1}^{p} \beta_d^{(M_k)} \mid \boldsymbol{z}_d - \boldsymbol{z}'_d \mid^{\alpha_d^{(M_k)}}\right) .$$

- Modular approach:

$$\left(w_k^M(\boldsymbol{z}) \mid \text{Data}, \hat{\mu}^{M_k}, \hat{\sigma}^{2M_k}, \hat{\boldsymbol{\alpha}}^{M_k}, \hat{\boldsymbol{\beta}}^{M_k}\right) \sim \text{N}\left(\widehat{m}_k^M(\boldsymbol{z}), \widehat{V}_k^M(\boldsymbol{z})\right) .$$

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$
\begin{aligned}
w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right)\,, \\
w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\,. \\
w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= b_k(\boldsymbol{v}_i) + \epsilon^b_{ijk}
\end{aligned}
$$

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$\begin{aligned} w_{kr}^F(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) &= w_k^R(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma_k^{2F}\right)\,, \\ w_k^R(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) &= w_k^M(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*) + w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*)\,. \\ w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) &= b_k(\boldsymbol{v}_i) + \epsilon_{ijk}^b \end{aligned}$$

- Data:
  - $\bar{w}_{ijk}^F = \frac{1}{r_{ij}} \sum_{r=1}^{r_{ij}} w_{kr}^F(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*)$.
  - $S_{ijk}^2 = \sum_{r=1}^{r_{ij}} (w_{kr}^F(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) - \bar{w}_{ijk}^F)^2$.
  - $\widehat{m}_k(\cdot), \widehat{V}_k(\cdot)$.

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$\begin{aligned} w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right)\,, \\ w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\,. \\ w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= b_k(\boldsymbol{v}_i) + \epsilon^b_{ijk} \end{aligned}$$

- The bias,

$$b_k(\boldsymbol{v}_i) \sim \mathrm{GP}\left(\mu^B_k, \sigma^{2B}_k \mathbb{C}\mathrm{orr}^B_k(\cdot,\cdot)\right), \qquad \epsilon^b_{ijk} \sim \mathrm{N}(0, \sigma^{2B^\epsilon}_k)\,,$$

with correlation,

$$\mathbb{C}\mathrm{orr}^B_k(\boldsymbol{v}, \boldsymbol{v}') = \exp\left(-\sum_{d=1}^{p_v} \beta^{(B_k)}_d \mid \boldsymbol{v}_d - \boldsymbol{v}'_d \mid^{\alpha^{(B_k)}_d}\right).$$

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$
\begin{aligned}
w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right)\,, \\
w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\,. \\
w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= b_k(\boldsymbol{v}_i) + \epsilon^b_{ijk}
\end{aligned}
$$

- Unknowns:
  - Inputs: $\boldsymbol{u}^*$ and δ^*_{ij}.
  - Bias: $\{b_k(\cdot)\}$, $w^B_k(\boldsymbol{v}_i, \delta^*_{ij})$.
  - Model: $w^M_k(\boldsymbol{v}_i, \delta^*_{ij}, \boldsymbol{u}^*)$.
  - Reality: $\{w^R_k(\boldsymbol{v}_i, \delta^*_{ij})\}$
  - Hyper-parameters: σ^{2B}_k, $\sigma^{2B^\epsilon}_k$, σ^{2F}_k, μ^B_k.

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$w^F_{kr}(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}) = w^R_k(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right),$$

$$w^R_k(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}) = w^M_k(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}, \mathbf{u}^*) + w^B_k(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}).$$

$$w^B_k(\mathbf{v}_i, \boldsymbol{\delta}^*_{ij}) = b_k(\mathbf{v}_i) + \epsilon^b_{ijk}$$

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  - Model: $w^M_k(\mathbf{v}_i, \delta^*_{ij}, \mathbf{u}^*)$.
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  - Hyper-parameters: σ^{2B}_k, $\sigma^{2B^\epsilon}_k$, σ^{2F}_k, μ^B_k.

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) = w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right)\,,$$

$$w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) = w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\,.$$

$$w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) = b_k(\boldsymbol{v}_i) + \epsilon^b_{ijk}$$

- Unknowns:
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  - Bias: $\{b_k(\cdot)\}$, $w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})$.
  - Model: $w^M_k(\boldsymbol{v}_i, \delta^*_{ij}, \boldsymbol{u}^*)$.
  - Reality: $\{w^R_k(\boldsymbol{v}_i, \delta^*_{ij})\}$
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Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$\begin{aligned} w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right)\,, \\ w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\,. \\ w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) &= b_k(\boldsymbol{v}_i) + \epsilon^b_{ijk} \end{aligned}$$

- Unknowns:
  - Inputs: $\boldsymbol{u}^*$ and $\boldsymbol{\delta}^*_{ij}$.
  - Bias: $\{b_k(\cdot)\}$, $w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})$.
  - Model: $w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*)$.
  - Reality: $\{w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\}$
  - Hyper-parameters: σ^{2B}_k, $\sigma^{2B^\epsilon}_k$, σ^{2F}_k, μ^B_k.

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$w_{kr}^F(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) = w_k^R(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) + \epsilon_{ijkr}\,, \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma_k^{2F}\right)\,,$$

$$w_k^R(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) = w_k^M(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*) + w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*)\,.$$

$$w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*) = b_k(\boldsymbol{v}_i) + \epsilon_{ijk}^b$$

- Unknowns:
  - Inputs: $\boldsymbol{u}^*$ and $\boldsymbol{\delta}_{ij}^*$.
  - Bias: $\{b_k(\cdot)\}$, $w_k^B(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*)$.
  - Model: $w_k^M(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*, \boldsymbol{u}^*)$.
  - Reality: $\{w_k^R(\boldsymbol{v}_i, \boldsymbol{\delta}_{ij}^*)\}$
  - Hyper-parameters: σ_k^{2B}, $\sigma_k^{2B^\epsilon}$, σ_k^{2F}, μ_k^B.

Bayesian analysis

For each $k = 1, \ldots, W_0$,

$$w^F_{kr}(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) = w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) + \epsilon_{ijkr} , \qquad \epsilon_{ijkr} \sim \mathrm{N}\left(0, \sigma^{2F}_k\right) ,$$

$$w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) = w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*) + w^B_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}) .$$

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- Unknowns:
  - Inputs: $\boldsymbol{u}^*$ and $\boldsymbol{\delta}^*_{ij}$.
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  - Model: $w^M_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij}, \boldsymbol{u}^*)$.
  - Reality: $\{w^R_k(\boldsymbol{v}_i, \boldsymbol{\delta}^*_{ij})\}$
  - Hyper-parameters: σ^{2B}_k, $\sigma^{2B^\epsilon}_k$, σ^{2F}_k,μ^B_k.

Outline

The road load data 1

- Time history data at $T = 90843$ time points.
- Inputs include:
  - One configuration $\boldsymbol{v} = \boldsymbol{x}_{nom}$.
  - Seven characteristics $\boldsymbol{x} = (x_1, x_2, \ldots, x_7)$, $\boldsymbol{x} = \boldsymbol{x}_{nom} + \delta$.
  - Two calibration parameters $\boldsymbol{u} = (u_1, u_2)$.

The road load data 2

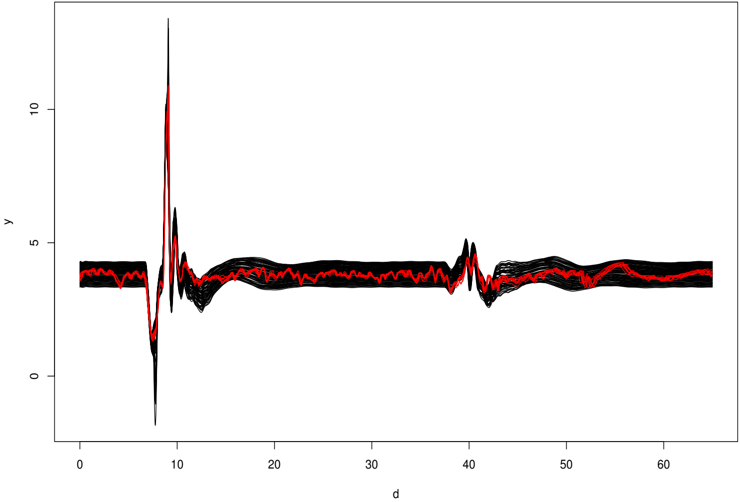
- 64 design points in 9-d space for computer model runs.

$$\{y^M(\boldsymbol{z}, t), \boldsymbol{z} \in \mathrm{D}^M, t \in 1, \ldots, T\}, \qquad \boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{u}).$$

- 7 field replicates.

$$\{y_r^F(\boldsymbol{x}^*, t), r \in (1, \ldots, 7)\}, \qquad \boldsymbol{x}^* = \boldsymbol{x}_{nom} + \delta^*.$$

The road load data 3



Wavelet representation

- Represent the time history data by wavelets:

$$y^M(\boldsymbol{z}_j; t) = \sum_{k=1}^{W} w_k^M(\boldsymbol{z}_j)\psi_k(t), \qquad j = 1, \ldots, 64;$$

$$y_r^F(\boldsymbol{x}^*; t) = \sum_{k=1}^{W} w_{kr}^F(\boldsymbol{x}^*)\psi_k(t), \qquad r = 1, \ldots, 7.$$

- Apply hard thresholding to reduce the computational expense.

  keep $W_0 = 289$ nonzero coefficients.

Emulators

For each wavelet coefficient,

$$w_k^M(\cdot) \sim \mathrm{GP}\left(\mu_k, \frac{1}{\lambda_k^M}\mathbb{C}\mathrm{orr}_k(\cdot,\cdot)\right).$$

- $\mathbb{C}\mathrm{orr}_k(\cdot,\cdot)$: power exponential family,

$$\mathbb{C}\mathrm{orr}_k(\boldsymbol{z},\boldsymbol{z}') = \exp\left(-\sum_{d=1}^{p} \beta_d^{(k)} \mid \boldsymbol{z}_d - \boldsymbol{z}_d' \mid^{\alpha_k^{(k)}}\right).$$

- Response Surface:

$$\left(w_k^M(\boldsymbol{z}) \mid \mathrm{Data}, \hat{\mu}_k, \hat{\lambda}_k^M, \hat{\boldsymbol{\alpha}}_k, \hat{\boldsymbol{\beta}}_k\right) \sim \mathrm{N}\left(\widehat{m}_k(\boldsymbol{z}), \widehat{V}_k(\boldsymbol{z})\right).$$

Bayesian analysis

- For each wavelet coefficient,

$$w_i^R(\boldsymbol{x}^*) = w_i^M(\boldsymbol{x}^*, \boldsymbol{u}^*) + b_i(\boldsymbol{x}^*), \qquad i = 1, \ldots, W,$$

$$w_{ir}^F(\boldsymbol{x}^*) = w_i^R(\boldsymbol{x}^*) + \epsilon_{ir}, \qquad r = 1, \ldots, f.$$

- The bias,

$$b_i(\boldsymbol{x}^*) \sim \mathrm{N}\left(0, \tau_j^2\right) \quad \text{or} \quad b_i(\boldsymbol{x}^*) \sim \mathrm{C}\left(0, \tau_j^2\right).$$

j: wavelet resolution level .

- The error,

$$\epsilon_{ir} \sim \mathrm{N}\left(0, \sigma_i^2\right).$$

Prior distributions

- The Input/Uncertainty Map,

Parameter	Type	Variability	Uncertainty
Damping_1	Calibration	Uncertain	15%
Damping_2	Calibration	Uncertain	15%
Stiffness_1	Manufacturing	Uncertain	10%
Stiffness_2	Manufacturing	Uncertain	10%
Front-rebound_1	Manufacturing	Uncertain	7%
Front-rebound_2	Manufacturing	Uncertain	8%
Sprung-Mass	Manufacturing	Uncertain	5%
Unsprung-Mass	Manufacturing	Uncertain	12%
Body-Pitch-Inertia	Manufacturing	Uncertain	8%

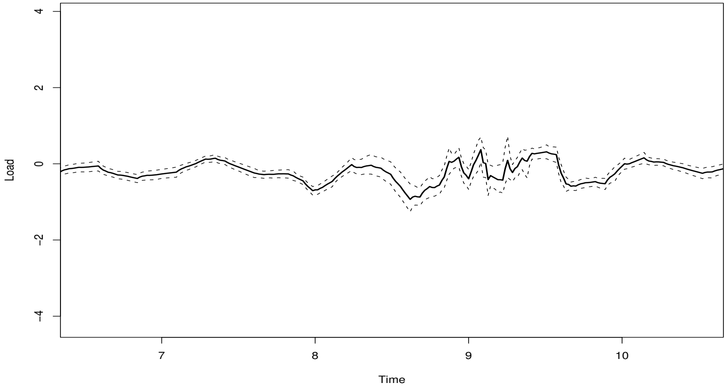
  Calibration: uniform over specified range.

  Manufacturing: truncated normals over the ranges.

- $\pi(\sigma_i^2) \propto 1/\sigma_i^2$, $\pi(\tau_j^2 \mid \{\sigma_i^2\}) \propto \frac{1}{\tau_j^2 + \frac{1}{7}\bar{\sigma}_j^2}$.

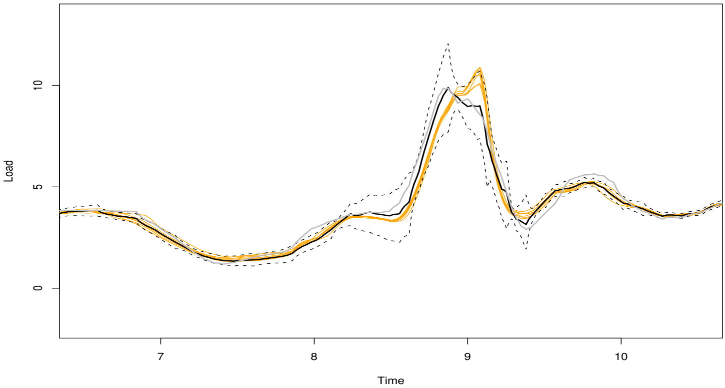
Bias under Gaussian assumption (Full Bayes)

$$b^h(t) = \sum_{i=1}^{W} b_i^h \psi_i(t), h = 1, \ldots, N$$



Reality under Gaussian assumption (Full Bayes)

$$y^{Rh}(\boldsymbol{u}^{*h}, \boldsymbol{x}^{*h}, t) = \sum_{i=1}^{W} \left(w_i^{Mh}(\boldsymbol{u}^{*h}, \boldsymbol{x}^{*h}) + b_i^h \right) \psi_i(t), h = 1, \ldots, N$$



Issue with the Gaussian bias

Confounding between $\boldsymbol{\sigma}^2$ and $\boldsymbol{\tau}^2$. We consider:

$$y_{ir} = \mu_i + b_i + \epsilon_{ir}, i = 1, \ldots, K; r = 1, \ldots, r_i$$

$$b_i \sim \mathrm{N}\left(0, \tau^2\right) \qquad \epsilon_{ir} \sim \mathrm{N}\left(0, \sigma_i^2\right) \ .$$

- The likelihood is

$$\prod_{i=1}^{K} \frac{\sigma_i^{1-n}}{\sqrt{\tau^2 + \frac{1}{n}\sigma_i^2}} \exp\left(-\frac{\left(\bar{y}_i - \mu_i\right)^2}{2\left(\tau^2 + \frac{1}{n}\sigma_i^2\right)} - \frac{s_i^2}{2\sigma_i^2}\right)$$

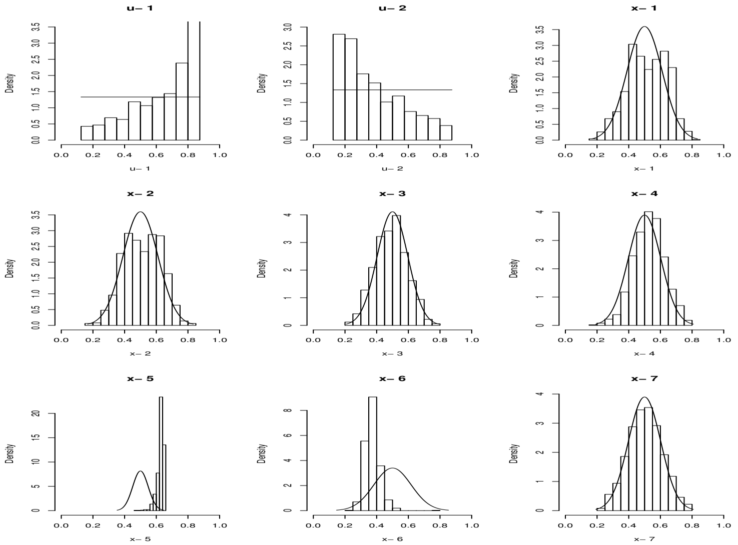
- For large K, the bias will be shrunk towards 0.
- *Modularization*: making inference about the $\{\sigma_i^2\}$ only from the replicate observations.

Analysis with Gaussian bias

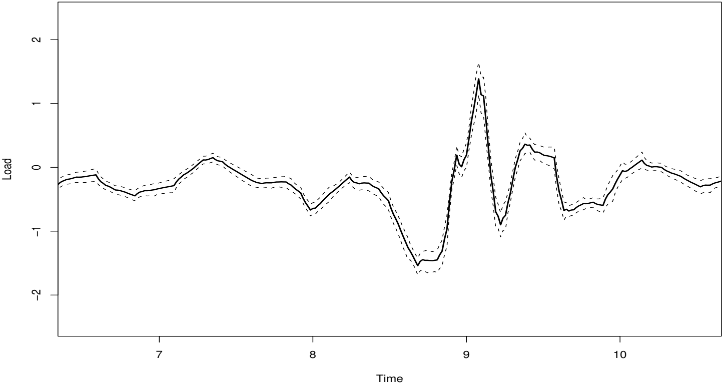
- Conditional on $\boldsymbol{\sigma}^2$, use Gibbs sampling for the rest parameters.
- Determine the posteriors for the σ_i^2 simply by the replicate observations.
- The posterior for $\boldsymbol{\sigma}^2$ is

$$\pi_{post}(\boldsymbol{\sigma}^2 \mid \boldsymbol{D}) \propto \left[\prod_{i \in I} \frac{1}{(\sigma_i^2)^3} \exp\left\{-\frac{s_i^2}{2\sigma_i^2}\right\}\right] \times \int L(\overline{\boldsymbol{w}}^F, \boldsymbol{s}^2 \mid \delta^*, \boldsymbol{u}^*, \boldsymbol{\sigma}^2, \boldsymbol{\tau}^2)\, d\delta^*\, d\boldsymbol{u}^*\, d\boldsymbol{\tau}^2 .$$

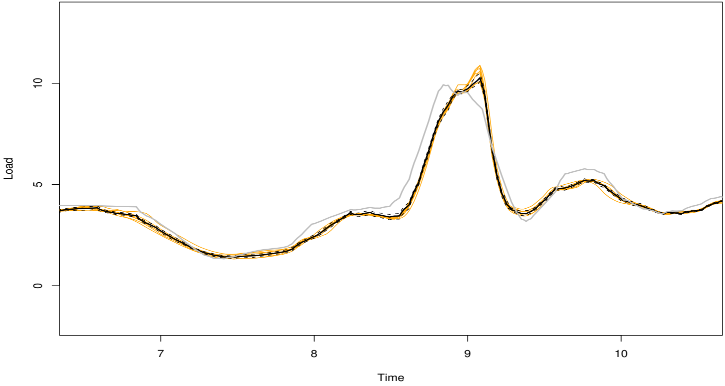
Marginal priors and marginal posteriors



Bias function (under Gaussian bias)



Reality (under Gaussian bias)



Analysis with Cauchy bias

Model the bias by robust distribution

$$\pi(w_i^b \mid \tau_{j(i)}^2) \sim \mathrm{Cauchy}\left(0, \tau_{j(i)}^2\right) .$$

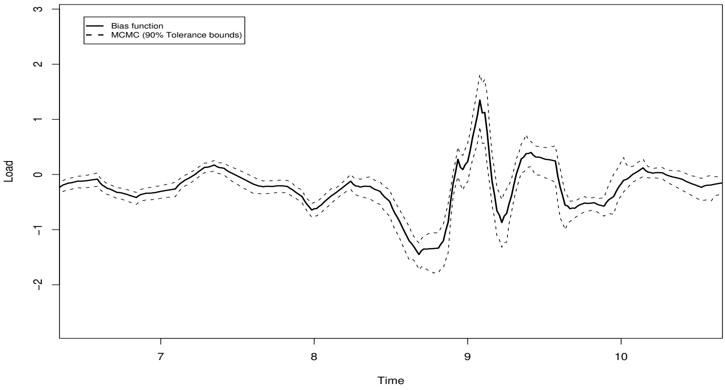
- Normal mixture

$$\pi(w_i^b \mid \tau_{j(i)}^2, \lambda_i) \sim \mathrm{N}\left(0, \tau_{j(i)}^2/\lambda_i\right) ,$$

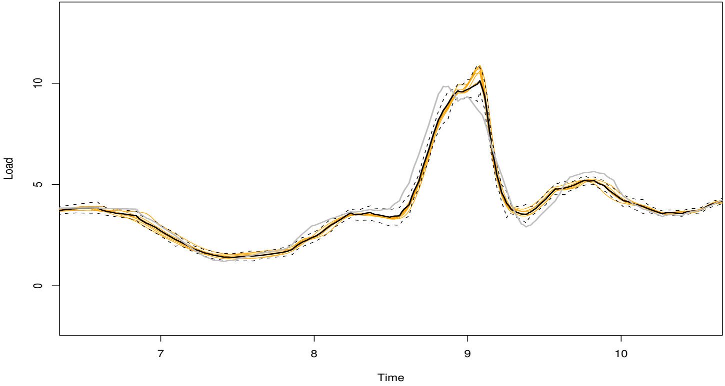
$$\lambda_i \sim \mathrm{Gamma}(\frac{1}{2}, 2) .$$

- Use the regular MCMC.

Bias function (under Cauchy bias)



Reality (under Cauchy bias)



Outline

Multiple computer codes

- Structural input $\boldsymbol{x} \in \boldsymbol{X}^M$.
- Build an emulator across all codes,

$$\begin{aligned} a_k^M(\boldsymbol{x}, \boldsymbol{\delta}, \boldsymbol{u}) \sim &\quad \mathrm{GP}\left(\mu_k, \sigma_k^{2M} \mathbb{C}\mathrm{orr}_k^{M_1}(\cdot,\cdot) \mathbb{C}\mathrm{orr}_k^{M_2}(\cdot,\cdot)\right) \,, \\ \mathbb{C}\mathrm{orr}_k^{M_1}(\cdot,\cdot) : &\quad \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R} \,, \\ \mathbb{C}\mathrm{orr}_k^{M_2}(\cdot,\cdot) : &\quad \mathbb{D}^M \times \mathbb{D}^M \rightarrow \mathbb{R} \,. \end{aligned}$$

Eigen-basis representation

- Represent the functional data by $\xi_k(t) = \sum_{i \in I} b_{ki} \Psi_i(t)$ (Ramsay, 1997),

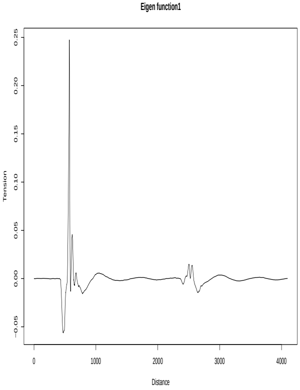
$$\sum_{i \in I} w_i^M(\boldsymbol{v}, \delta, \boldsymbol{u}) \Psi_i(t) \approx \sum_{k=1}^{p} a_k^M(\boldsymbol{v}, \delta, \boldsymbol{u}) \xi_k(t)$$

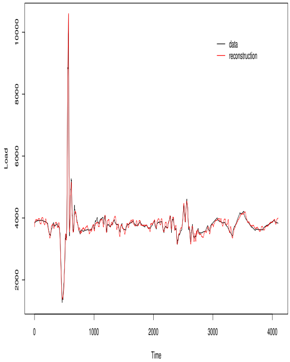
$$\sum_{i \in I} w_{ir}^F(\boldsymbol{v}, \delta) \Psi_i(t) \approx \sum_{k=1}^{p} a_{kr}^F(\boldsymbol{v}, \delta) \xi_k(t) \,.$$

- To obtain $\xi_k(t)$, we have

$$N^{-1} \boldsymbol{W}^t \boldsymbol{W} \boldsymbol{b}_k = \rho_k \boldsymbol{b}_k \,.$$

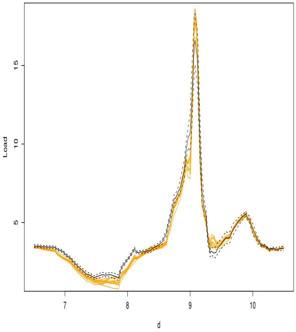
- Emulators for $\{a_k^M(\boldsymbol{v}, \delta, \boldsymbol{u})\}$.

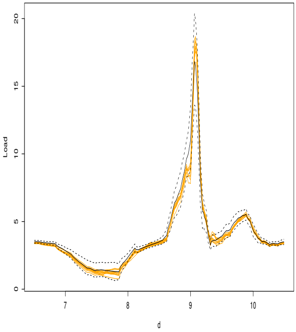

Eigen function1
Tension
Distance
0
1000
2000
3000
4000
-0.05
0.00
0.05
0.10
0.15
0.20
0.25


data
reconstruction
Load
Time
0
1000
2000
3000
4000
2000
4000
6000
8000
10000

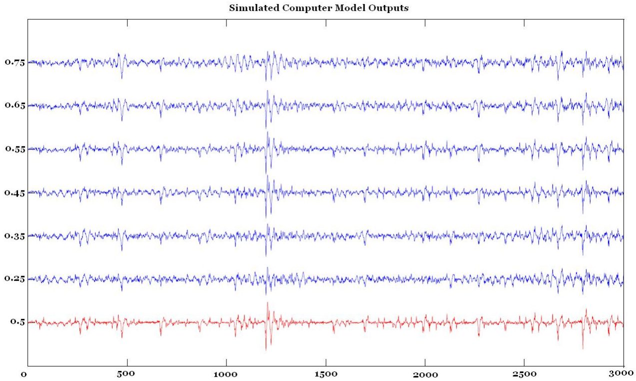
Result

Interpolate the bias/reality into new settings.





Dynamic Linear models

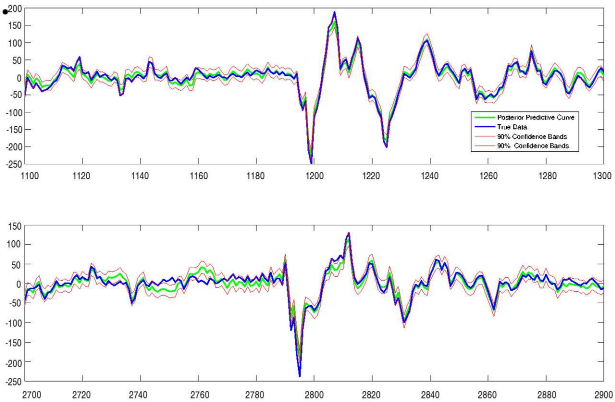


- Model the computer model run at $\boldsymbol{z}$ by multivariate TVAR (West and Harrison, 1997),

$$y^M(\boldsymbol{z}, t) = \sum_{j=1}^{p} \phi_{t,j} y^M(\boldsymbol{z}, t-j) + \underbrace{\epsilon_t^M(\boldsymbol{z})}_{\Downarrow \atop \mathrm{GP}(0, \sigma_t^2 \mathbb{C}\mathrm{orr}(\cdot,\cdot))},$$

- Interpolator with forecasting capability.
- Computation is done by Forward filtering backward sampling algorithm.
- Predict at untried input $\boldsymbol{z} = 0.5$.

Result


Posterior Predictive Curve
True Data
90% Confidence Bands
90% Confidence Bands
200
150
100
50
0
-50
-100
-150
-200
-250
1100
1120
1140
1160
1180
1200
1220
1240
1260
1280
1300
2700
2720
2740
2760
2780
2800
2820
2840
2860
2880
2900

Outline

Summary

- We developed various Bayesian functional data analysis approaches to computer model validation.
- The approaches automatically take into account model discrepancy and model calibration.
- Unknown (field) inputs can be incorporated.
- Bias functions are modeled using hierarchical structures when needed.

On-going work : Spatio-Temporal Outputs

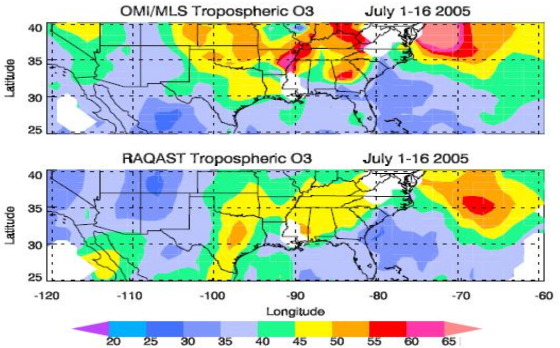


Figure: Regional Air Quality forecAST (RAQAST) Over the U.S. (S. Guillas et al., 2006

- The model,

$$y^F(s, \boldsymbol{\delta}^*; t) = y^M(s, \boldsymbol{\delta}^*, \boldsymbol{u}^*; t) + b(s, \boldsymbol{\delta}^*; t) + \epsilon_t^F .$$

  - s: location (configuration).
  - $\boldsymbol{u}$: calibration parameters.
  - $\boldsymbol{\delta}$: meteorology.
  - t: time.

- Spatial interpolation,

$$y^M(s, \boldsymbol{\delta}, \boldsymbol{u}; t) = \sum_{k \in \mathbb{K}} a_k(s, \boldsymbol{\delta}, \boldsymbol{u}) \psi_k(t) .$$

- Forecasting,

$$b(s, \boldsymbol{\delta}; t) = \sum_{j=1}^{p} \phi_{t,j} b(s, \boldsymbol{\delta}; t - j) + \epsilon_t^b(s, \boldsymbol{\delta}) .$$

On-going work: Time-dependent parameters

- Time-dependent parameters (Reichert, 2006)

$$y_t^F = \underbrace{y_t^M(\boldsymbol{z}^F + \phi_t^z)}_{\Downarrow} + \phi_t^F + \epsilon_t^F \, , \phi_t^z \sim \text{Stochastic process} \, ,$$

$$y_t^M(\boldsymbol{z}^F + \phi_t^z) \approx y_t^M(\boldsymbol{z}^F) + \nabla y_t^M(\boldsymbol{z}^F)\phi_t^z \, .$$

- Build emulators for $y_t^M(\boldsymbol{z}^F)$ and $\nabla y_t^M(\boldsymbol{z}^F)$.

Thank you!