Calibration of computer models

Bayesian Calibration

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Outline

Field data

- Field data provided by physical experiments:

$$\mathbf{y}^e = y^e(\mathbf{x}_1^e), \ldots, y^e(\mathbf{x}_{n_e}^e)\,,$$

- n_e is small, $\mathbf{x}_1, \ldots \mathbf{x}_{n_e} \in \mathcal{X}$ hard to set, sometimes uncontrollable, included in a small domain...

- Model:

$$y^e(\mathbf{x}_i^e) = \zeta(\mathbf{x}_i^e) + \epsilon(\mathbf{x}_i^e)\,,$$

  where
  - $\zeta(\cdot)$ real physical process (unknown),
  - $\epsilon(\mathbf{x}_i^e)$ often assumed i.i.d. $\mathcal{N}(0, \sigma^2)$,
  - σ^2 sometimes treated as known...

Relationship between the simulator and the data

for $i = 1, \ldots, n_e$,

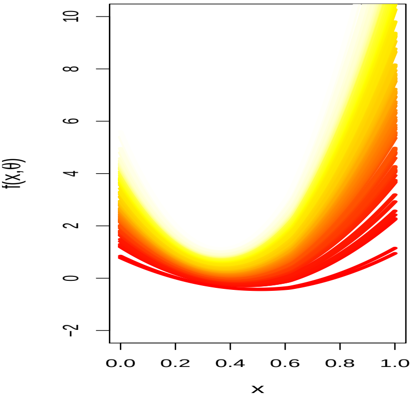
- if the simulator sufficiently represents the physical system:

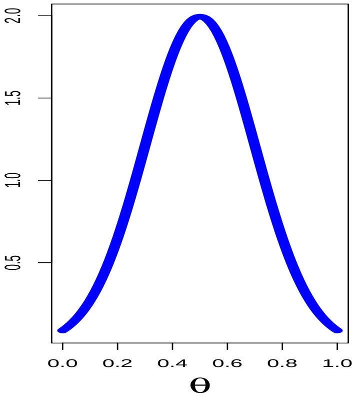
$$y_i^e = f(\mathbf{x}_i^e, \boldsymbol{\theta}^*) + \epsilon(\mathbf{x}_i^e)\,,$$

i.e. for the unknown value $\boldsymbol{\theta} = \boldsymbol{\theta}^*$: $f(\mathbf{x}, \boldsymbol{\theta}^*) = \zeta(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{X}$,

A calibration example

Prior:
prior distribution on unknown $\boldsymbol{\theta}$: $\pi(\cdot)$
from expert judgment, past experiments...
Possible choice $\pi(\boldsymbol{\theta}) = \mathcal{N}(\theta_0, \sigma_0^2) = \mathcal{N}(0.5, 0.04)$.





A calibration example

Data:
Couples $(\mathbf{x}_1^e, y_1^e), \ldots, (\mathbf{x}_{n_e}^e, y_{n_e}^e)$ from physical experiments.

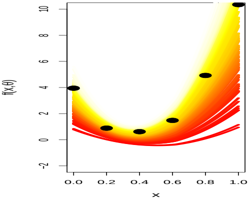
Posterior distribution:

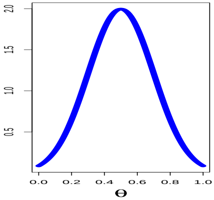
$$\begin{aligned}\pi(\boldsymbol{\theta}|\mathbf{y}^e) &\propto \mathcal{L}(\boldsymbol{\theta}|\mathbf{y}^e)\cdot\pi(\boldsymbol{\theta})\\ &\propto \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n_e}(y_i^e - f(\mathbf{x}_i^e,\boldsymbol{\theta}))^2 - \frac{1}{2\sigma_0^2}(\boldsymbol{\theta}-\boldsymbol{\theta}_0)^2\right)\end{aligned}$$

- Analytical posterior if $\boldsymbol{\theta} \mapsto f(\mathbf{x}, \boldsymbol{\theta})$ is a linear map,
- Otherwise MH sampling to simulate according to the posterior distribution. [Robert et al., 1999]

A calibration example

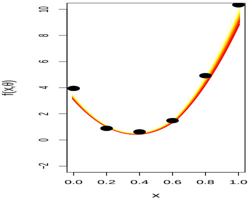
Prior with data:

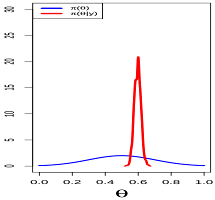




⇓ Metropolis-Hastings algorithm ⇓

Posterior on θ:





More details on the MH algorithm

Initialisation:
$\boldsymbol{\theta}^0$ chosen.

Update:
iterations $t = 1, \dots,$

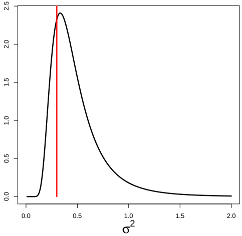
1. Proposal: $\tilde{\boldsymbol{\theta}}^{t+1} = \boldsymbol{\theta}^t + \mathcal{N}(0, \tau^2)$.
2. Compute
$$\alpha(\boldsymbol{\theta}^t, \tilde{\boldsymbol{\theta}}^{t+1}) = \frac{\pi(\tilde{\boldsymbol{\theta}}^{t+1}|\mathbf{y}^e)}{\pi(\boldsymbol{\theta}^t|\mathbf{y}^e)}$$
3. Acceptation:
$$\boldsymbol{\theta}^{t+1} = \begin{cases} \tilde{\boldsymbol{\theta}}^{t+1} & \text{with probability } \alpha(\boldsymbol{\theta}^t, \tilde{\boldsymbol{\theta}}^{t+1}) \\ \boldsymbol{\theta}^t & \text{otherwise.} \end{cases}$$

Note that the ratio $\alpha(\boldsymbol{\theta}^t, \tilde{\boldsymbol{\theta}}^{t+1})$ needs several computations of $f(\mathbf{x}, \boldsymbol{\theta})$ at each step since

$$\pi(\boldsymbol{\theta}|\mathbf{y}^e) \propto \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n_e}(y_i^e - f(\mathbf{x}_i^e, \boldsymbol{\theta}))^2 - \frac{1}{2\sigma_0^2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^2\right).$$

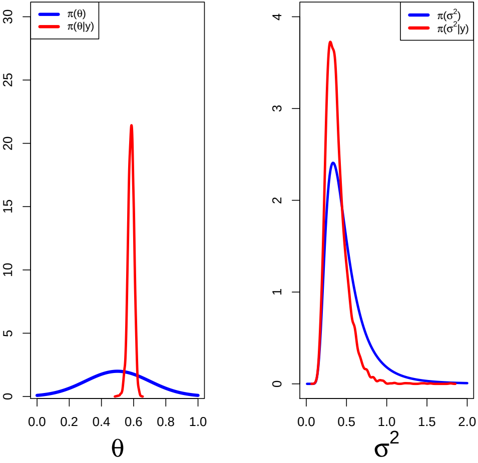
Unknown σ^2

- prior distribution on σ^2: $\pi(\sigma^2) = \mathcal{IG}(5, 2)$



- Gibbs algorithm to simulate couples $(\boldsymbol{\theta}, \sigma^2)$ from $\pi(\boldsymbol{\theta}, \sigma^2|\mathbf{y}^e)$. Iterate :
  1. MH algorithm to simulate $\boldsymbol{\theta}_t$ from $\pi(\cdot|\mathbf{y}^e, \sigma^2_{t-1})$,
  2. conditional simulation of σ^2_t from $\pi(\cdot|\mathbf{y}^e, \boldsymbol{\theta}_t)$.

Posterior distributions



Comparison

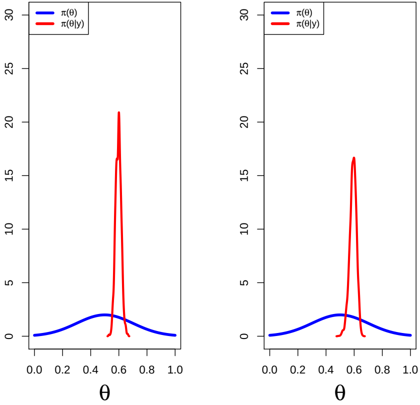


Figure: known σ^2 vs unknown σ^2

Outline

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Relationship between the simulator and the data

for $i = 1, \dots, n_e$,

- if the simulator represents sufficiently well the physical system:

$$y_i^e = f(\mathbf{x}_i^e, \boldsymbol{\theta}^*) + \epsilon(\mathbf{x}_i^e)\,,$$

  i.e. for the unknown value $\boldsymbol{\theta} = \boldsymbol{\theta}^*$: $f(\mathbf{x}, \boldsymbol{\theta}^*) = \zeta(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{X}$,

- if the field observations are inconsistent with the simulations (irreducible model discrepancy):

$$y_i^e = f(\mathbf{x}_i^e, \boldsymbol{\theta}^*) + \delta(\mathbf{x}_i^e) + \epsilon(\mathbf{x}_i^e)\,.$$

  $\delta(\cdot)$ models the difference between the simulator and the physical system:

$$\delta(\mathbf{x}) = \zeta(\mathbf{x}) - f(\mathbf{x}, \theta^*)\,.$$

Limited computational budget:

Limited number M of runs of the simulator.

Ref.: [Kennedy and O'Hagan, 2001, Higdon et al., 2004]

Statistical models

Notation proposed in [Carmassi et al., 2019]:

$$
\begin{aligned}
\mathcal{M}_0 &: \forall i \in [\![1,\dots,n_e]\!] \quad y_i^e = \zeta(\mathbf{x}_i^e) + \epsilon_i\\
\mathcal{M}_1 &: \forall i \in [\![1,\dots,n_e]\!] \quad y_i^e = f_c(\mathbf{x}_i^e, \boldsymbol{\theta}) + \epsilon_i,\\
\mathcal{M}_2 &: \forall i \in [\![1,\dots,n_e]\!] \quad y_i^e = F(\mathbf{x}_i^e, \boldsymbol{\theta}) + \epsilon_i,\\
\mathcal{M}_3 &: \forall i \in [\![1,\dots,n_e]\!] \quad y_i^e = f_c(\mathbf{x}_i^e, \boldsymbol{\theta}) + \delta(\mathbf{x}_i^e) + \epsilon_i,\\
\mathcal{M}_4 &: \forall i \in [\![1,\dots,n_e]\!] \quad y_i^e = F(\mathbf{x}_i^e, \boldsymbol{\theta}) + \delta(\mathbf{x}_i^e) + \epsilon_i.
\end{aligned}
$$

where

- $\epsilon_i \overset{iid}{\sim} \mathcal{N}(0, \sigma_{err}^2)$,
- $F(\bullet,\bullet) \sim \mathcal{GP}\Big(m_S(\bullet,\bullet), c_S\{(\bullet,\bullet),(\bullet,\bullet)\}\Big)$, on $\mathcal{X} \times \Theta$ [Sacks et al., 1989],
- $\delta(\bullet) \sim \mathcal{GP}\Big(\boldsymbol{m}_\delta(\bullet), c_\delta(\bullet,\bullet)\Big)$ on $\mathcal{X}$.

Likelihood for $\mathcal{M}_1$ and $\mathcal{M}_3$

$$\mathcal{L}^F(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta; \mathbf{y}^e, \mathbf{X}^e) = \frac{1}{(2\pi)^{n_e/2} |\boldsymbol{V}_{exp}(\mathbf{X}^e)|^{1/2}} \exp\Bigg\{ -\frac{1}{2}\Big(\mathbf{y}^e - \boldsymbol{m}_{exp}(\mathbf{X}^e, \boldsymbol{\theta})\Big)^T \boldsymbol{V}_{exp}(\mathbf{X}^e)^{-1} \Big(\mathbf{y}^e - \boldsymbol{m}_{exp}(\mathbf{X}^e, \boldsymbol{\theta})\Big)\Bigg\}.$$

$$\mathbb{E}[\mathbf{y}^e | \boldsymbol{\theta}, \boldsymbol{\beta}_\delta; \mathbf{X}^e] = \boldsymbol{m}_{exp}^{\boldsymbol{\beta}_\delta}(\mathbf{X}^e, \boldsymbol{\theta}) = \boldsymbol{m}_{exp}(\mathbf{X}^e, \boldsymbol{\theta}) = f_c(\mathbf{X}^e, \boldsymbol{\theta}) + \boldsymbol{H}_\delta(\mathbf{X}^e)\boldsymbol{\beta}_\delta.$$

Then, the expression of the variance is given by

$$\mathbb{V}ar[\mathbf{y}^e | \Phi_\delta; \mathbf{X}^e] = \boldsymbol{V}_{exp}^{\Phi_\delta, \sigma^2_{err}}(\mathbf{X}^e) = \boldsymbol{V}_{exp}(\mathbf{X}^e) = \boldsymbol{\Sigma}_\delta(\mathbf{X}^e) + \sigma^2_{err} \boldsymbol{I}_{n_e},$$

with $\forall (i,j) \in [\![1, \dots, n]\!]^2 : (\boldsymbol{\Sigma}_\delta(\mathbf{X}^e))_{i,j} = (\boldsymbol{\Sigma}_\delta^{\Phi_\delta}(\mathbf{X}^e))_{i,j} = \sigma^2_\delta c_\delta(\{\boldsymbol{x}_i, \boldsymbol{x}_j\})$.

For $\mathcal{M}_1$

$\boldsymbol{m}_{exp}(\mathbf{X}^e, \boldsymbol{\theta}) = f_c(\mathbf{X}^e, \boldsymbol{\theta})$ and $\boldsymbol{V}_{exp}(\mathbf{X}^e) = \sigma^2_{err} \boldsymbol{I}_{n_e}$.

When the code is slow

Data:

1. DoNE: Design of Numerical Experiments: $D^c = \{(\mathbf{x}_1, \boldsymbol{\theta}_1), \ldots, (\mathbf{x}_N, \boldsymbol{\theta}_N)\}$ with corresponding evaluations of the computer model (time-consuming):

$$\mathbf{y}^c = f(D^c) = \{f(\mathbf{x}_1, \boldsymbol{\theta}_1), \ldots, f(\mathbf{x}_N, \boldsymbol{\theta}_N)\}.$$

2. DoFE: Design of Field Experiments: $\mathbf{X}^e = \{\mathbf{x}_1^e, \ldots, \mathbf{x}_{n_e}^e\}$ with corresponding noisy observation of ζ:

$$\mathbf{y}^e = \{y_1^e = \zeta(\mathbf{x}_1^e) + \epsilon_1, \ldots, y_{n_e}^e = \zeta(\mathbf{x}_{n_e}^e) + \epsilon_{n_e}\}.$$

Model: $\forall 1 \leq i \leq n_e, \quad y_i^e = f(\mathbf{x}_i^e, \boldsymbol{\theta}) + \delta(\mathbf{x}_i^e) + \epsilon_i$ where:

- f is emulated via a GP Emulator [Sacks et al., 1989] : $f \sim \mathcal{GP}(m_S(\cdot), c_S(\cdot,\cdot))$, $f|f(D^c) \sim \mathcal{GP}$ is the emulator/surrogate/metamodel,
- δ the discrepancy modeled as a GP: $\delta \sim \mathcal{GP}(H_\delta(\cdot)\boldsymbol{\beta}_\delta, \sigma_\delta^2 C_\delta(\cdot,\cdot))$,
- $\epsilon \overset{iid}{\sim} \mathcal{N}(0, \sigma_{err}^2)$ are measurement errors.

Likelihood for $\mathcal{M}_2$ and $\mathcal{M}_4$

$\Phi = (\sigma_c^2, \phi_c, \sigma_\delta^2, \phi_\delta)$, and $\boldsymbol{\beta} = (\boldsymbol{\beta}_S, \boldsymbol{\beta}_\delta)$
Full Likelihood written for $\mathbf{y} = (\mathbf{y}^e, \mathbf{y}^c)$:

$$\begin{aligned}
&\mathcal{L}^F(\boldsymbol{\theta}, \boldsymbol{\beta}, \Phi, \sigma_{err}^2; \boldsymbol{y}, \mathbf{X}^e, D^c)\\
=&\frac{1}{(2\pi)^{(n_e+N)/2}|\boldsymbol{V}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)|^{1/2}}\\
&\exp\left\{ -\frac{1}{2}\Big(\boldsymbol{y} - \boldsymbol{m_y}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\Big)^T \boldsymbol{V}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)^{-1}\Big(\boldsymbol{y} - \boldsymbol{m_y}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\Big)\right\}.
\end{aligned}$$

with

$$\begin{aligned}
\mathbb{E}[\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{\beta}; \mathbf{X}^e, D^c] = \boldsymbol{m}_{\boldsymbol{y}}^{\boldsymbol{\beta}}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) =& \boldsymbol{m_y}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) = \boldsymbol{H}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\boldsymbol{\beta}\\
&= \begin{pmatrix} \boldsymbol{H}_S(\mathbf{X}^e, \boldsymbol{\theta}) & \boldsymbol{H}_\delta(\mathbf{X}^e) \\ \boldsymbol{H}_S(D^c) & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\beta}_S \\ \boldsymbol{\beta}_\delta \end{pmatrix}.
\end{aligned}$$

$$\begin{aligned}
\mathbb{V}ar[\boldsymbol{y}|\boldsymbol{\theta}, \Phi, \sigma_{err}^2; \mathbf{X}^e, D^c] &= \boldsymbol{V}^{\Phi, \sigma_{err}^2}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) = \boldsymbol{V}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\\
&= \begin{pmatrix} \boldsymbol{\Sigma}_{exp,exp}(\mathbf{X}^e, \boldsymbol{\theta}) + \boldsymbol{\Sigma}_\delta(\mathbf{X}^e) + \sigma_{err}^2 \boldsymbol{I}_{n_e} & \boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) \\ \boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)^T & \boldsymbol{\Sigma}_{c,c}(D^c) \end{pmatrix}
\end{aligned}$$

- $\forall (i,j) \in [\![1,\dots,n_e]\!]^2 : (\boldsymbol{\Sigma}_{exp,exp}(\mathbf{X}^e,\boldsymbol{\theta}))_{i,j} = c_S\{(\mathbf{x}_i^e,\boldsymbol{\theta}),(\mathbf{x}_j^e,\boldsymbol{\theta})\}$,
- $\forall (i,j) \in [\![1,\dots,n_e]\!] \times [\![1,\dots,N]\!] : (\boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c))_{i,j} = c_S\{(\mathbf{x}_i^e,\boldsymbol{\theta}),(\mathbf{x}_j,\boldsymbol{\theta}_j)\}$,
- $\forall (i,j) \in [\![1,\dots,n_e]\!]^2 : (\boldsymbol{\Sigma}_\delta(\mathbf{X}^e))_{i,j} = c_\delta\{(\mathbf{x}_i^e,\mathbf{x}_j^e)\}$,
- $\forall (i,j) \in [\![1,\dots,N]\!]^2 : (\boldsymbol{\Sigma}_{c,c}(D^c))_{i,j} = c_S\{(\mathbf{x}_i,\boldsymbol{\theta}_i),(\mathbf{x}_j,\boldsymbol{\theta}_j)\}$.

For $\mathcal{M}_2$

Mean

$$\mathbb{E}[\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{\beta}_S; \mathbf{X}^e, D^c] = \boldsymbol{m}_{\boldsymbol{y}}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) = \boldsymbol{H}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\boldsymbol{\beta}_S = \begin{pmatrix} \boldsymbol{H}_S(\mathbf{X}^e, \boldsymbol{\theta}) \\ \boldsymbol{H}_S(D^c) \end{pmatrix} \boldsymbol{\beta}_S$$

and the covariance

$$\mathbb{V}ar[\boldsymbol{y}|\boldsymbol{\theta}, \Phi, \sigma^2_{err}; \mathbf{X}^e, D^c] = \boldsymbol{V}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) = \begin{pmatrix} \boldsymbol{\Sigma}_{exp,exp}(\mathbf{X}^e, \boldsymbol{\theta}) + \sigma^2_{err}\boldsymbol{I}_{n_e} & \boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) \\ \boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)^T & \boldsymbol{\Sigma}_{c,c}(D^c) \end{pmatrix}$$

Modularization

Advocated in [Liu et al., 2009].

- From $\mathbf{y}^c$, compute the GP emulator from the partial Likelihood $\mathcal{L}^M(\boldsymbol{\beta}_S, \Phi_S; \mathbf{y}^c, D^c)$,
- Plug the GP emulator in the conditional Likelihood of $\mathbf{y}^e$:
  $\mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta; \boldsymbol{\beta}_S, \Phi_S, \mathbf{y}^e|\mathbf{y}^c, \mathbf{X}^e, D^c)$.

[Gramacy, 2020] “Modularization or Compartmentalization is an engineering practice such that Components should perform robustly in isolation, irrespective of their anticipated role in a larger system.”

MLE estimates

MLE for $\boldsymbol{\beta}_S, \Phi_S$ from the partial likelihood:

$$\mathcal{L}^M(\boldsymbol{\beta}_S, \Phi_S; \mathbf{y}^c, D^c)$$
$$= \frac{1}{(2\pi)^{N/2}|\boldsymbol{V}_c(D^c)|^{1/2}} \exp\left\{ -\frac{1}{2}\Big(\mathbf{y}^c - \boldsymbol{m}_c(D^c)\Big)^T \boldsymbol{V}_c(D^c)^{-1}\Big(\mathbf{y}^c - \boldsymbol{m}_c(D^c)\Big)\right\}.$$

$$\mathbb{V}ar[\mathbf{y}^c|\Phi_S; D^c] = \boldsymbol{V}_c^{\Phi_S}(D^c) = \boldsymbol{V}_c(D^c) = \boldsymbol{\Sigma}_{c,c}(D^c),$$

$$\mathbb{E}[\mathbf{y}^c|\boldsymbol{\beta}_S; D^c] = \boldsymbol{m}_c(D^c) = \boldsymbol{H}_S(D^c)\boldsymbol{\beta}_S\,.$$

GP emulation

We derive

$$\mathbf{y}^e|\mathbf{y}^c \sim \mathcal{N}(\boldsymbol{\mu}_{exp|c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c),\boldsymbol{\Sigma}_{exp|c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c))$$

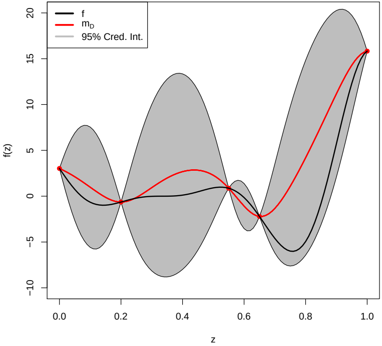
with

$$\begin{aligned}&\boldsymbol{\mu}_{exp|c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c)\\&=\boldsymbol{H}_S(\mathbf{X}^e,\theta)\boldsymbol{\beta}_S+\boldsymbol{H}_\delta(\mathbf{X}^e)\beta_\delta+\boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e,\theta),D^c)\boldsymbol{\Sigma}_{c,c}(D^c)^{-1}(\mathbf{y}^c-\boldsymbol{m}_c(D^c)),\end{aligned}$$

$$\boldsymbol{\Sigma}_{exp|c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c)=\boldsymbol{V}_{exp,exp}(\mathbf{X}^e,\boldsymbol{\theta})-\boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c)\boldsymbol{\Sigma}_{c,c}(D^c)^{-1}\boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e,\boldsymbol{\theta}),D^c)^T,$$

with
$\boldsymbol{V}_{exp,exp}(\mathbf{X}^e,\boldsymbol{\theta})=\boldsymbol{\Sigma}_{exp,exp}(\mathbf{X}^e,\boldsymbol{\theta})+\boldsymbol{\Sigma}_\delta(\mathbf{X}^e)+\sigma^2_{err}\boldsymbol{I}_{n_e}.$

GP emulator illustrated



Conditional Likelihood

GP emulator plugged into

$$\mathcal{L}^{C}(\boldsymbol{\theta}, \boldsymbol{\beta}_{\delta}, \Phi_{\delta}, \sigma^2_{err}; \hat{\boldsymbol{\beta}}_{S}, \hat{\Phi}_{S}, \mathbf{y}^{e} | \mathbf{y}^{c}, \mathbf{X}^{e}, D^{c})$$
$$\propto |\Sigma_{exp|c}((\mathbf{X}^{e}, \boldsymbol{\theta}), D^{c})|^{-1/2}$$
$$\exp\Big\{ -\frac{1}{2}(\mathbf{y}^{e} - \mu_{exp|c}((\mathbf{X}^{e}, \boldsymbol{\theta}), D^{c}))^{T} \Sigma_{exp|c}((\mathbf{X}^{e}, \boldsymbol{\theta}), D^{c})^{-1} (\mathbf{y}^{e} - \mu_{exp|c}((\mathbf{X}^{e}, \boldsymbol{\theta}), D^{c}))\Big\}.$$

Outline

Frequentist estimation: least squares estimation

[Cox et al., 2001, Wong et al., 2017]

$$\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}\in\mathcal{Q}}{argmin}\, M_n(\boldsymbol{\theta}) \quad \text{with} \quad M_n(\boldsymbol{\theta}) = \frac{1}{n_e}\sum_{i=1}^{n_e}\{y_i^e - f(\mathbf{x}_i^e, \boldsymbol{\theta})\}^2, \tag{1}$$

and
estimation of δ_0 applying any nonparametric regression method to the “data”

$$\{\mathbf{x}_i, y_i^e - f(\mathbf{x}_i^e, \hat{\boldsymbol{\theta}})\}_{i=1,\dots,n_e}.$$

Bayesian estimation for $\mathcal{M}_4$

Prior information:

$$\pi(\boldsymbol{\theta}, \boldsymbol{\beta}, \Phi, \sigma^2_{err}) = \pi(\boldsymbol{\theta}) \times 1 \times \pi(\Phi) \times \pi(\sigma^2_{err}).$$

Estimation

- Full Bayesian: For a full Bayesian analysis, integrating other parameters out is needed to finally get $\pi(\boldsymbol{\theta}|\boldsymbol{y})$,
- Modular:
  1. maximizing the likelihood $\mathcal{L}^M(\boldsymbol{\beta}_S, \Phi_S|\mathbf{y}^c; D^c)$ to get the maximum likelihood estimates (MLE) $\hat{\boldsymbol{\beta}}_S$ and $\hat{\Phi}_S$ of $\boldsymbol{\beta}_S$ and Φ_S
  2. plugged into the conditional likelihood $\mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta, \sigma^2_{err}; \hat{\boldsymbol{\beta}}_S, \hat{\Phi_S}, \mathbf{y}^e|\mathbf{y}^c, \mathbf{X}^e, D^c)$
  3. sampled with MCMC methods: $\pi(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta, \sigma^2_{err}|\mathbf{y}^e, \mathbf{y}^c, \mathbf{X}^e, D^c) \propto$ $\mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta, \sigma^2_{err}; \hat{\boldsymbol{\beta}}_S, \hat{\Phi_S}, \mathbf{y}^e|\mathbf{y}^c, \mathbf{X}^e, D^c) \cdot \pi(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \Phi_\delta, \sigma^2_{err})$
- Generate explicitely realizations of $(\delta(\mathbf{x}_i^e))_{1\leq i\leq n_e}$ conditionally on the current parameters values in a Gibbs sampling algorithm. [Bayarri et al., 2007].

for other models

For $\mathcal{M}_1$ and $\mathcal{M}_3$ no modularization use the actual code in the likelihood.

Outline

A word on history matching

- common alternative to KOH calibration [Craig et al., 1997, Vernon et al., 2010, Boukouvalas et al., 2014, Andrianakis et al., 2017].
- searches for inputs where the simulator outputs closely match observed data, while recognizing the presence of the various uncertainties, including model discrepancy
- rules out "implausible" inputs,

$\boldsymbol{\theta}$ is deemed implausible if:

$$\frac{||y^e - f(\mathbf{x}^e, \boldsymbol{\theta})||}{\sqrt{\sigma_S^2(\mathbf{x}^e, \boldsymbol{\theta}) + \sigma_\delta^2(\mathbf{x}^e) + \sigma_{err}^2}} \geq 3, \tag{2}$$

where $\sigma_S^2, \sigma_\delta^2$, and σ_{err}^2 are the variances of the surrogate, the model discrepancy, and the observational error.

- number 3 comes from [Pukelsheim, 1994] who shows that at least 95% of any unimodal distribution is contained within three standard deviations,
- HM can be repeated in so-called "waves", using non-implausible $\boldsymbol{\theta}$ found at one wave to generate simulation runs for the next wave
- simulator not valid if plausible space is void.

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