

Calibration of computer models

Bayesian Calibration

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Outline

- 1 A simple example
- 2 More complex models
- 3 Additional comments

Field data

- Field data provided by physical experiments:

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

- n_e is small, $\mathbf{x}_1, \dots, \mathbf{x}_{n_e} \in \mathcal{X}$ 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 $i = 1, \dots, n_e$,

- if the simulator sufficiently represents the physical system:

$$y_i^\theta = f(\mathbf{x}_i^\theta, \theta^*) + \epsilon(\mathbf{x}_i^\theta), \quad (1)$$

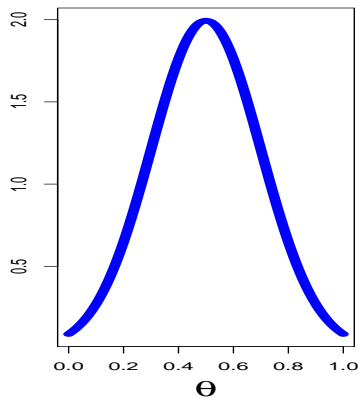
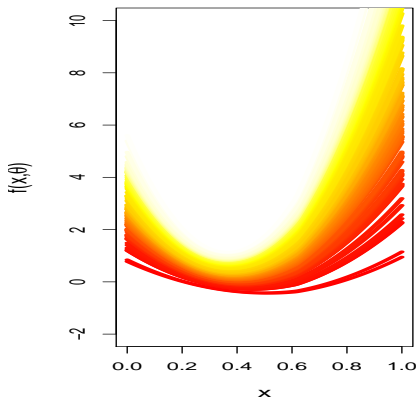
i.e. for the unknown value $\theta = \theta^* : f(\mathbf{x}, \theta^*) = \zeta(\mathbf{x})$ for any $\mathbf{x} \in \mathcal{X}$,

A calibration example

Prior:

prior distribution on unknown θ : $\pi(\cdot)$
from expert judgment, past experiments...

Possible choice $\pi(\theta) = \mathcal{N}(\theta_0, \sigma_0^2) = \mathcal{N}(0.5, 0.04)$.



A calibration example

Data:

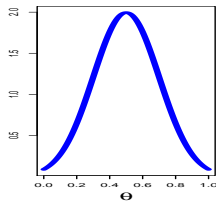
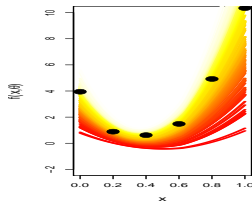
Couples $(\mathbf{x}_1^e, y_1^e), \dots, (\mathbf{x}_{n_e}^e, y_{n_e}^e)$ from physical experiments.

Posterior distribution:

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

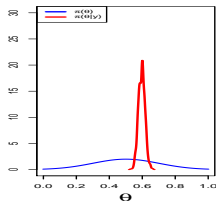
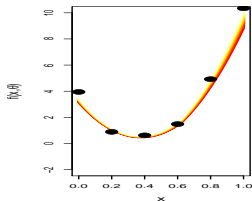
- Analytical posterior if $\boldsymbol{\theta} \mapsto f(\mathbf{x}, \boldsymbol{\theta})$ is a linear map,
- Otherwise MH sampling to simulate according to the posterior distribution.
[Robert et al., 1999]

A calibration example



Prior with data:

↓ Metropolis-Hastings algorithm ↓



Posterior on θ :

More details on the MH algorithm

Initialisation:

θ^0 chosen.

Update:

iterations $t = 1, \dots$,

1 Proposal: $\tilde{\theta}^{t+1} = \theta^t + \mathcal{N}(0, \tau^2)$.

2 Compute

$$\alpha(\theta^t, \tilde{\theta}^{t+1}) = \frac{\pi(\tilde{\theta}^{t+1} | \mathbf{y}^e)}{\pi(\theta^t | \mathbf{y}^e)}$$

3 Acceptation:

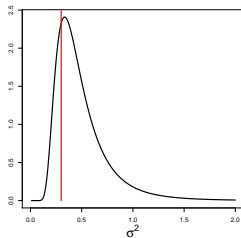
$$\theta^{t+1} = \begin{cases} \tilde{\theta}^{t+1} & \text{with probability } \alpha(\theta^t, \tilde{\theta}^{t+1}) \\ \theta^t & \text{otherwise.} \end{cases}$$

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

$$\pi(\theta | \mathbf{y}^e) \propto \exp \left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i^e - f(\mathbf{x}_i^e, \theta))^2 - \frac{1}{2\sigma_0^2} (\theta - \theta_0)^2 \right).$$

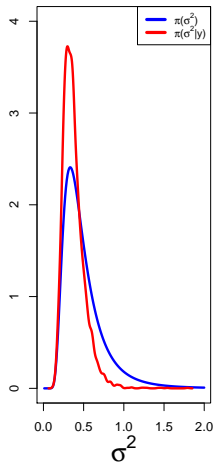
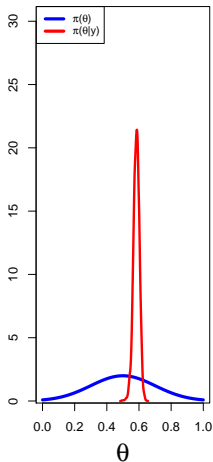
Unknown σ^2

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



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

Posterior distributions



Comparison

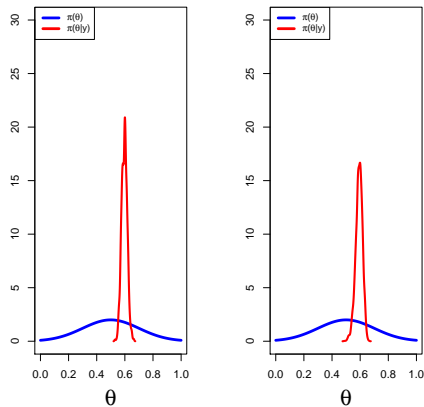


Figure: known σ^2 vs unknown σ^2

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Relationship between the simulator and the data

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

- if the simulator represents sufficiently well the physical system:

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

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

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

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

$\delta(\cdot)$ 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

$$\mathcal{M}_0 : \forall i \in \llbracket 1, \dots, n_e \rrbracket \quad y_i^\theta = \zeta(\mathbf{x}_i^\theta) + \epsilon_i$$

$$\mathcal{M}_1 : \forall i \in \llbracket 1, \dots, n_e \rrbracket \quad y_i^\theta = f_c(\mathbf{x}_i^\theta, \theta) + \epsilon_i,$$

$$\mathcal{M}_2 : \forall i \in \llbracket 1, \dots, n_e \rrbracket \quad y_i^\theta = F(\mathbf{x}_i^\theta, \theta) + \epsilon_i,$$

$$\mathcal{M}_3 : \forall i \in \llbracket 1, \dots, n_e \rrbracket \quad y_i^\theta = f_c(\mathbf{x}_i^\theta, \theta) + \delta(\mathbf{x}_i^\theta) + \epsilon_i,$$

$$\mathcal{M}_4 : \forall i \in \llbracket 1, \dots, n_e \rrbracket \quad y_i^\theta = F(\mathbf{x}_i^\theta, \theta) + \delta(\mathbf{x}_i^\theta) + \epsilon_i.$$

where

- $\epsilon_i \stackrel{iid}{\sim} \mathcal{N}(0, \sigma_{err}^2),$
- $F(\bullet, \bullet) \sim \mathcal{GP}\left(m_S(\bullet, \bullet), c_S\{(\bullet, \bullet), (\bullet, \bullet)\}\right),$ on $\mathbb{X} \times \Theta$
- $\delta(\bullet) \sim \mathcal{GP}\left(\mathbf{m}_\delta(\bullet), c_\delta(\bullet, \bullet)\right)$ on $\mathbb{X}.$

[Carmassi et al., 2019]

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

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

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

Then, the expression of the variance is given by

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

with $\forall (i, j) \in \llbracket 1, \dots, n \rrbracket^2 : (\Sigma_\delta(\mathbf{X}^e))_{i,j} = (\Sigma_\delta^{\Phi_\delta}(\mathbf{X}^e))_{i,j} = \sigma_\delta^2 c_\delta(\{\mathbf{x}_i, \mathbf{x}_j\})$.

For \mathcal{M}_1

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

When the code is slow

Data:

- 1 DoNE: Design of Numerical Experiments: $D^c = \{(\mathbf{x}_1, \theta_1), \dots, (\mathbf{x}_N, \theta_N)\}$ with corresponding evaluations of the computer model (time-consuming):

$$\mathbf{y}^c = f(D^c) = \{f(\mathbf{x}_1, \theta_1), \dots, f(\mathbf{x}_N, \theta_N)\}.$$

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

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

Model: $\forall 1 \leq i \leq n_e, \quad y_i^e = f(\mathbf{x}_i^e, \theta) + \delta(\mathbf{x}_i^e) + \epsilon_i$ 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: $\delta \sim \mathcal{GP}(H_\delta(\cdot)\beta_\delta, \sigma_\delta^2 C_\delta(\cdot, \cdot))$,
- $\epsilon \stackrel{iid}{\sim} \mathcal{N}(0, \sigma_{err}^2)$ are measurement errors.

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

$\Phi = (\sigma_c^2, \phi_c, \sigma_\delta^2, \phi_\delta)$, and $\beta = (\beta_S, \beta_\delta)$

Full Likelihood written for $\mathbf{y} = (\mathbf{y}^e, \mathbf{y}^c)$:

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

with

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

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

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

For \mathcal{M}_2

Mean

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

and the covariance

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

Modularization

Advocated in [Liu et al., 2009].

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

[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 β_S, Φ_S from the partial likelihood:

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

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

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

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

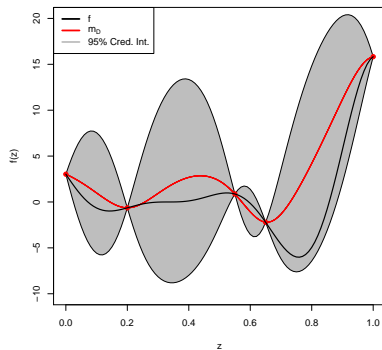
$$\begin{aligned} \boldsymbol{\mu}_{exp|c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c) \\ = \mathbf{H}_S(\mathbf{X}^e, \boldsymbol{\theta})\boldsymbol{\beta}_S + \mathbf{H}_\delta(\mathbf{X}^e)\boldsymbol{\beta}_\delta + \boldsymbol{\Sigma}_{exp,c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)\boldsymbol{\Sigma}_{c,c}(D^c)^{-1}(\mathbf{y}^c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

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

with

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

GP emulator illustrated



Conditional Likelihood

GP emulator plugged into

$$\begin{aligned} & \mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \boldsymbol{\Phi}_\delta, \sigma_{err}^2; \hat{\boldsymbol{\beta}}_S, \hat{\boldsymbol{\Phi}}_S, \mathbf{y}^e | \mathbf{y}^c, \mathbf{X}^e, D^c) \\ & \propto |\boldsymbol{\Sigma}_{exp|c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)|^{-1/2} \\ & \exp \left\{ -\frac{1}{2} (\mathbf{y}^e - \mu_{exp|c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c))^T \boldsymbol{\Sigma}_{exp|c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)^{-1} (\mathbf{y}^e - \mu_{exp|c}((\mathbf{X}^e, \boldsymbol{\theta}), D^c)) \right\}. \end{aligned}$$

Frequentist estimation: least squares estimation

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

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

and

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

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

Bayesian estimation for \mathcal{M}_4

Prior information:

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

Estimation

- Full Bayesian: For a full Bayesian analysis, integrating other parameters out is needed to finally get $\pi(\boldsymbol{\theta}|\mathbf{y})$,
- Modular:
 - 1 maximizing the likelihood $\mathcal{L}^M(\boldsymbol{\beta}_S, \boldsymbol{\Phi}_S|\mathbf{y}^c; D^c)$ to get the maximum likelihood estimates (MLE) $\hat{\boldsymbol{\beta}}_S$ and $\hat{\boldsymbol{\Phi}}_S$ of $\boldsymbol{\beta}_S$ and $\boldsymbol{\Phi}_S$
 - 2 plugged into the conditional likelihood $\mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \boldsymbol{\Phi}_\delta, \sigma_{err}^2; \hat{\boldsymbol{\beta}}_S, \hat{\boldsymbol{\Phi}}_S, \mathbf{y}^e|\mathbf{y}^c, \mathbf{X}^e, D^c)$
 - 3 sampled with MCMC methods:

$$\pi(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \boldsymbol{\Phi}_\delta, \sigma_{err}^2|\mathbf{y}^e, \mathbf{y}^c, \mathbf{X}^e, D^c) \propto \mathcal{L}^C(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \boldsymbol{\Phi}_\delta, \sigma_{err}^2; \hat{\boldsymbol{\beta}}_S, \hat{\boldsymbol{\Phi}}_S, \mathbf{y}^e|\mathbf{y}^c, \mathbf{X}^e, D^c) \cdot \pi(\boldsymbol{\theta}, \boldsymbol{\beta}_\delta, \boldsymbol{\Phi}_\delta, \sigma_{err}^2)$$
- Generate explicitly 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.

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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,

θ is deemed implausible if:

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

where σ_S^2 , σ_δ^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 θ found at one wave to generate simulation runs for the next wave
- simulator not valid if plausible space is void.



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