Sequential designs for computer experiments

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Outline

Plan

Field data

- Field data provided by physical experiments:

$$\mathbf{y}^F = y^F(\mathbf{x}_1), \ldots, y^F(\mathbf{x}_n) ,$$

- n is small, $\mathbf{x}_1, \ldots \mathbf{x}_n \in \mathbb{X}$ hard to set, sometimes uncontrollable, included in a small domain...

- Model:

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

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

Computer model / simulator

Computer experiments:

Computer model (simulator) $(\mathbf{x}^*, \boldsymbol{\theta}) \mapsto f(\mathbf{x}^*, \boldsymbol{\theta}) \in \mathbb{R}^s$ where

- **physical parameters**: $\mathbf{x}^* \in \mathbb{X} \subset \mathbb{R}^m$ observable and often controllable inputs
  - $\mathbf{x}^*$ same meaning as in field data,
  - extrapolation if $\mathbf{x}^* > \max(\mathbf{x}_i)$ or $\mathbf{x}^* < \min(\mathbf{x}_i)$.
- **simulator parameters**: $\boldsymbol{\theta} \in \Theta \subset \mathbb{R}^d$ non-observable parameters, required to run the simulator.

  2 types:
  - "calibration parameters": physical meaning but unknown, necessary to make the code mimic the reality,
  - "tuning parameters": no physical interpretation.

f designed to mimic the unknown physical process $\zeta(\cdot)$ for a value of $\boldsymbol{\theta}$.
The simulator is often an **expensive black-box function**.
$\Rightarrow$ limited number N_{run} of runs of the simulator.

Relationship between the simulator and the data

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

- if the simulator sufficiently represents the physical system:

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

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

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

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

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

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

  but
  - What does θ^* mean ?
  - A best fitting ?
  - identifiability issues ?
  - usually assumed to be smoother than the real physical process $\zeta(\cdot)$

Ref.: Kennedy and O'Hagan (2001), Hidgon et al. (2005)...

Plan

A calibration example

Hypotheses:

- The simulator represents sufficiently well the physical system:

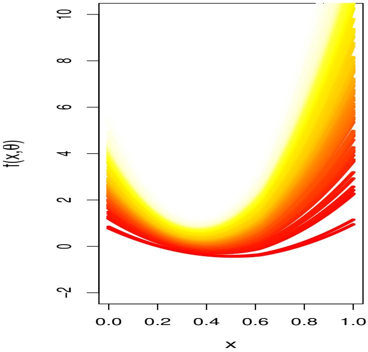
$$y^F(\mathbf{x}_i) = f(\mathbf{x}_i, \boldsymbol{\theta}^*) + \epsilon_i, \quad i = 1, \dots, n.$$

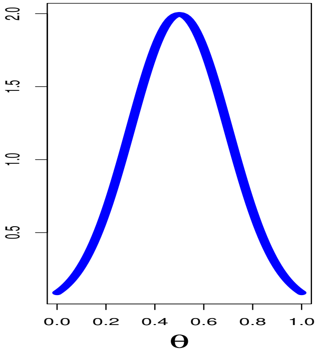
- But unknown $\boldsymbol{\theta}^*$.
- $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$ i.i.d. with known σ^2.
- $\sigma^2 = 0.3$
- $n = 6$,
- $\theta^* = 0.6$

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 $(\mathbf{x}_1, y_1^F), \ldots, (\mathbf{x}_n, y_n^F)$ from physical experiments.

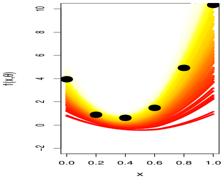
Posterior distribution:

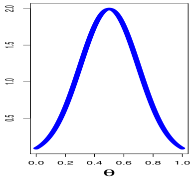
$$\begin{aligned}\pi(\boldsymbol{\theta}|\mathbf{y}^F) &\propto l(\boldsymbol{\theta}|\mathbf{y}^F) \cdot \pi(\boldsymbol{\theta}) \\ &\propto \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y^F(\mathbf{x}_i) - f(\mathbf{x}_i, \boldsymbol{\theta}))^2 - \frac{1}{2\sigma_0^2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^2\right)\end{aligned}$$

- 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.

A calibration example

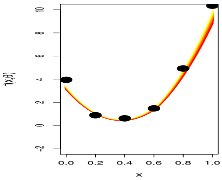
Prior with data:

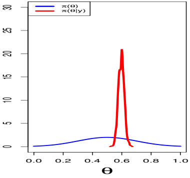




⇓ Metropolis-Hastings algorithm ⇓

Posterior on θ:





More details on the MH algorithm

Initialisation:
θ^0 chosen.

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

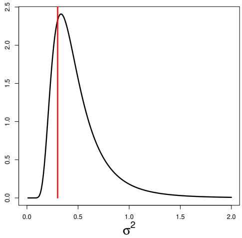
1. Proposal: $\tilde{\theta}^{t+1} = \theta^t + \mathcal{N}(0, \tau^2)$.
2. Compute
$$\alpha(\theta^t, \tilde{\theta}^{t+1}) = \frac{\pi(\tilde{\theta}^{t+1}|\mathbf{y}^F)}{\pi(\theta^t|\mathbf{y}^F)}$$
3. Acceptation:
$$\theta^{t+1} = \begin{cases} \tilde{\theta}^{t+1} & \text{with probability } \alpha(\theta^t,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

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

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

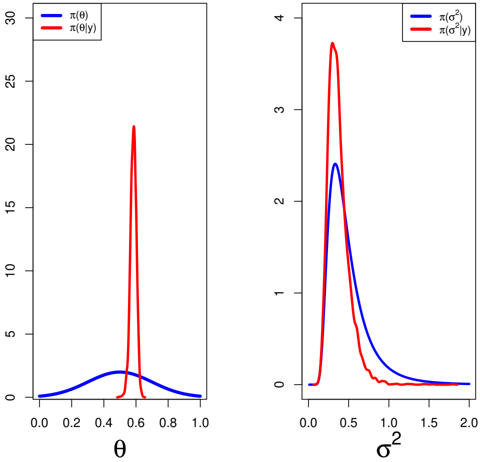
Unknown σ^2

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



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

Posterior distributions



Comparison

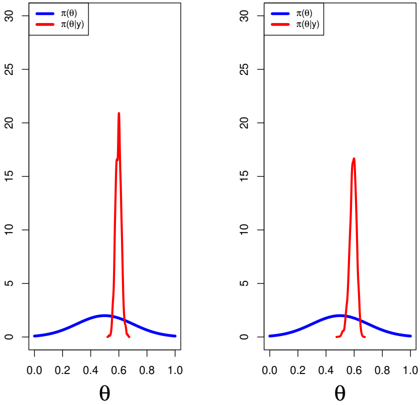


Figure : known σ^2 vs unknown σ^2

with a bad prior....

prior on θ: $\pi(\theta) = \mathcal{N}(0.2, 0.04)$ and $n = 12$ field data

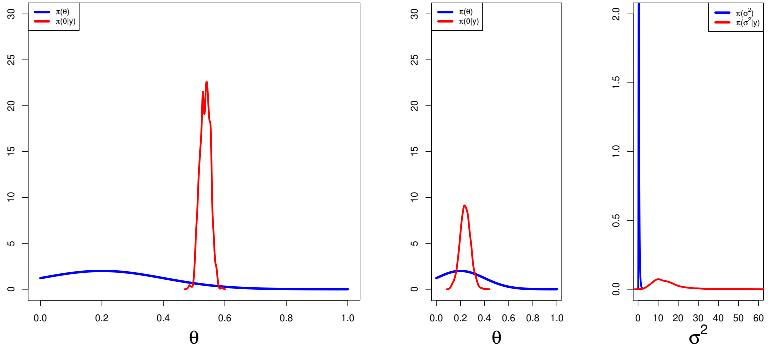


Figure : known σ^2 vs unknown σ^2

Plan

Expensive black-box computer code

- Run the simulator for a given $(\mathbf{x}^*, \boldsymbol{\theta})$ is time-consuming / expensive.
- The simulator is a black-box, no intrusive methods are possible.

$\Rightarrow$ Only few runs of the simulator are possible then we cannot apply algorithms (as in Bayesian calibration) which make a massive use of simulator runs.

Using an emulator / metamodel / coarse model / approximation of the simulator which is fast to compute, but:

- loss on precision of prediction,
- new uncertainty source: accuracy of the model approximation,
- taken into account.

Choosing a design of experiments

Choose N_{run} couples

$$(\mathbf{x}_j^*, \theta_j)$$

- space filling for x,
- with respect to the prior distribution on θ,
- $\mathbf{x}_j^* = \mathbf{x}_i$?

where the simulator is called.

Emulator using Gaussian Process:

- Very popular in computer experiments.
- integrated in a Bayesian framework: appears in the likelihood function and a prior on the parameters of the Gaussian process are chosen.
- model uncertainty coming from approximation of f.
- After the calibration step, used in prediction for a new point $\mathbf{x}$.

Meta-modeling: prior distribution on f

Sacks et al. (1989).
f realization of a Gaussian process F:
$\forall(\mathbf{x}^*, \boldsymbol{\theta}) \in E$,

$$F((\mathbf{x}^*, \boldsymbol{\theta})) = \sum_{k=1}^{Q} \beta_k h_k((\mathbf{x}^*, \boldsymbol{\theta})) + Z((\mathbf{x}^*, \boldsymbol{\theta})) = H((\mathbf{x}^*, \boldsymbol{\theta}))^T \boldsymbol{\beta} + Z((\mathbf{x}^*, \boldsymbol{\theta})),$$

où

- $h_1, \ldots, h_Q$ regression functions and $\boldsymbol{\beta}$ parameters vector,
- Z centered Gaussians process with covariance function:

$$\mathrm{Cov}(Z((\mathbf{x}_1^*, \boldsymbol{\theta}_1)), Z((\mathbf{x}_2^*, \boldsymbol{\theta}_2))) = \sigma^2 K((\mathbf{x}_1^*, \boldsymbol{\theta}_1), (\mathbf{x}_2^*, \boldsymbol{\theta}_2)),$$

where K is correlation kernel.

Hypotheses

- $K((\mathbf{x}_1^*, \boldsymbol{\theta}_1), (\mathbf{x}_2^*, \boldsymbol{\theta}_2)) = \sigma_K^2 \exp(-\xi_{\mathbf{x}^*} \sum |\mathbf{x}_1^* - \mathbf{x}_2^*|^\alpha - \xi_{\boldsymbol{\theta}} \sum |\boldsymbol{\theta}_1 - \boldsymbol{\theta}_2|^\alpha)$
- parameters $\phi = (\boldsymbol{\beta}, \sigma^2, K \text{ parameters})$ assumed fixed (in practice, maximum likelihood estimators);

Meta-modeling: posterior

- $v_1 = f((\mathbf{x}^*, \boldsymbol{\theta})_1), \ldots, v_{N_{run}} = f((\mathbf{x}^*, \boldsymbol{\theta})_{N_{run}})$ evaluations of f on a design $D_{N_{run}}$
- Process $F^{D_{N_{run}}}$: Conditioning F to $F((\mathbf{x}^*_1, \boldsymbol{\theta}_1)) = v_1, \ldots, F(\mathbf{x}^*_{N_{run}}, \boldsymbol{\theta}_{N_{run}})) = v_{N_{run}}$.
  Gaussian Process with mean $m((\mathbf{x}^*, \boldsymbol{\theta}))$ and covariance $C((\mathbf{x}^*, \boldsymbol{\theta}), (\mathbf{x}^*, \boldsymbol{\theta})') \; \forall (\mathbf{x}^*, \boldsymbol{\theta}), (\mathbf{x}^*, \boldsymbol{\theta})'$.

  For all $(\mathbf{x}^*, \boldsymbol{\theta}) \in E$,
  - $m((\mathbf{x}^*, \boldsymbol{\theta}))$ approximates $f((\mathbf{x}^*, \boldsymbol{\theta}))$,
  - $C((\mathbf{x}^*, \boldsymbol{\theta}), (\mathbf{x}^*, \boldsymbol{\theta}))$ uncertainty on this approximation.

For all $(\mathbf{x}^*_i, \boldsymbol{\theta}_i) \in D_{N_{run}}$,

- $m(\mathbf{x}^*_i, \boldsymbol{\theta}_i) = f(\mathbf{x}^*_i, \boldsymbol{\theta}_i)$,
- $C((\mathbf{x}^*_i, \boldsymbol{\theta}_i), (\mathbf{x}^*_i, \boldsymbol{\theta}_i)) = 0$.

Gaussian process emulator: illustration

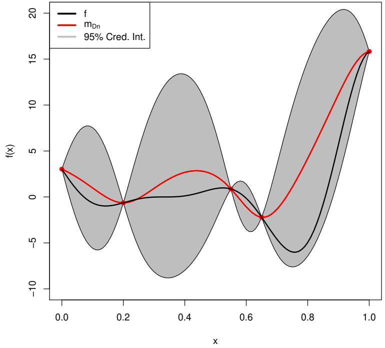


Figure : Posterior mean and pointwise credible interval

Plan

Likelihood with a Gaussian process hypothesis on f

- $\mathbf{z} = (\mathbf{y}_1^F, \ldots, \mathbf{y}_n^F, f(\mathbf{x}_1^*, \boldsymbol{\theta}_1), \ldots, f(\mathbf{x}_{N_{run}}^*, \boldsymbol{\theta}_{N_{run}}))$
- likelihood on $\mathbf{z}$

$$l(\boldsymbol{\theta}, \sigma^2 | \mathbf{z}) \propto |\Sigma_{\mathbf{z}}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{z} - \mu)^T \Sigma_{\mathbf{z}}^{-1} (\mathbf{z} - \mu)\right)$$

where

- μ is the mean of the Gaussian process,
- $$\Sigma_{\mathbf{z}} = \Sigma_f + \begin{pmatrix} \Sigma_y & 0 \\ 0 & 0 \end{pmatrix}$$

  with $\Sigma_y = \sigma^2 I_n$ and Σ_f is obtained as the covariance matrix corresponding to the points: $(\mathbf{x}_1, \boldsymbol{\theta}), \ldots, (\mathbf{x}_n, \boldsymbol{\theta}), (\mathbf{x}_1^*, \boldsymbol{\theta}_1), \ldots, (\mathbf{x}_{N_{run}}^*, \boldsymbol{\theta}_{N_{run}})$.

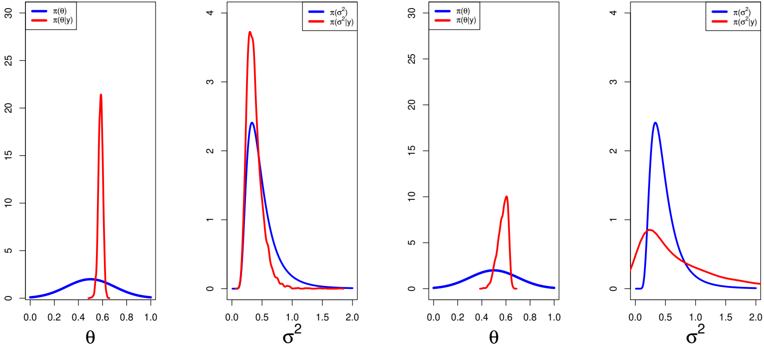
Dealing with GP parameters

- prior distribution on μ and covariance parameters Hidgon et al. (2005) $\Rightarrow$ MCMC inference

- MLE estimators Kennedy and O'Hagan (2001)
  - treated as fixed,
  - only computer data $f(\mathbf{x}_1^*, \boldsymbol{\theta}_1), \ldots, f(\mathbf{x}_{N_{run}}^*, \boldsymbol{\theta}_{N_{run}})$ are used ($n < N_{run}$) for MLE
  - likelihood $l(\boldsymbol{\theta}, \sigma^2 | \mathbf{z})$:

$$l(\boldsymbol{\theta}, \sigma^2 | \mathbf{z}) \propto |\tilde{\Sigma}_{\mathbf{y}^F}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{y}^F - m(\mathbf{x}, \boldsymbol{\theta}))^T \tilde{\Sigma}_{\mathbf{y}^F}^{-1} (\mathbf{y}^F - m(\mathbf{x}, \boldsymbol{\theta}))\right)$$

    where
    - $m(\cdot)$ is the mean of the GP conditioned to simulator data,
    - $\tilde{\Sigma}_{\mathbf{y}^F} = \Sigma_{\mathbf{y}^F} + \tilde{\Sigma}_f = \sigma^2 I_n + \tilde{\Sigma}_f$ where $\tilde{\Sigma}_f$ is constructed with the covariance function $\tilde{C}$ of the conditioned GP.



unlimited runs versus $N_{run} = 12$

Outline

Principle

1. Construct a first exploratory design: D_n s. t. $n \leq N$,
2. For $i = n + 1 ... N$ do $D_i = D_{i-1} \cup \{\mathbf{x}_i\}$ where

$$\mathbf{x}_i \in \arg\max Crit(D_{i-1}, f) .$$

$Crit(D_{i-1}, f)$ can be adapted to the applied goal (optimization, estimation of probability of rare event).

Plan

Expected Improvement criterion

- Goal: Find the global extremum (here minimum e.g.) of f,
- Expected improvement criterion proposed by Jones et al. (1998):

$$EI_n(\mathbf{x}) = \mathbb{E}((min_n - F(\mathbf{x}))^+ | F(D_n)) \,,$$

where min_n is the current minimum value:

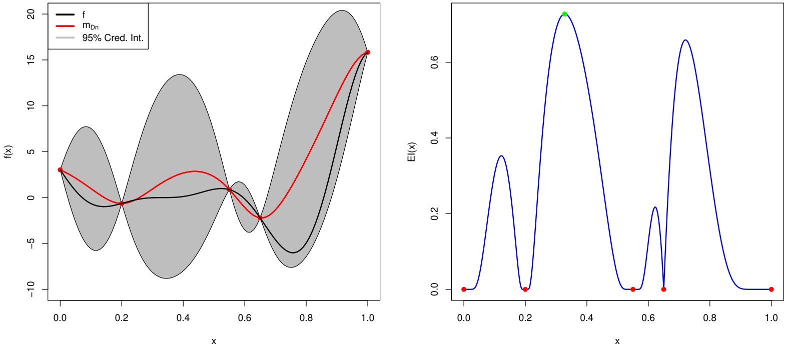
$$min_n = \min_{1,\dots,n} f(\mathbf{x}_i)$$

- Closed-form computation:

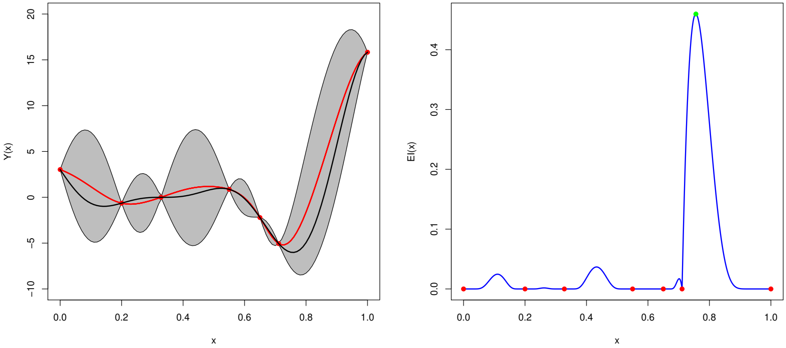
$$EI_n(\mathbf{x}) = (min_n - m_{D_n}(\mathbf{x}))\Phi\left(\frac{min_n - m_{D_n}(\mathbf{x})}{\sqrt{C_{D_n}(\mathbf{x},\mathbf{x})}}\right) + \sqrt{C_{D_n}(\mathbf{x},\mathbf{x})}\phi\left(\frac{min_n - m_{D_n}(\mathbf{x})}{\sqrt{C_{D_n}(\mathbf{x},\mathbf{x})}}\right)$$

where Φ and ϕ are respectively the cdf and the pdf of $\mathcal{N}(0,1)$.

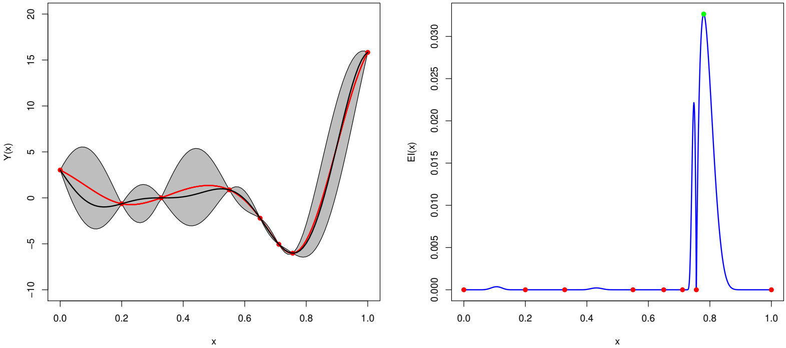
Example step 1



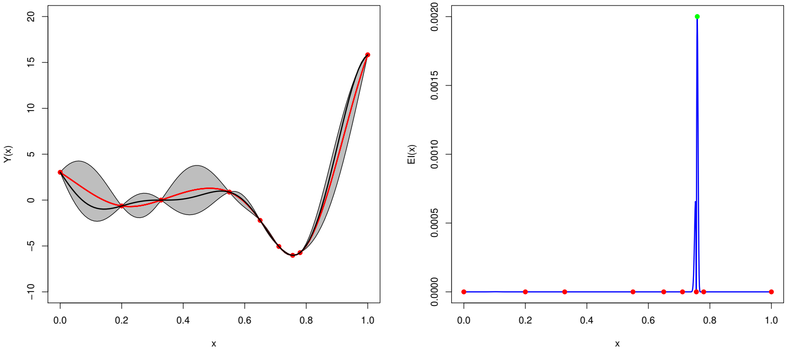
Example step 2



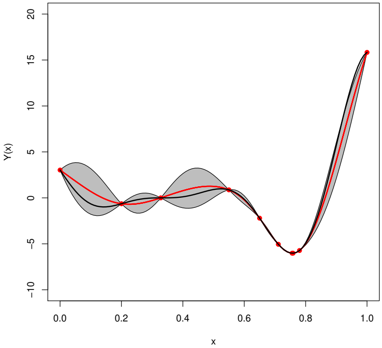
Example step 3

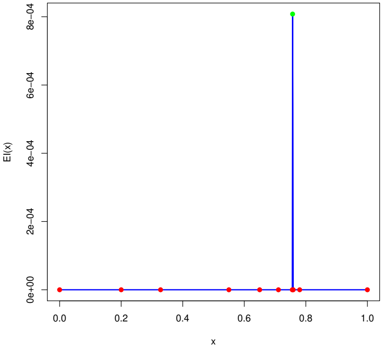


Example step 4



Example step 5

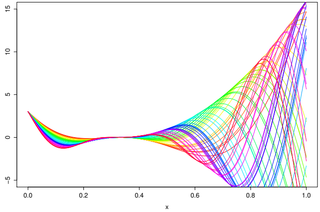




Plan

Example:

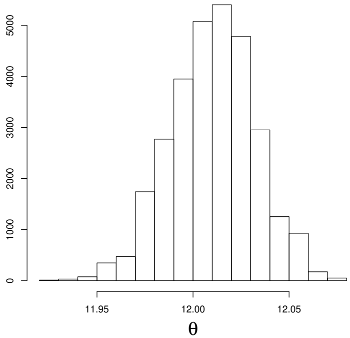
- $\theta = 12$,
- $(x_1, x_2, x_3) = (0.1, 0.3, 0.8)$,
- $f(x, \theta) = (6 \cdot x - 2)^2 \cdot \sin(\theta \cdot x - 4) + \epsilon$,
- $\epsilon_i \sim \mathcal{N}(0, 0.1^2)$ i.i.d.,
- prior $\theta \sim \mathcal{U}[5, 15]$,
- $y_i = f(x_i, \theta) + \epsilon_i$.



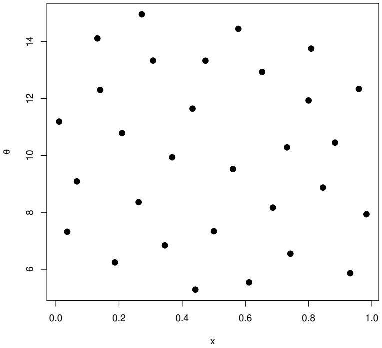
Motivation for adaptive designs in calibration

Quality of calibration (Bayesian or ML) is affected by choice in the numerical design.

- Calibration with unlimited runs of *f*

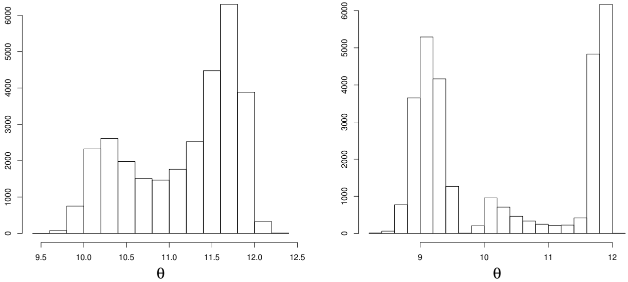


LHS maximin design



Motivation for adaptive designs in calibration

- Calibration with emulator built from a design with $N = 30$ calls to f



Likelihood for calibration

$l(\boldsymbol{\theta}|\mathbf{z})$:

$$l(\boldsymbol{\theta}|\mathbf{z}) \propto |\tilde{\Sigma}_{\mathbf{y}^F}|^{-1/2} \exp\left(-\frac{1}{2}(\mathbf{y}^F - m(\mathbf{x},\boldsymbol{\theta}))^T \tilde{\Sigma}_{\mathbf{y}^F}^{-1}(\mathbf{y}^F - m(\mathbf{x},\boldsymbol{\theta}))\right)$$

where

- $\mathbf{y}^F$ is the vector of field data,
- $m(\cdot)$ is the mean of the GP conditioned to simulator data,
- $\tilde{\Sigma}_{\mathbf{y}^F} = \Sigma_{\mathbf{y}^F} + \tilde{\Sigma}_f = \sigma^2 I_n + \tilde{\Sigma}_f$ where $\tilde{\Sigma}_f$ is constructed with the covariance function C of the conditioned GP.

Optimization goal : maximize the likelihood $\Rightarrow$ Expected Improvement for calibration.

EI

Maximize the likelihood $l(\boldsymbol{\theta}|\mathbf{z})$ over $\boldsymbol{\theta} \Leftrightarrow$ Minimize $MC(\boldsymbol{\theta}) = \|\mathbf{y}^F - f(\mathbf{x}, \boldsymbol{\theta})\|^2$ over $\boldsymbol{\theta}$.

For given:

- field experiments $\mathbf{y}^F = y^F(\mathbf{x}_1), \dots, y^F(\mathbf{x}_n)$,
- D_k numerical design on $\mathbb{X} \times \Theta$ with M points,
- m_0 current minimal value of $MC(\boldsymbol{\theta})$.

EI criterion:

$$EI_{D_k}(\boldsymbol{\theta}) = \mathbb{E}_{D_k}\left((m_0 - MC(\boldsymbol{\theta}))^+\right) ,$$

to be minimised.

EI criterion is applied to a function of f.

EI computation

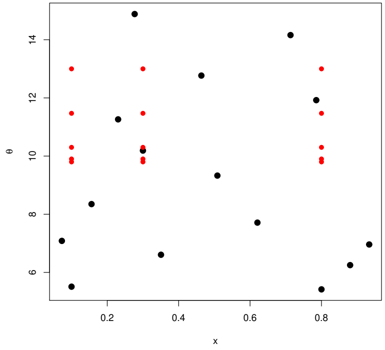
$$
\begin{aligned}
EI_{D_k}(\boldsymbol{\theta}) &= \int_{B(0,\sqrt{m_0})} \left(m_0 - MC(\boldsymbol{\theta})\right) dF_{D_M} \\
&= m_0 \cdot \mathbb{P}_{D_M}(MC(\boldsymbol{\theta}) \leq m_0) - \mathbb{E}_{D_M}\left(MC(\boldsymbol{\theta})\mathbb{I}_{MC(\boldsymbol{\theta})\leq m_0}\right)
\end{aligned}
$$

- no close form computation,
- $\mathbb{P}_{D_M}(MC(\boldsymbol{\theta}) \leq m_0)$ is an upper bound and easier to compute,
- importance sampling may be used for the second term.

Algorithm

1. Build a first space-filling design D_0 on $\mathbb{X} \times \Theta$,
2. Find the maximum: $\tilde{\boldsymbol{\theta}}_0$ of $l(\boldsymbol{\theta}|\mathbf{z})$,
3. Evaluate $f(\mathbf{x}_1, \tilde{\boldsymbol{\theta}}_0), \dots, f(\mathbf{x}_n, \tilde{\boldsymbol{\theta}}_0)$.
4. Set $m_0 = MC(\tilde{\boldsymbol{\theta}}_0)$,
5. for k=1..., repeat
    1. Compute EI_{D_k} on a grid on Θ,
    2. $\tilde{\boldsymbol{\theta}}_k = \arg\max_\Theta EI_{D_k}(\boldsymbol{\theta})$,
    3. Evaluate $f(\mathbf{x}_1, \tilde{\boldsymbol{\theta}}_k), \dots, f(\mathbf{x}_n, \tilde{\boldsymbol{\theta}}_k)$

Adapted design



Bayesian calibration based on the adapted design

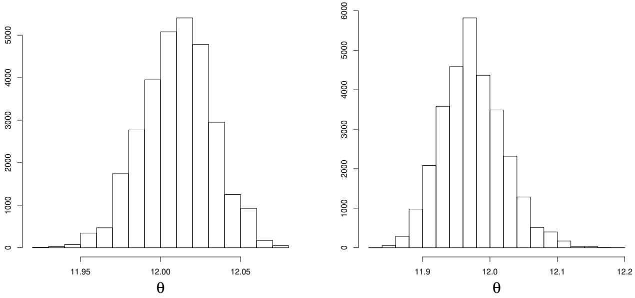


Figure : Bayesian calibration with unlimited runs vs Bayesian calibration with $N = 30$ chosen by EGO

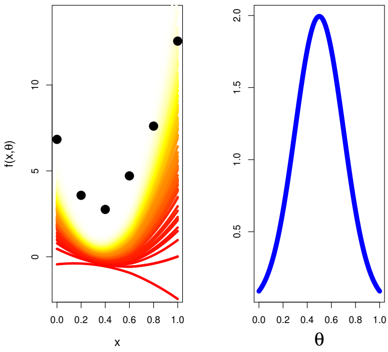
Outline

Conclusion

- Designs of numerical experiments adapted to calibration purpose,
- Robustness in calibration.
- Higher dimension questions, number of field experiments, dimension of $\boldsymbol{\theta}$...
- New field experiments ?
- discrepancy issues ?

Model discrepancy

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



No value of $\boldsymbol{\theta}$ makes the simulator corresponding to the fied data

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Calibration of computer models

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