A New Bayesian Approach for Statistical Calibration of Computer Models

Frédérick Delay[1], Thierry A. Mara[2], Anis Younès[1,3]

[1]LHyGeS, UMR CNRS 7517 (France),[2]University of La Reunion (France),[3]IRD UMR LISAH, Montpellier (France)

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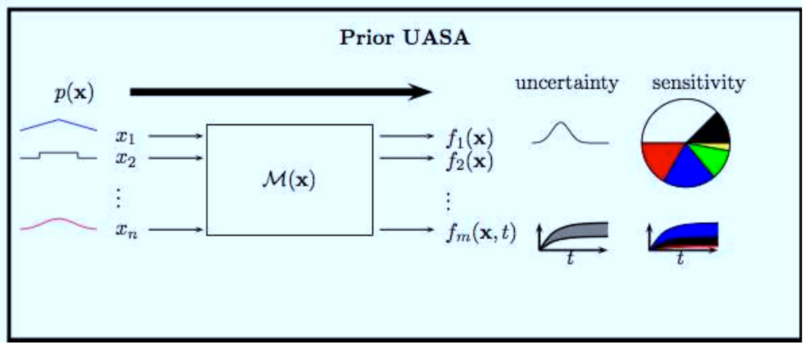
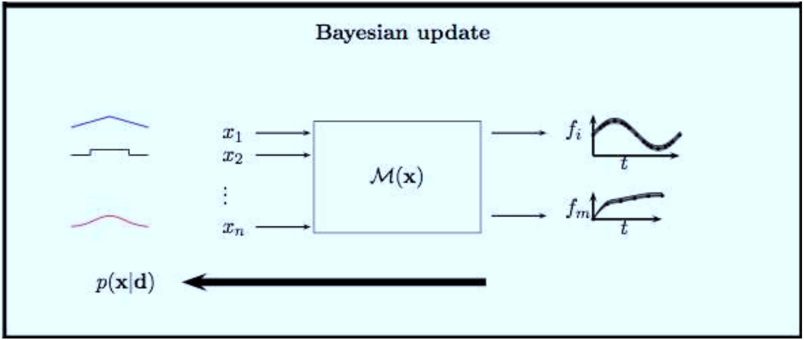
The setting: The Forward Problem (UASA)



Given $p(\mathbf{x})$ find $p(y)$ + Sensitivity Indices

The setting: The Inverse Problem (Statistical Calibration)



Given $p(\mathbf{y}|\mathbf{x}) + p(\mathbf{x})$ find $p(\mathbf{x}|\mathbf{y})$

Bayesian inference

Bayesian inference relies on the axiom of conditional probability:
$p(\mathbf{y},\mathbf{x}) = p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = p(\mathbf{x}|\mathbf{y})p(\mathbf{y})$
and writes:

$$p(\mathbf{x}|\mathbf{y}) \propto p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) \tag{1}$$

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The most probable (best) solution is,

$$\mathbf{X}_{MAP} = \underset{\mathbf{x}}{\operatorname{argmax}} \{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})\} \tag{2}$$

called the maximum a posteriori estimate (MAP).

MCMC sampling

Evaluating $\mathbf{X}_{MAP}$ can be computationally fast but:

- can be hampered by the presence of local optima
- do not provide the posterior pdf of the inputs (except under Laplace approximation)

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Markov chains Monte Carlo (MCMC) can sample $\mathbf{x}$ from (1). It is a rejection/acceptance sampling technique that explores the probable region of the input space.

But MCMC remains computationally demanding.

The maximal conditional posterior distribution (MCPD) approach of Mara et al. (2015) - cheaper alternative approach.

MCPD sampling

The maximal conditional posterior distribution (MCPD) is defined as:

$$\mathcal{P}(x_i) = \max_{\mathbf{x}_{\sim i}} \left(p(\mathbf{x}_{\sim i} | \mathbf{y}, x_i) \right) \times p(x_i | \mathbf{y}) \tag{3}$$

First introduced in Mara et al. (AWR, 2015) for statistical calibration of computer models as an alternative to MCMC.

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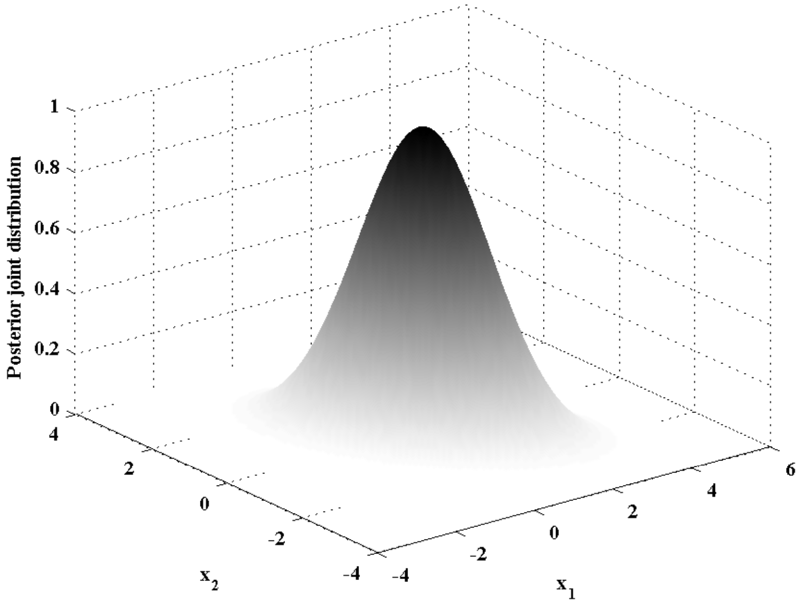
Definition: $\mathcal{P}(x_i)$ represents the distribution of x_i knowing that the remaining inputs $\mathbf{x}_{\sim i}$ maximize the conditional posterior pdf.

Consequence: Any draw $\mathbf{X}_k$ drawn from $p(\mathbf{x})$ is such that, $(X_{ki}, p(\mathbf{X}_k|\mathbf{y}))$ is located beneath $\mathcal{P}(x_i)$, $\forall i = 1, \ldots, n$.


Posterior joint distribution
1
0.8
0.6
0.4
0.2
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-2
-4
x2
-4
-2
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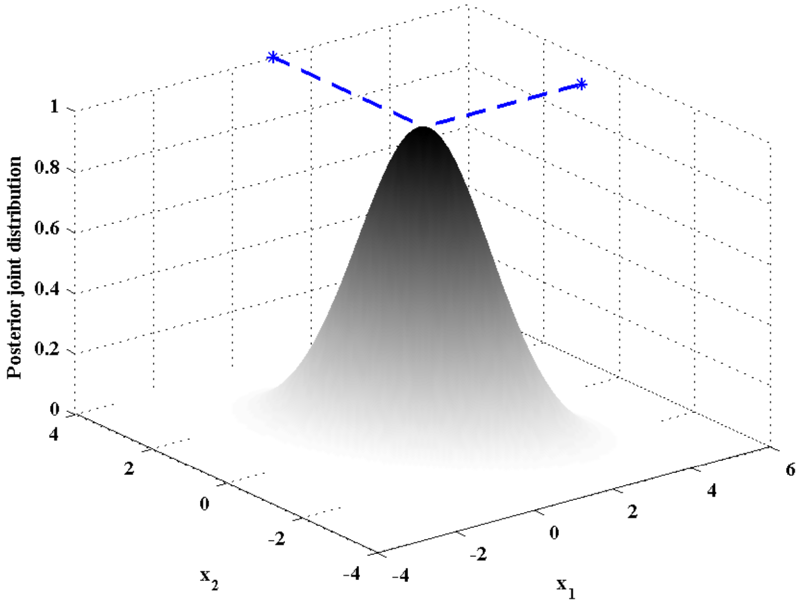
2
4
6
x1



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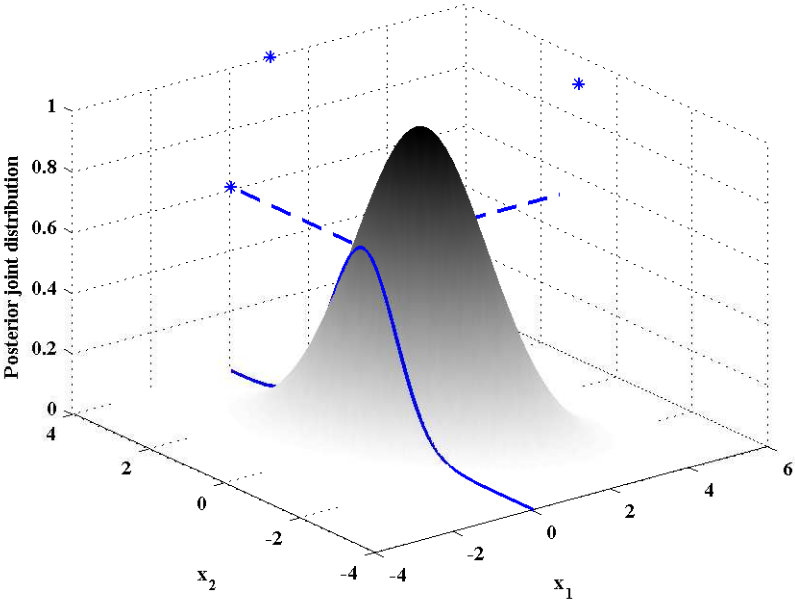

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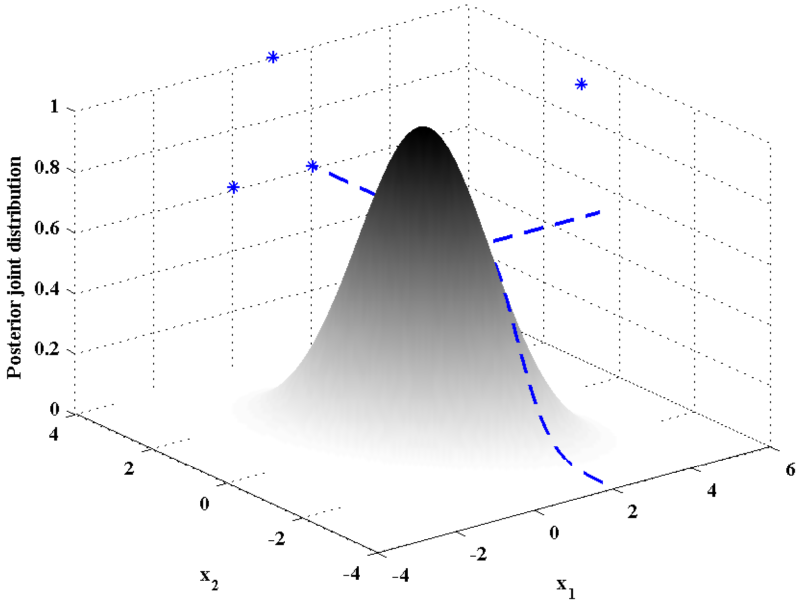

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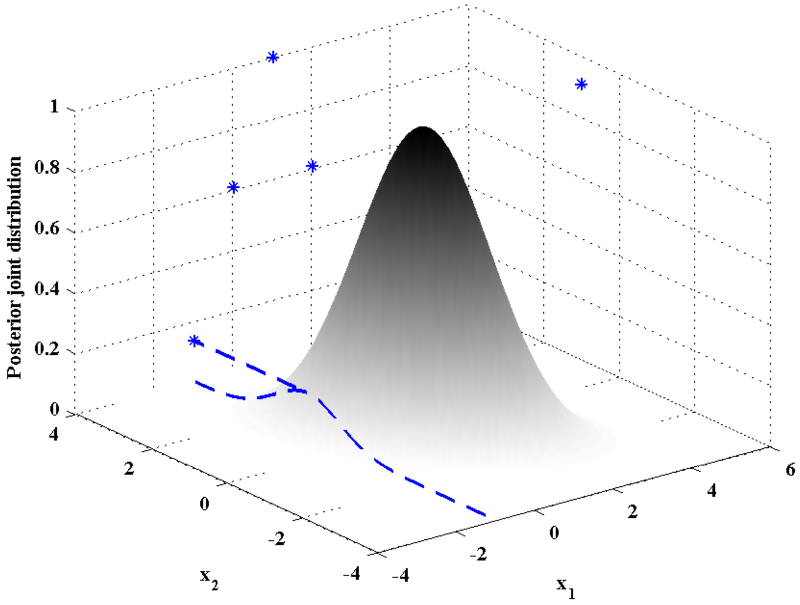
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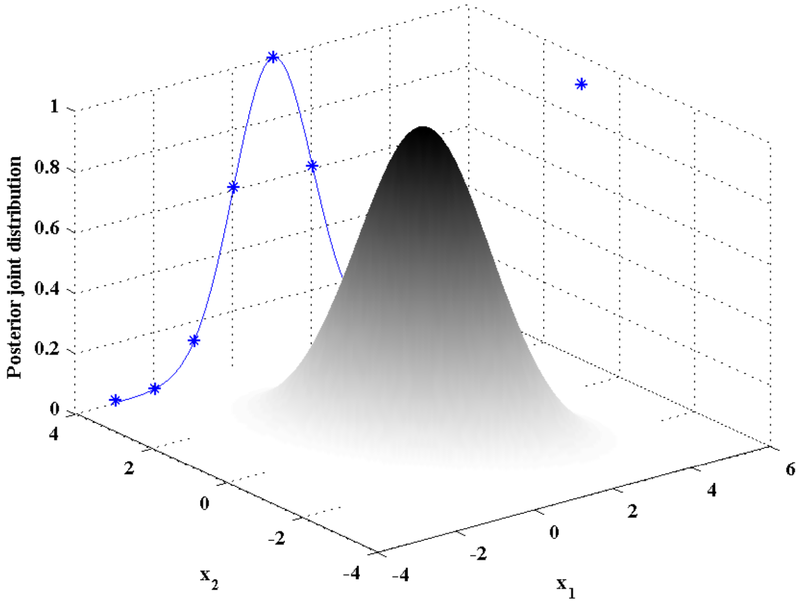
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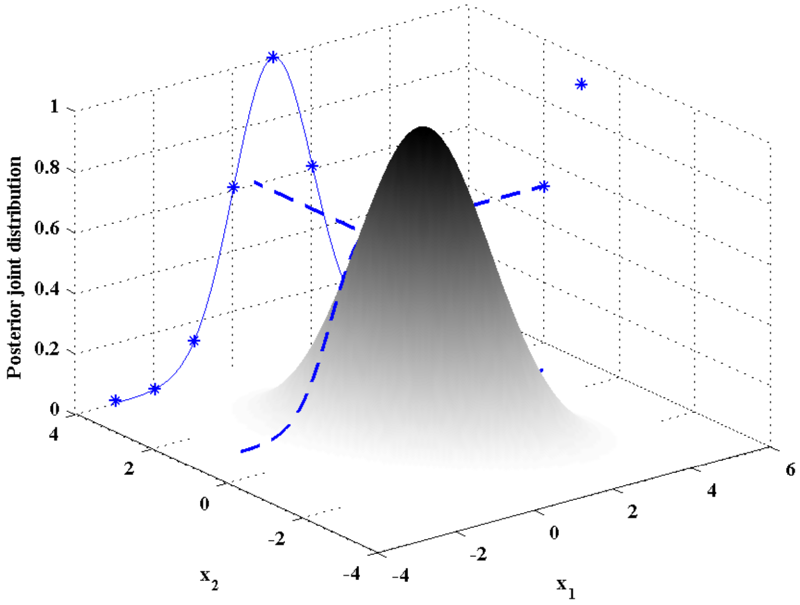
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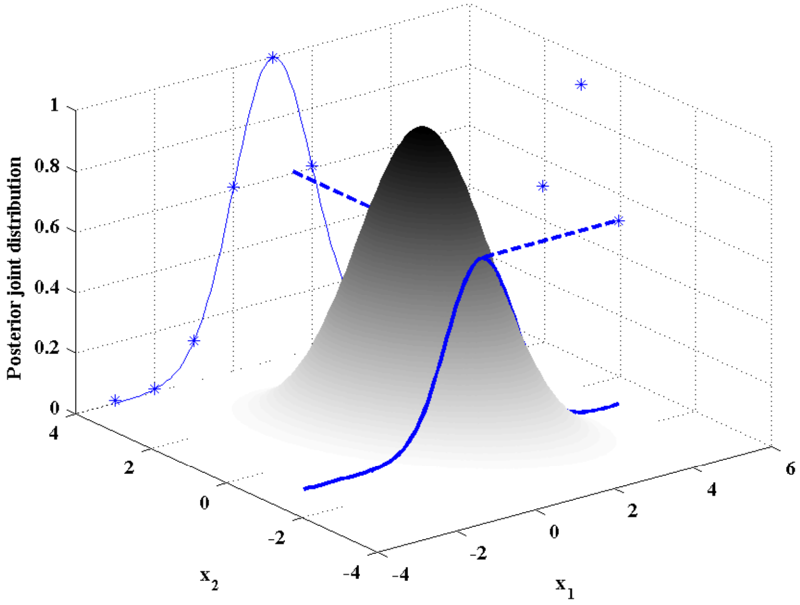

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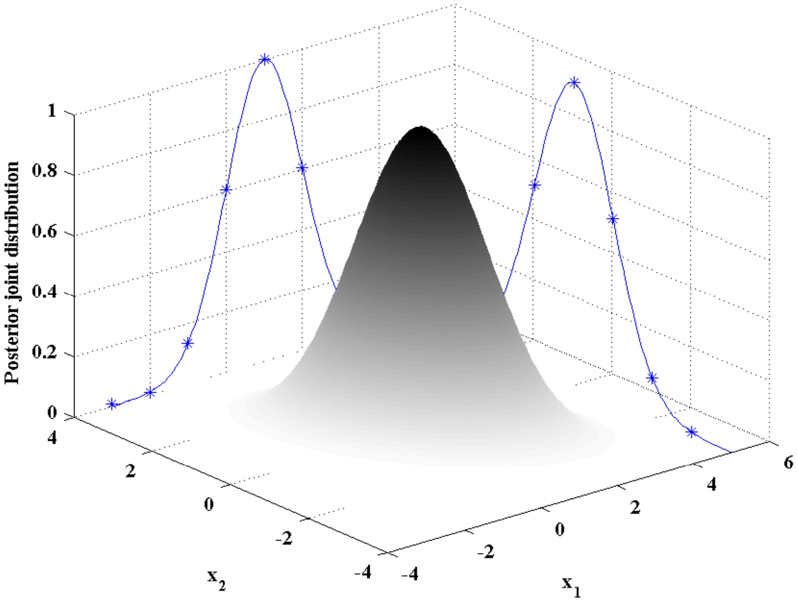

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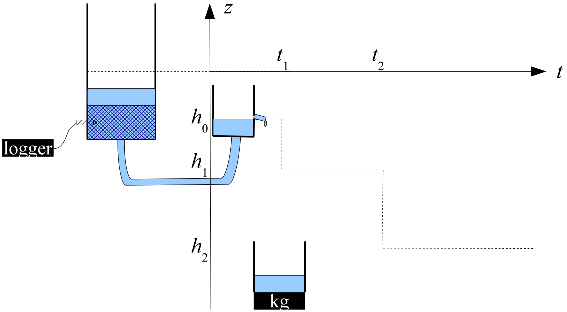
Drainage experiment: MCMC vs MCPD



Obj: From the observed data, find the hydraulic parameters:
$K_s, \omega_r, \omega_s, \alpha, n, \lambda)$

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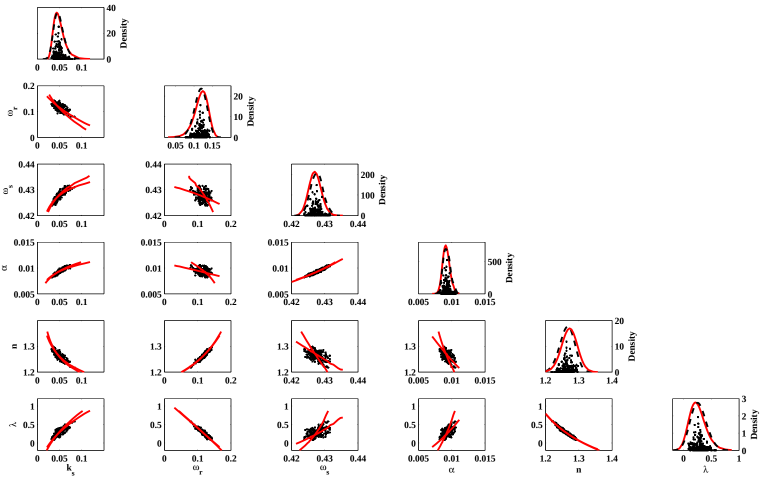

MCMC: 8x8000 model runs, CTU=8000

MCPD: 7500 runs, CTU = 2000

MCPD sampler versus MCMC sampler

Pros of MCPD:

- Computationally cheap
- Easy to use (free available MATLAB programs)
- Assessment of the MCPDs can be parallelized (cost independent of the dimension n)

Cons of MCPD:

- Likelihood dependent ($p(\mathbf{x}|\mathbf{y})$ must have finite modes), so far, only implemented for Gaussian likelihood
- May need to modify $\mathcal{M}$ to compute the Jacobian (for efficiency purposes)
- Few probabilistic draws provided (while MCMC provides large stochastic draws)