



Bayesian Inference of Model Error in Imprecise Models

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DE LA RECHERCHE À L'INDUSTRIE

BAYESIAN INFERENCE OF MODEL ERROR IN IMPRECISE MODELS

January 2021, ECCOMAS Congress (online)

Nicolas Leoni ^{1 2} Pietro Congedo ² Olivier Le Maître ³ Maria-Giovanna Rodio ¹

¹CEA SACLAY, DES/ISAS/DM2S/STMF/LMSF ²INRIA SACLAY-ÎLE-DE-FRANCE ³CNRS, CMAP, PALAISEAU

Context

Model error and Calibration

Analytical example with gaussian posteriors

Numerical example

Conclusion

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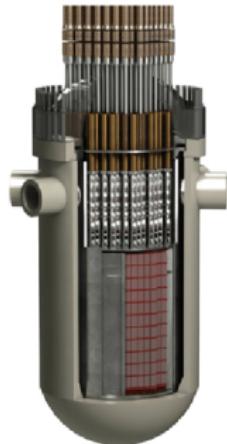


Image source : Framatome

- ▶ A reliable simulation of the reactor is needed for risk prevention ;
- ▶ Physical models exist for each component of the reactor,
- ▶ These models are calibrated separately then used together,
- ▶ Modelling assumptions can lead to inaccurate predictions.

To make more realistic predictions :

Need to estimate uncertainties linked to modeling assumptions, namely "model error".

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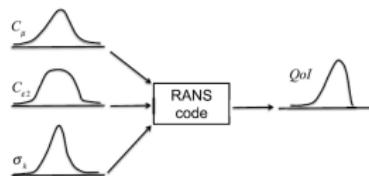
Conclusion

Calibration of a computer code

Use observations obtained from an experiment to find out the best values of coefficients in the numerical model.

It is an **inverse problem**.

Bayesian framework : the parameters are unknown and **random**. They follow a probability distribution, from **prior** (before seeing the data) to **posterior** (after seeing the data).



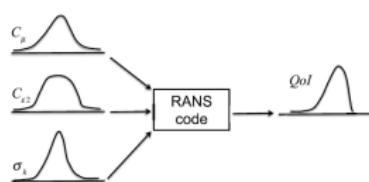
(a) Direct problem

Calibration of a computer code

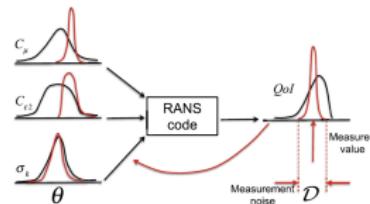
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(a) Direct problem



(b) Inverse problem

Image source : [XC19]

Traditional decomposition : ([KO01])

- ▶ **Parametric uncertainty** : due to the imperfect knowledge of coefficients in the model.
- ▶ **Model error** : due to modeling assumptions to construct the physical model.
- ▶ **Experimental uncertainty** : results from inexact measurements of quantities of interest.
- ▶ **Numerical error** : results from solving a physical model with numerical methods (discrete schemes, finite elements, . . .).

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In Uncertainty Quantification studies, **model error** is often not included.

In this work : How can we accurately estimate **model error** and take it into account in the result of a computer code ?

Calibration with model error [KO01] :

$$y_{obs}(x) = f(x, \theta^{best}) + z(x) + \epsilon_{exp} \quad (1)$$

- ▶ No numerical error.
- ▶ Model error : defined as difference between reality and model *taken at its best parameters*.
- ▶ What is the "best parameters" value ?

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Calibration with flexible prior [Plu17] :

$$y_{obs}(x) = f(x, \theta) + z(x, \theta) + \epsilon_{exp} \quad (2)$$

- ▶ Model bias depends on model parameters.

Common hypotheses : $\epsilon_{exp} \sim N(0, \sigma_{exp}^2)$; $z|\psi \sim GP(\mu, c_\psi)$; $z \perp \epsilon_{exp}$.

With previous hypotheses, the likelihood function is gaussian :

$$\mathbf{y}_{obs} | \theta, \psi \sim N(\mathbf{f}_\theta, \mathbf{C}_\psi + \sigma_{\text{exp}}^2 \mathbf{I}_n). \quad (3)$$

And the full posterior distribution is given by Bayes' Theorem :

$$p(\theta, \psi | \mathbf{y}_{obs}) \propto p(\theta, \psi) p(\mathbf{y}_{obs} | \theta, \psi). \quad (4)$$

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KOH approximation :

A single value of hyperparameters is estimated with maximum a posteriori :

$$\psi_{MAP} = \arg \max_{\psi} p(\psi | \mathbf{y}_{obs}). \quad (5)$$

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KOH approximation :

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Full Maximum Posterior approximation :

Multiple values of hyperparameters are estimated :

$$\psi_{FMP}(\theta) = \arg \max_{\psi} p(\psi) p(\mathbf{y}_{obs} | \theta, \psi). \quad (6)$$

The posterior density of parameters is then estimated by :

$$p(\theta | \mathbf{y}_{obs}) \propto p(\theta) p(\mathbf{y}_{obs} | \theta, \psi = \psi_{FMP}(\theta)) \quad (7)$$

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The model can be used for prediction at a new point x^* :

$$p(f(x^*) | \mathbf{y}_{obs}) = \int_{\theta} p(f(x^*) | \theta, \mathbf{y}_{obs}) p(\theta | \mathbf{y}_{obs}) d\theta \quad (8)$$

Algorithm 1: FMP calibration

- Build a DoE $\{\theta_i\}$ in the model parameters space;
 - Run the computer model to get $\{f(\theta_i)\}$ and perform the optimisations to get $\{\psi_{FMP}(\theta_i)\}$ (eq. (6));
 - Store the optimized values and multiply by $p(\theta)$ to get the posterior density $p(\theta|\mathbf{y}_{obs})$;
 - The posterior density is used to compute new predictions.
-

- ▶ More optimisations are required compared to traditional methods.
- ▶ Optimisations are independent and can be run in parallel.
- ▶ In this work we use a full grid sampling. Integrals are evaluated by quadrature.

Context

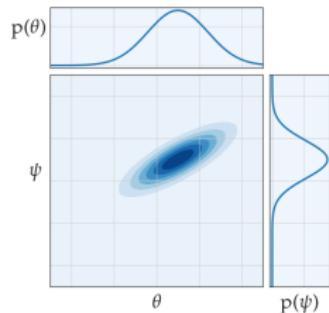
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Analytical example with gaussian posteriors

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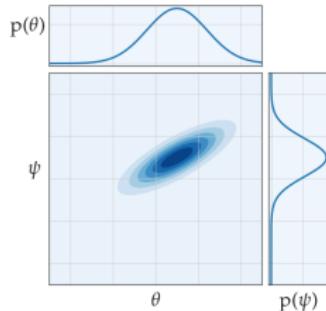
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Let us assume that the joint posterior $p(\theta, \psi | \mathbf{y}_{obs})$ is gaussian.

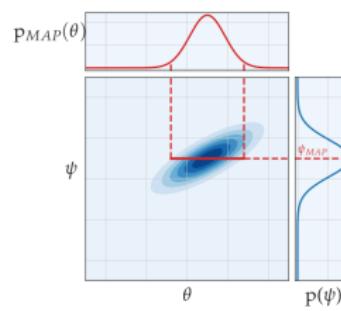


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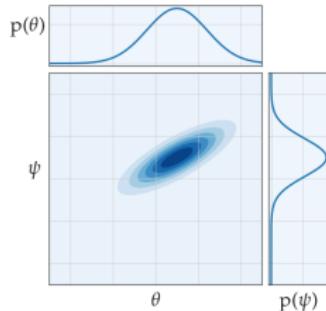


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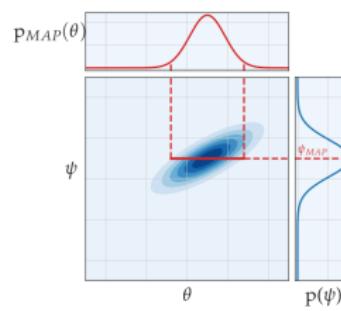


(b) MAP approximation

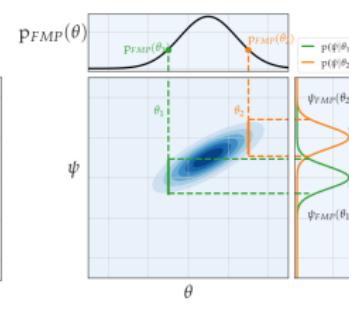
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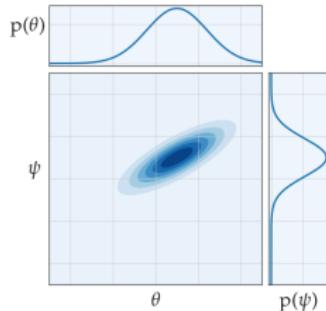


(b) MAP approximation

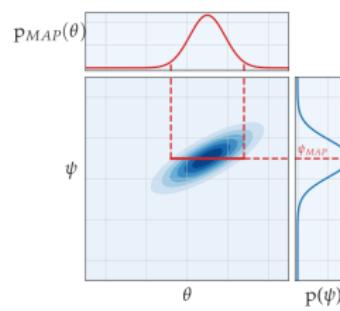


(c) FMP approximation

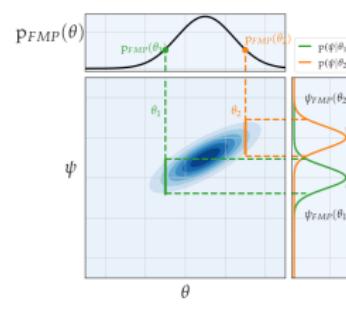
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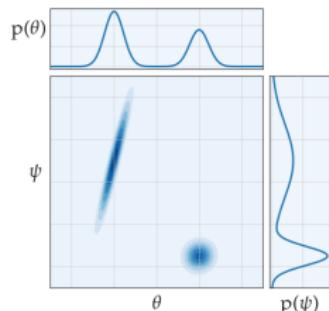
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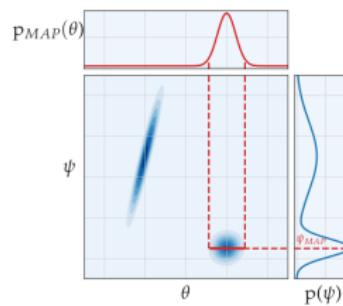
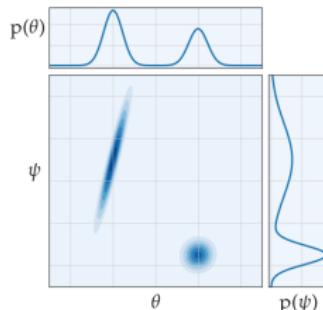
- The FMP method is exact on this case. With traditional MAP the parameter posterior shows reduced variance ("false certitude").

Suppose that $p(\theta, \psi | \mathbf{y}_{obs})$ is a mixture of gaussians, well-separated.

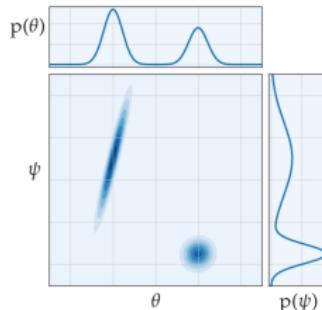


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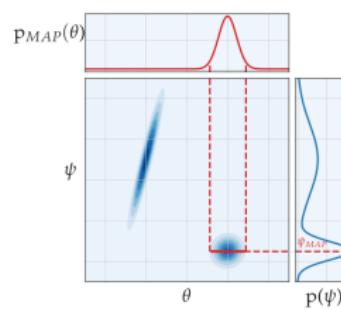
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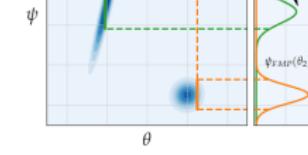
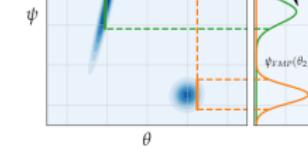
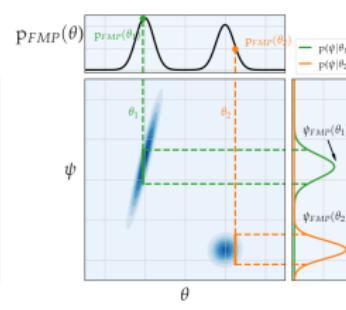
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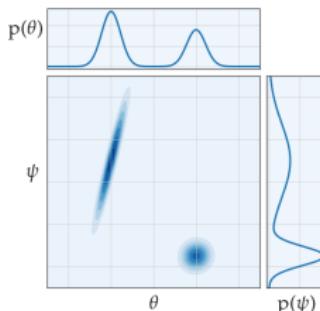


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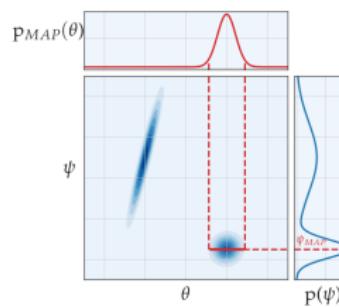


(c) FMP approximation

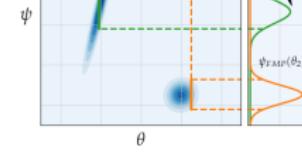
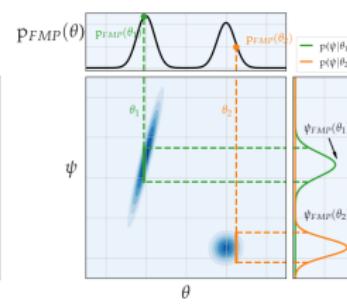
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(c) FMP approximation

- ▶ Traditional MAP might not see probability mass. The estimated variance is still reduced.
- ▶ FMP approximation finds all maxima with correct variance. Peak values might be incorrect due to volume effects.

Context

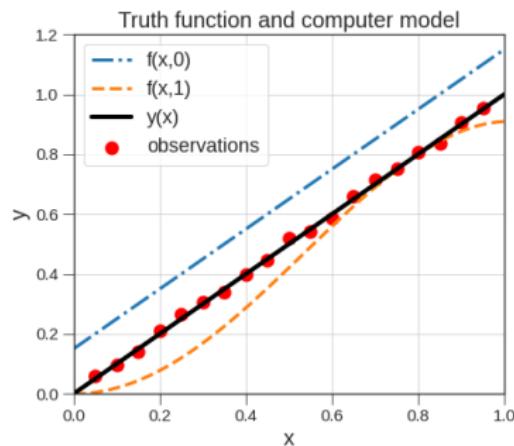
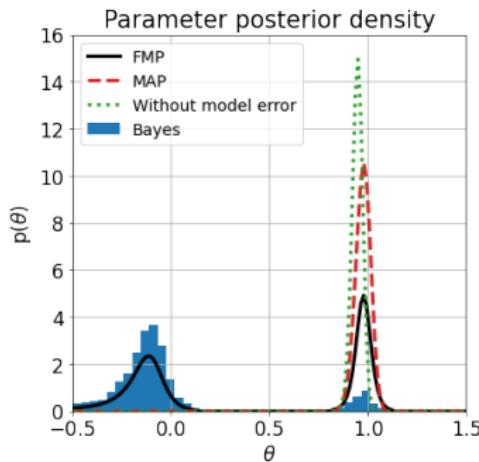
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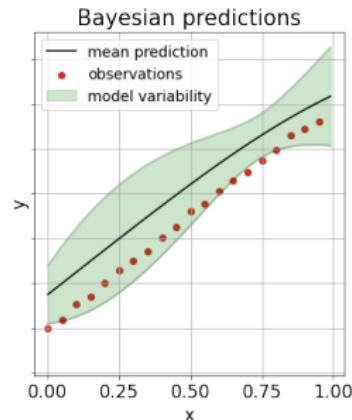
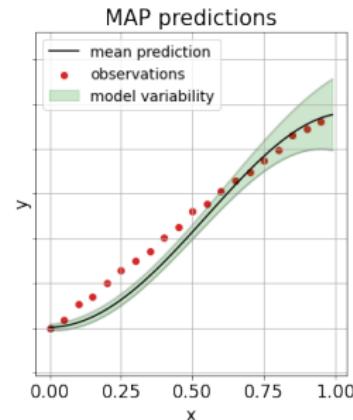
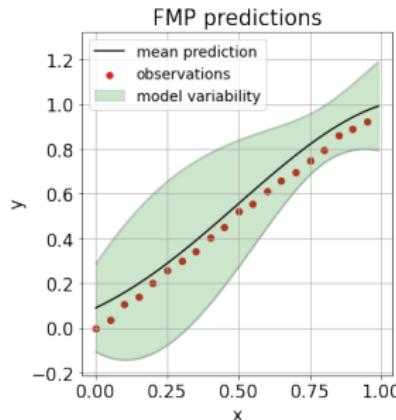
Conclusion

1D example. $y_{truth}(x) = x$ and $f(x, \theta) = x \sin(2\theta x) + (x + 0.15)(1 - \theta)$.
 $x \in [0, 1]$ and $\theta \in [-0.5, 1.5]$.



We use 20 observations from reality, with small noise $\sigma_{exp}^2 = 0.01$.
Statistical assumptions : $p(\sigma^2, \sigma_{exp}^2) \propto 1$, $I_{cor} \sim IG(5, 0.4)$, $\mu = 0$.
 $p(\theta) \propto 1$, squared exponential kernel.

Predictions with the calibrated model



Confidence intervals from FMP and Bayesian predictions are large enough to contain observations.

Map predictions provide an incorrectly thin confidence interval, "false certitude".

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- ▶ We solve the joint estimation problem that is overlooked in litterature because :
 - it is expensive to solve
 - it doesn't match with the traditional definition of model error.
- ▶ The FMP estimation reduces the cost and is still accurate with gaussian posteriors.
- ▶ The traditional MAP estimation might miss posterior probability mass.

Perspectives :

- ▶ Application to more complex cases,
- ▶ Study of smart sampling techniques to increase the dimension of the problem.



Marc C. KENNEDY et Anthony O'HAGAN. "Bayesian Calibration of Computer Models". In : *Journal of the Royal Statistical Society : Series B (Statistical Methodology)* 63.3 (2001), p. 425-464. ISSN : 1467-9868. DOI : 10.1111/1467-9868.00294. URL : <https://rss.onlinelibrary.wiley.com/doi/abs/10.1111/1467-9868.00294> (visité le 14/02/2020).



Matthew PLUMLEE. *Bayesian Calibration of Inexact Computer Models : Journal of the American Statistical Association : Vol 112, No 519*. 2017. URL : <https://www.tandfonline.com/doi/full/10.1080/01621459.2016.1211016> (visité le 14/02/2020).



Heng XIAO et Paola CINNELLA. "Quantification of Model Uncertainty in RANS Simulations : A Review". In : *Progress in Aerospace Sciences* 108 (1^{er} juil. 2019), p. 1-31. ISSN : 0376-0421. DOI : 10.1016/j.paerosci.2018.10.001. URL : <http://www.sciencedirect.com/science/article/pii/S0376042118300952> (visité le 14/02/2020).



Thanks for your attention!