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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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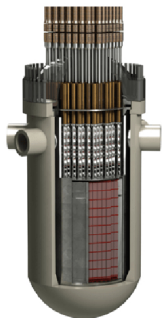


Image source : Framatome

- ▶ 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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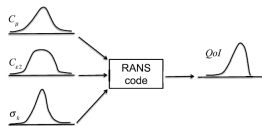
Conclusion

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).



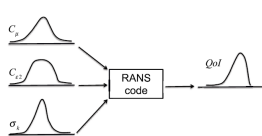
(a) Direct problem

Calibration of a computer code

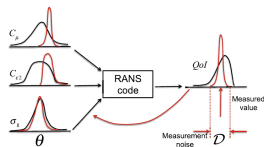
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(a) Direct problem



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

With previous hypotheses, the likelihood function is gaussian :

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

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

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

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KOH approximation :

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

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Full Maximum Posterior approximation :

Multiple values of hyperparameters are estimated :

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

The posterior density of parameters is then estimated by :

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

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

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

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

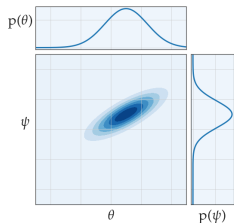
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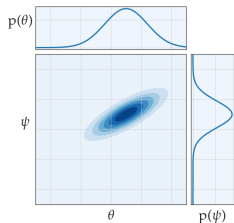
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Let us assume that the joint posterior $p(\boldsymbol{\theta}, \psi | \mathbf{y}_{obs})$ is gaussian.

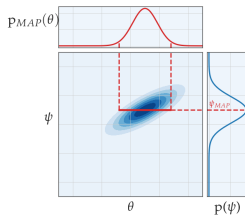


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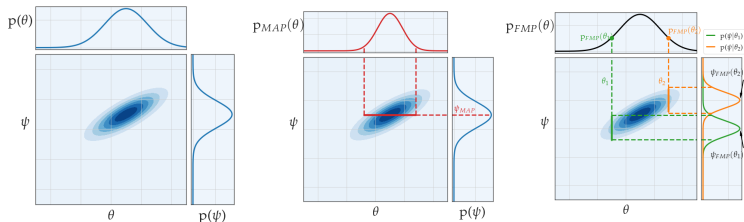


(a) Full Bayes



(b) MAP approximation

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

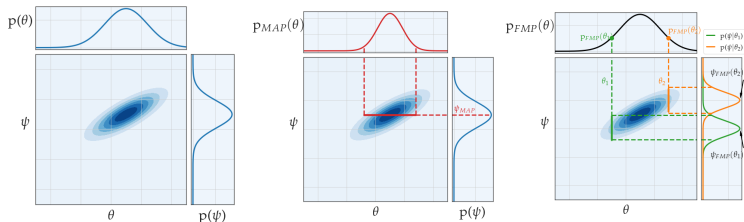


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(c) FMP approximation

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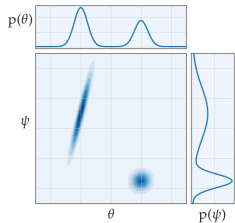
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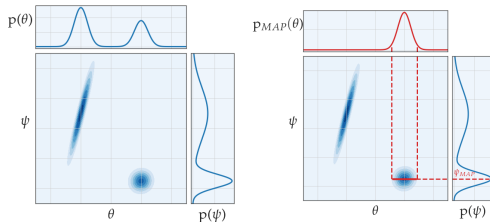
- The FMP method is exact on this case. With traditional MAP the parameter posterior shows reduced variance ("false certitude").

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



(a) Full Bayes

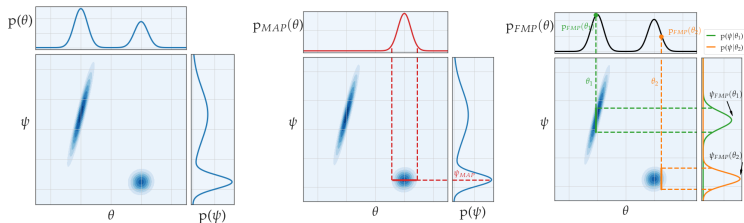
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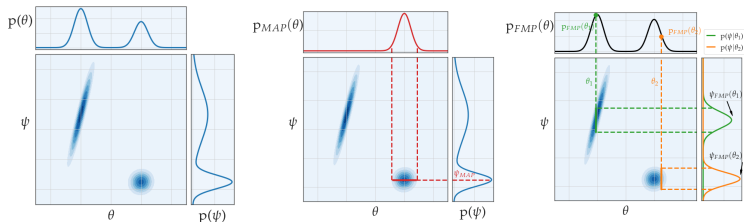


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Suppose that $p(\theta, \psi | \mathbf{y}_{obs})$ is a mixture of gaussians, well-separated.



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- ▶ 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

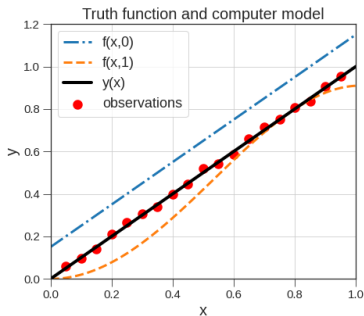
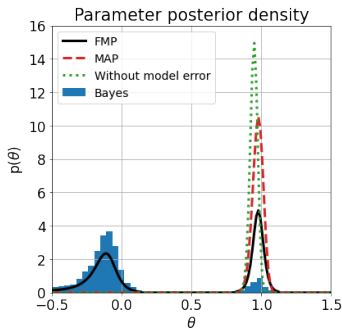
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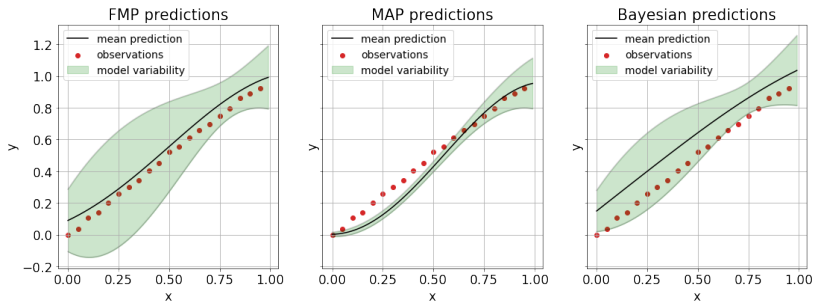
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1D example. $y_{truth}(x) = x$ and $f(x, \theta) = x \sin(2\theta x) + (x + 0.15)(1 - \theta)$.
 $x \in [0, 1]$ and $\theta \in [-0.5, 1.5]$.



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



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 literature 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!