Bayesian calibration of computer codes with Full Maximum a Posteriori (FMP) estimation of model error

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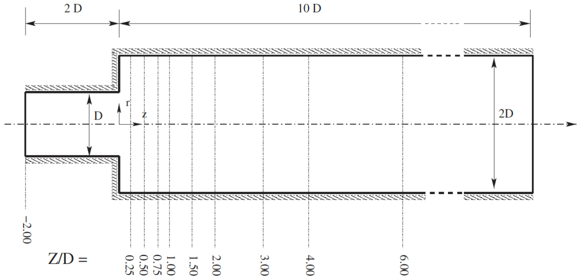
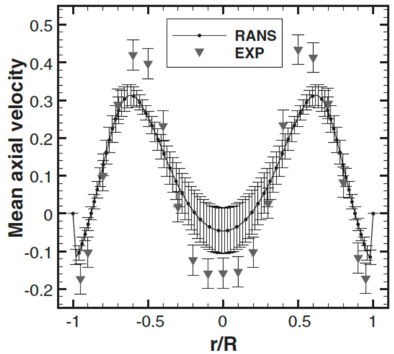
Workshop on calibration of numerical code
31 May 2023

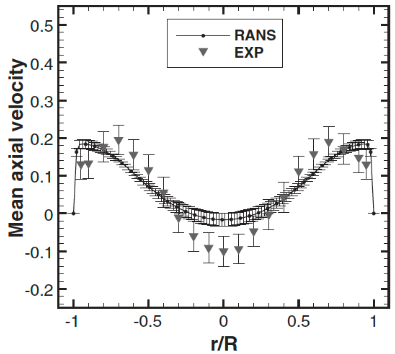
Prediction uncertainty for complex model is a big issue

Ex: IJNMF (2013)

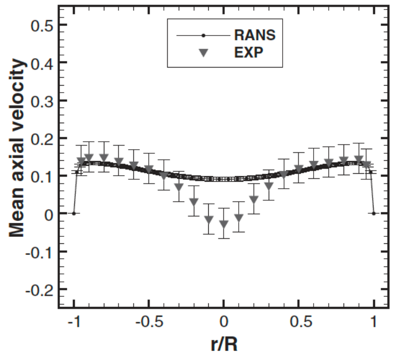




(a) L/D=0.75

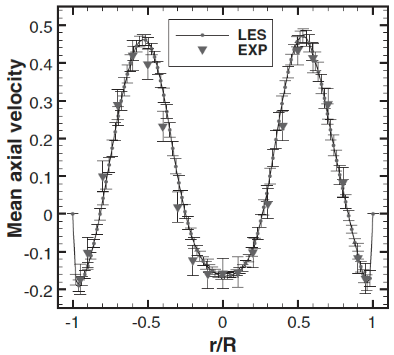


(b) L/D=1.5

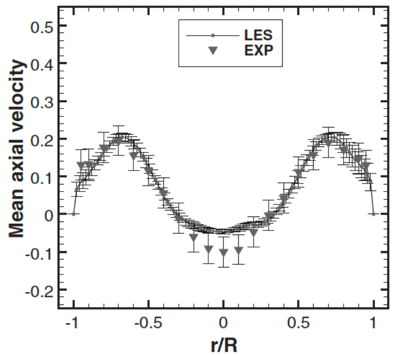


(c) L/D=4.0

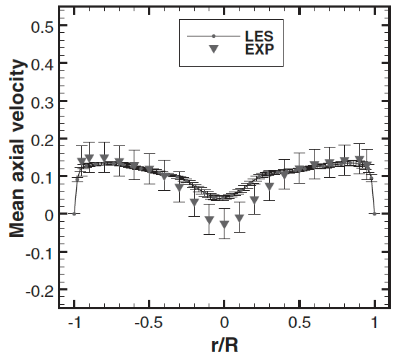
Impact of **tuning parameters** on the variability



(d) L/D=0.75



(e) L/D=1.5

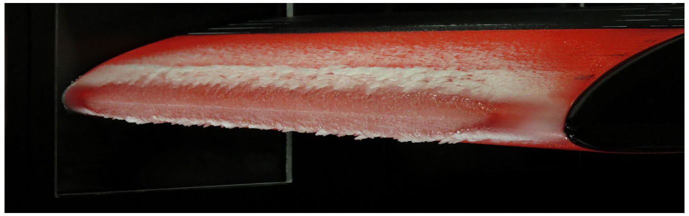


(f) L/D=4.0

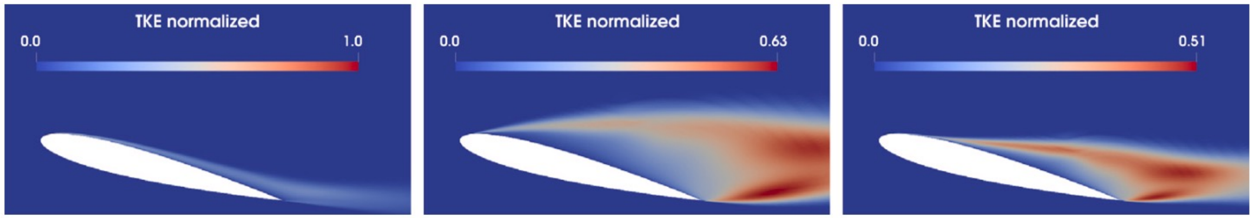
Prediction uncertainty for complex model is a big issue

Ex: Modelling of in-flight icing –EU-MSCA TRACES (2022-2026)

Objective: Assessment of performance in icing conditions, virtual certification



Impact of **structural uncertainty** (on turbulence model) – CandF (2022)



Need for reducing uncertainty through calibration when possible

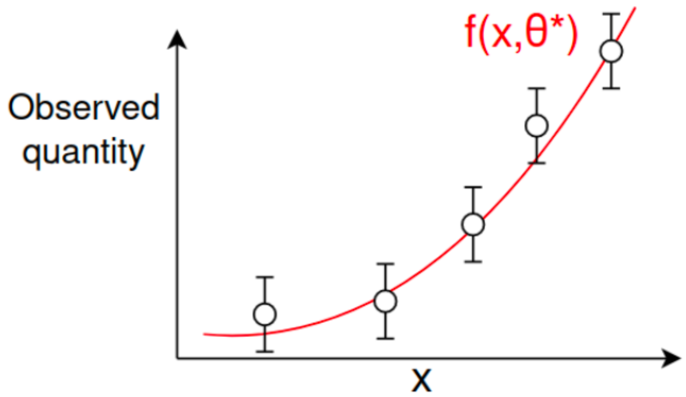
Long-term objective:

Develop a calibration framework with consideration of model error, appropriate for costly, strongly non-linear solvers

- Mostly in situation with few experimental data;
- Model predictions used usually for design (Extrapolation)
- Different levels of resolution in the models (discretization, fidelity)

Model predictions after calibration

Case #1: some parameter values fit the data well. ✓



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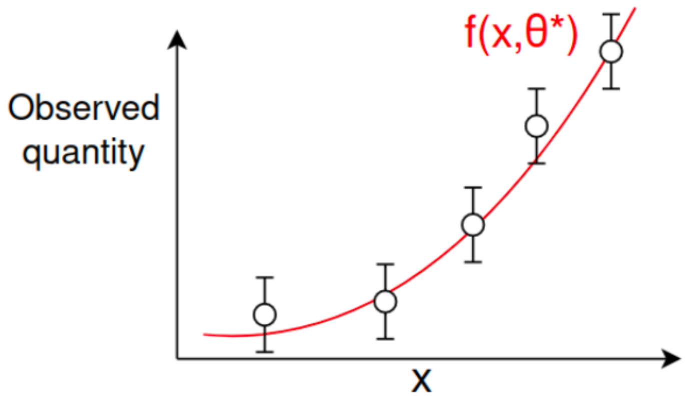
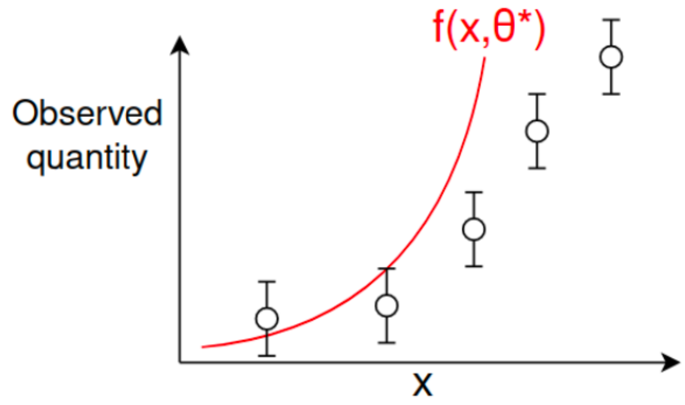


Case #2: best values are not consistent with the observations. ✗



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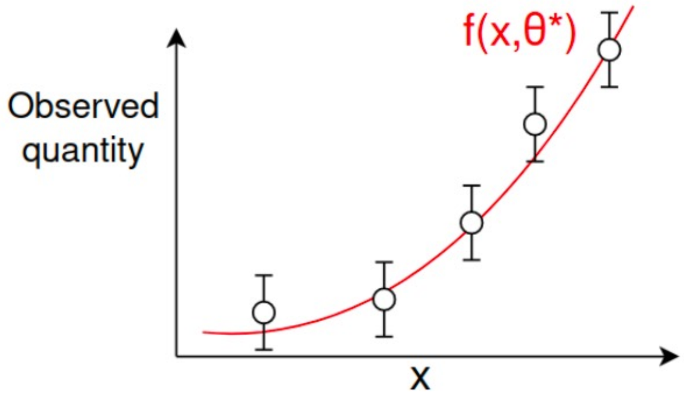

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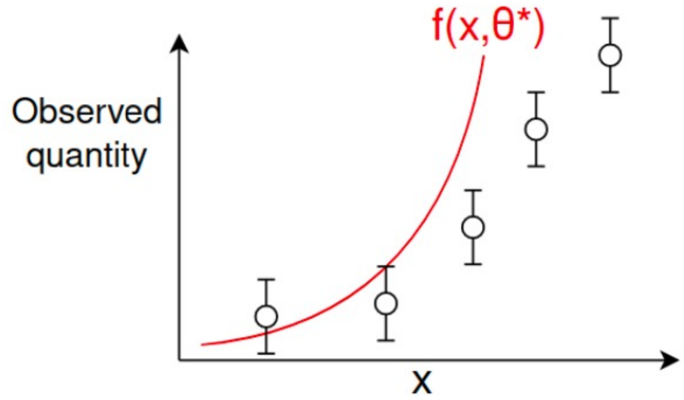

- Need to acknowledge **model error** in the calibration process.
  - Statistical correction on the model output (**KOH2001**).
  - Nature of model discrepancy and its treatment in the calibration process (**BOH2014**).
  - Representation of the model error (**Arhonditsis 2008**)
  - Potential use of the model during extrapolation (**Bayarri2007**)
  - Impact of priors (**BOH2014**)

Full Bayesian calibration

$$\overbrace{y_{\text{obs}}(x)}^{\text{observations}} = \overbrace{f(x,\boldsymbol{\theta})}^{\text{computer model}} + \cancel{\overbrace{z(x)}^{\text{model discrepancy}}} + \overbrace{\epsilon(x)}^{\text{measurement error}} \qquad (1)$$

Some statistical assumptions:

- Measurement error and model discrepancy usually supposed independent: $z(\mathbf{x}_i) \perp\!\!\!\perp \epsilon(\mathbf{x}_i)$.
- Model discrepancy taken as a GP: $z|\boldsymbol{\psi}_z \sim GP(\mu(\cdot), c(\cdot,\cdot))$, where μ and c are the prior mean and covariance of the process. Cov of z depends on hyperparameters $\boldsymbol{\psi}_z$.
- $\boldsymbol{\psi}$ vector of hyperparameters of the entire error model, then $\boldsymbol{\psi} = (\boldsymbol{\psi}_z, \sigma_\epsilon)$, where σ_ϵ^2 is the mean-squared measurement error.
- $\boldsymbol{\theta}$ and $\boldsymbol{\psi}$ considered as joint unknows.
- Choice of prior distributions for model parameters and hyperparameters.

Full Bayesian calibration

- Rigorous derivation, flexible framework.
- Calibration can not be solved precisely in most applications. Posterior density might exhibit substantial variations and many local maxima in the joint space.
- For calibrations with multiple quantities and experimental configurations, number of HP might become significant, making estimation in high dimensions very complex.
- Some advanced sampling techniques (**Robert2010**) employed to generate samples from high dimensional posterior distributions and approximate the required integrals.

$\Rightarrow$ **Modular approaches** (**Liu2009**) alternatives to full Bayesian calibration. They reduce dimensionality of the sample space by estimating point values for some hyperparameters.

Modular Approaches

Modular approaches: separate into groups (modules) the treatment of parameters and HP during the calibration and obtain a problem of sequential estimations.

Advantages: breaking high-dimensional calibration problem into smaller ones; more accessible to sample; improvement of the identifiability of the HP belonging to different modules.

Last module estimates $\mathrm{p}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{obs}}, \boldsymbol{\psi} = \hat{\boldsymbol{\psi}})$ where the estimator $\hat{\boldsymbol{\psi}}$ of $\boldsymbol{\psi}$ have been estimated in previous modules such that $\mathrm{p}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{obs}}, \boldsymbol{\psi} = \hat{\boldsymbol{\psi}}) \approx \mathrm{p}_{\mathrm{Bayes}}(\boldsymbol{\theta})$.

In Kennedy and O'Hagan (KOH), Maximum A Posteriori (MAP) estimate:

$$\widehat{\boldsymbol{\psi}}_{\mathrm{KOH}} = \underset{\boldsymbol{\psi}\in\Psi}{\arg\max}\ \mathrm{p}(\boldsymbol{\psi}|\mathbf{y}_{\mathrm{obs}}) = \underset{\boldsymbol{\psi}\in\Psi}{\arg\max}\ \mathrm{p}(\boldsymbol{\psi}) \int_{\Theta} \mathrm{p}(\boldsymbol{\theta})\mathrm{p}(\mathbf{y}_{\mathrm{obs}}|\boldsymbol{\theta}, \boldsymbol{\psi})\, \mathrm{d}\boldsymbol{\theta}, \qquad (5)$$

and the following estimation for the parameters posterior distribution:

$$\mathrm{p}_{\mathrm{KOH}}(\boldsymbol{\theta}) \propto \mathrm{p}(\boldsymbol{\theta})\mathrm{p}(\mathbf{y}_{\mathrm{obs}}|\boldsymbol{\theta}, \widehat{\boldsymbol{\psi}}_{\mathrm{KOH}}). \qquad (6)$$

Kennedy and O'Hagan Calibration

KOH calibration equation:

$$\overbrace{y_{\text{obs}}(x)}^{\textbf{observations}} = \overbrace{f(x,\boldsymbol{\theta}^*)}^{\textbf{computer model}} + \overbrace{z(x)}^{\textbf{model discrepancy}} + \overbrace{\epsilon(x)}^{\textbf{measurement error}} , \qquad (7)$$

with $\boldsymbol{\theta}^*$ the "best-fitting" $\boldsymbol{\theta}$, *representing the data faithfully according to the error structure specified for the residuals*.

- Pointwise estimation of z, supposed independent of $\boldsymbol{\theta}$: identifiability issue (**Liu2009, Arendt2012**).
- A single distribution is used for z, inappropriate as different model parameters values could correspond to different shapes of z.

Bayesian framework for Calibration with model error

Full Bayesian
Higdon et al SIAM JSC 2004

Modular approaches
Liu et al, Bayesian Analysis 2009

Need for a modular technique that approximates the fully Bayesian Calibration while retaining the advantage of reduced sample space

↓

Full Maximum A Posteriori Method

Our proposal: Full Maximum a Posteriori calibration

We relax the assumption of independence between z and $\boldsymbol{\theta}$.

$$y_{\text{obs}}(x) = f(x, \boldsymbol{\theta}) + z_{\boldsymbol{\theta}}(x) + \epsilon(x), \tag{8}$$

with **Full Maximum a Posteriori** hyperparameters estimated as a function of $\boldsymbol{\theta}$:

$$\widehat{\boldsymbol{\psi}}_{\text{FMP}}(\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\psi}} \; p(\boldsymbol{\psi} | \mathbf{y}_{\text{obs}}, \boldsymbol{\theta}). \tag{9}$$

- Answer to the Identifiability issue: no more ”best value” of parameters.
- Parametric estimation of model error: more flexibility.
- Eq. (8) first proposed by (**plumlee2017**), who used an external definition of $\boldsymbol{\theta}^*$ as the best fit value.

Full Maximum a Posteriori (FMP) calibration

Posterior predictive density: predictions of the true quantity y at a non-observed point x^*. It reads:

$$\mathrm{p}(y(x^*)|\mathbf{y}_{\mathrm{obs}}) \approx\approx \int_{\Theta} \mathrm{p}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{obs}})\mathrm{p}(y(\mathbf{x}^*)|\boldsymbol{\theta}, \boldsymbol{\psi} = \hat{\boldsymbol{\psi}}_{\mathrm{FMP}}(\boldsymbol{\theta}), \mathbf{y}_{\mathrm{obs}})\, \mathrm{d}\boldsymbol{\theta} \tag{12}$$

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with mean:

$$\mathrm{E}\left[y(x^*)|\mathbf{y}_{\text{obs}}\right] = \underbrace{\mathrm{E}_{\boldsymbol{\theta}}[f(\mathbf{x}_*, \boldsymbol{\theta})]}_{\text{averaged model prediction at } \mathbf{x}_*} + \underbrace{\mathrm{E}_{\boldsymbol{\theta}}[\mathbf{k}_*^T(\boldsymbol{\Sigma} + \sigma_\epsilon^2 \mathbf{I}_n)^{-1}(\mathbf{y}_{\text{obs}} - \mathbf{f}_{\boldsymbol{\theta}})]}_{\text{averaged model discrepancy at } \mathbf{x}_*}, \tag{13}$$

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and variance :

$$\mathrm{Var}\left[y(\mathbf{x}_*)|\mathbf{y}_{\text{obs}}\right] = \underbrace{\mathrm{Var}_{\boldsymbol{\theta}}[f(\mathbf{x}_*, \boldsymbol{\theta}) + \mathbf{k}_*^T(\Sigma_{\hat{\psi}_{\text{FMP}}(\boldsymbol{\theta})} + \sigma_\epsilon^2 \mathbf{I}_n)^{-1}(\mathbf{y}_{\text{obs}} - \mathbf{f}_{\boldsymbol{\theta}})]}_{\text{uncertainty in the corrected model}} \quad (14)$$

$$+ \underbrace{\mathrm{E}_{\boldsymbol{\theta}}[c_{\hat{\psi}_{\text{FMP}}(\boldsymbol{\theta})}(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}_*^T(\Sigma_{\hat{\psi}_{\text{FMP}}(\boldsymbol{\theta})} + \sigma_\epsilon^2 \mathbf{I}_n)^{-1}\mathbf{k}_*]}_{\text{residual uncertainty}} \quad (15)$$

Equations used to make predictions with the model after calibration.

Comparison between FMP and KOH

When the posterior distribution $p(\boldsymbol{\theta}, \psi|\mathbf{y}_{\text{obs}})$ is a **mixture of Gaussians with well-separated modes**, FMP calibration outperforms KOH calibration :

- KOH calibration underestimates posterior variance of $\boldsymbol{\theta}$ (**false certainty effect**),
- FMP can account for multiple parameter values that correspond to different shapes of model error.

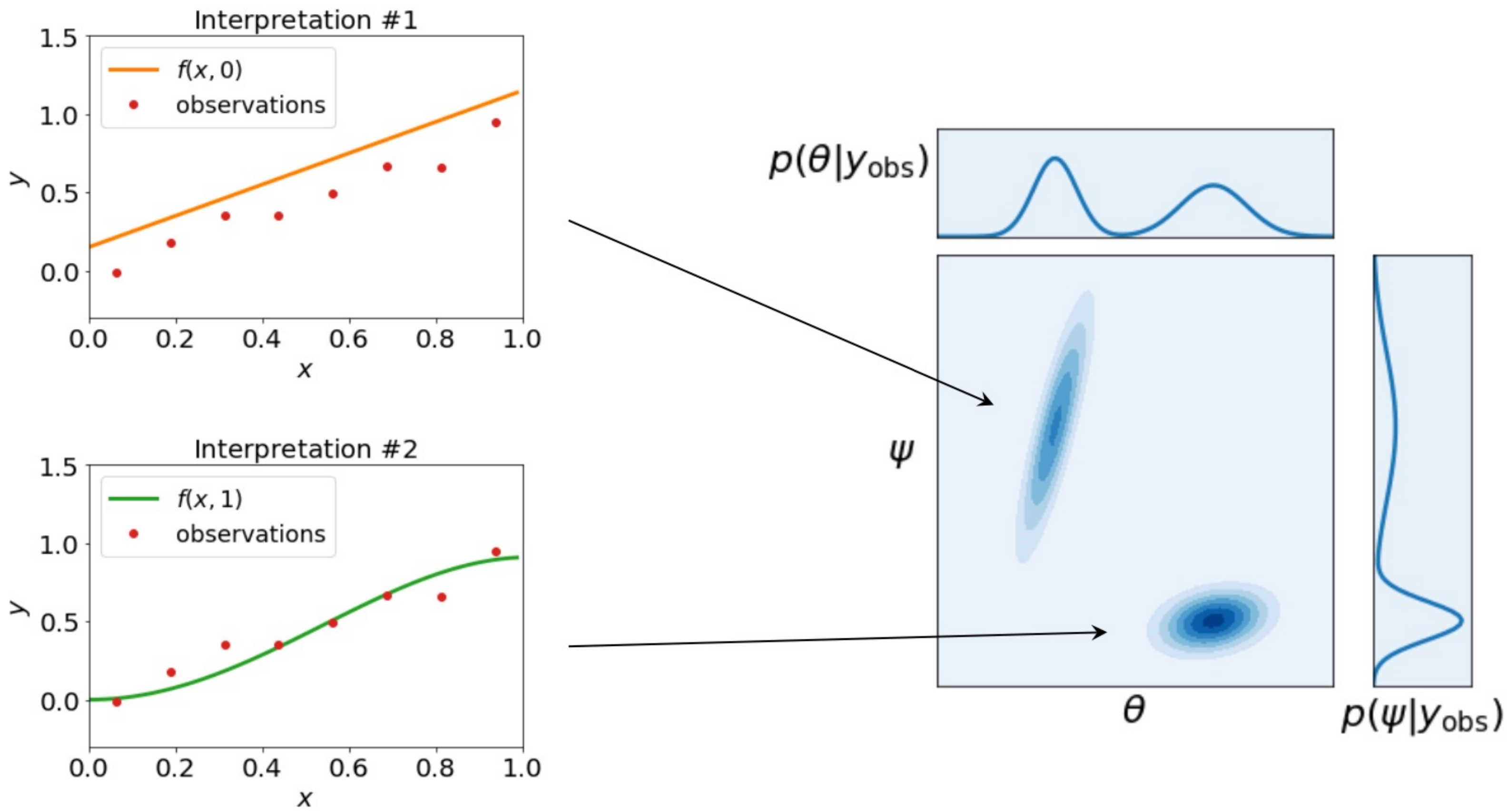
Let us illustrate multimodality on a simple numerical example.

Illustrative Example

"Truth" y, Computer model f, $(x, \theta) \in [0,1] \times [-0.5, 1.5]$.

$$y(x) = x, \tag{16}$$

$$f(x,\theta) = \underbrace{(x + 0.15)(1-\theta)}_{\textbf{affine term, null when } \theta = 1} + \underbrace{x\sin(2\theta x)}_{\textbf{oscillating term, null when } \theta = 0}. \tag{17}$$



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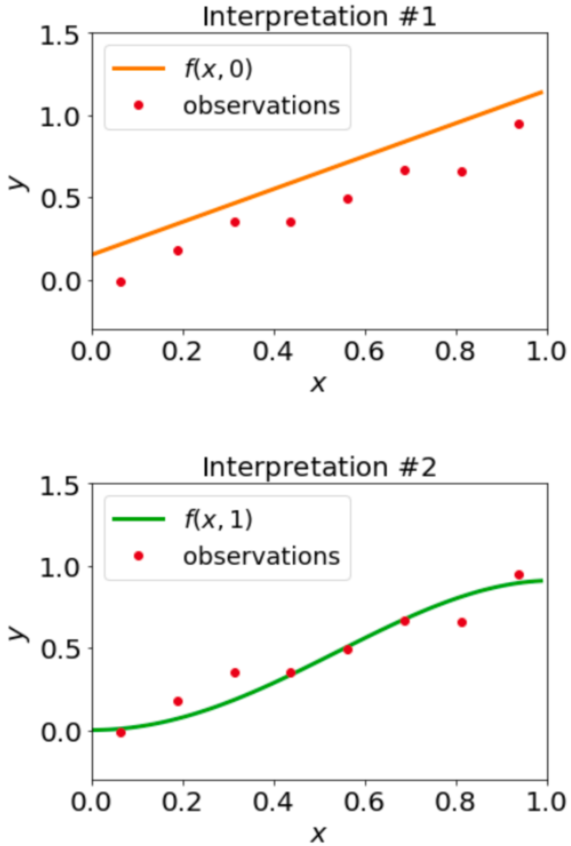

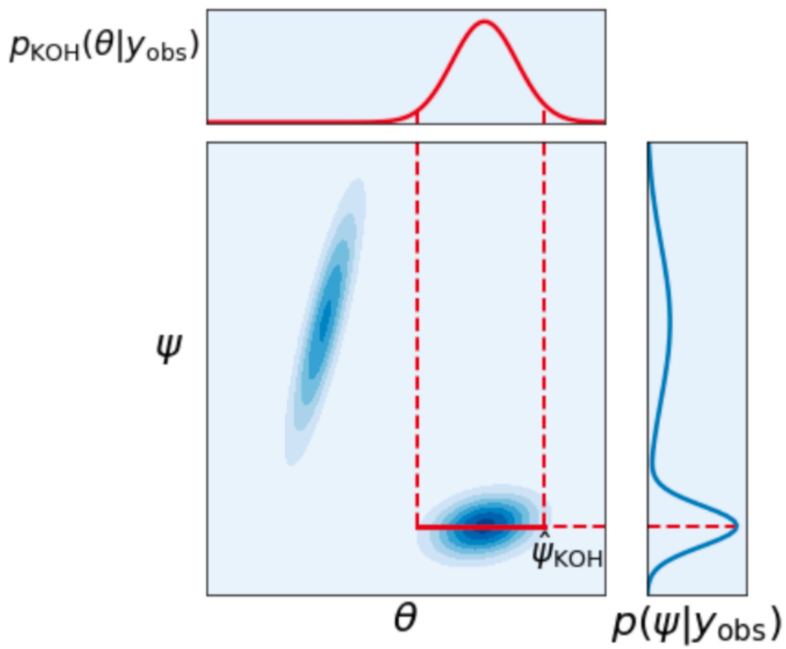

- KOH calibration misses half of the probability mass, and underestimates variance (*false certainty*).

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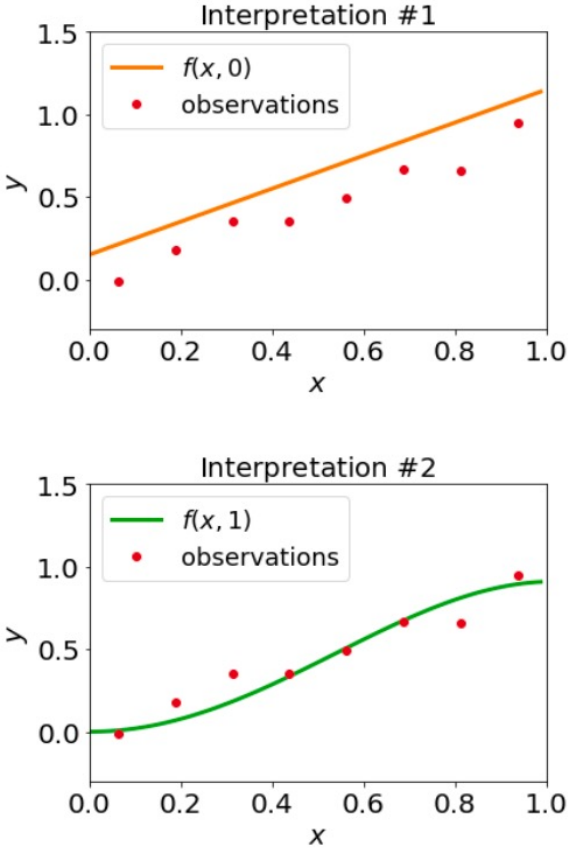

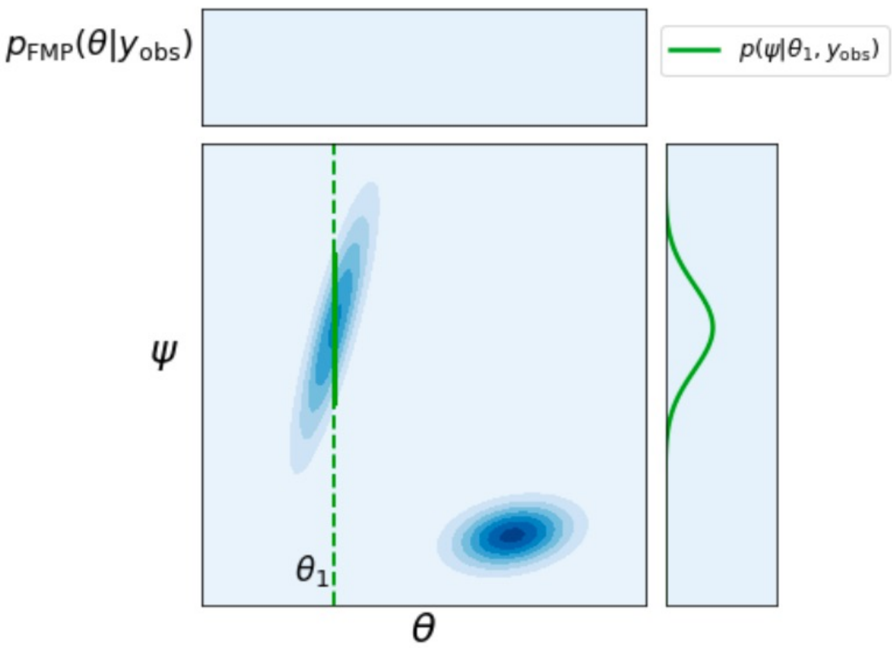

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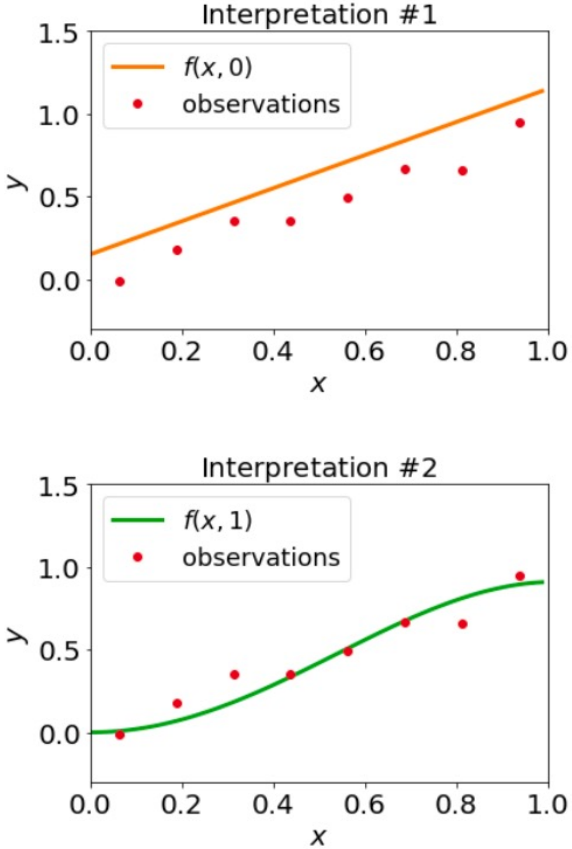

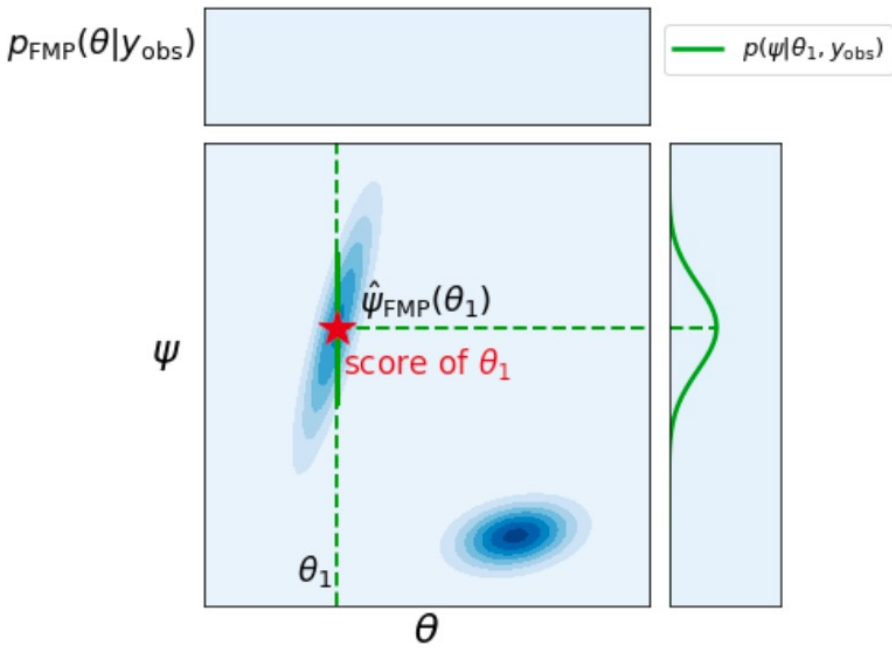

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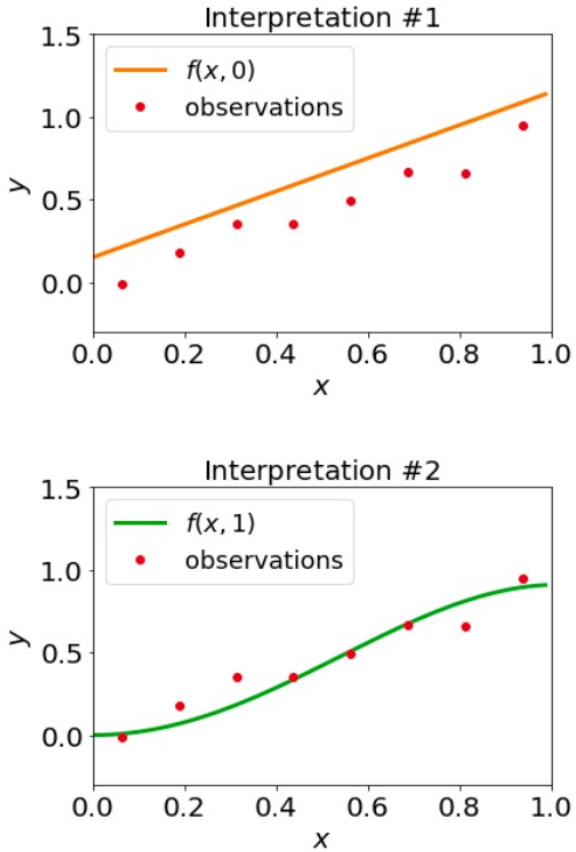

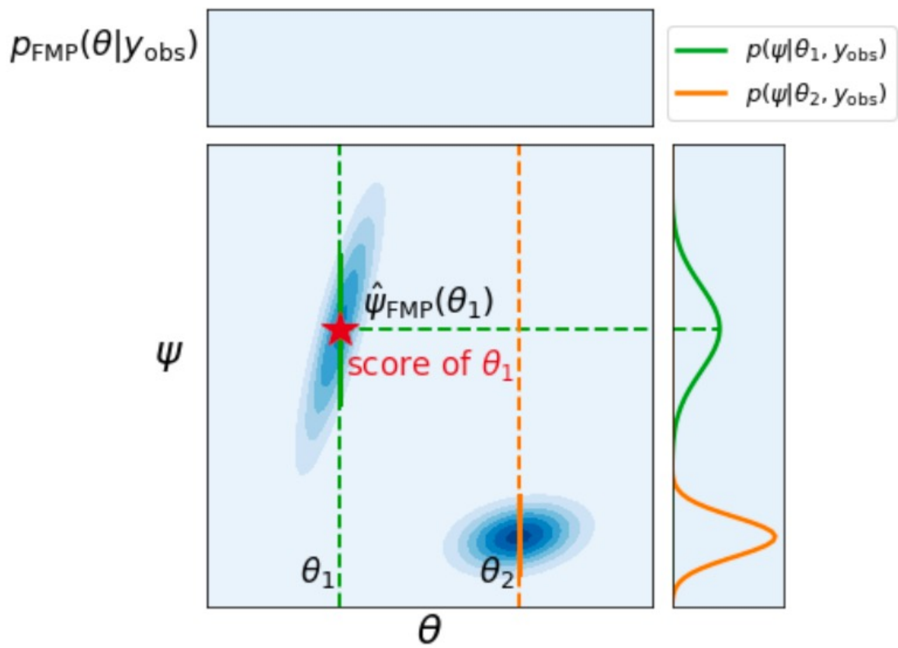

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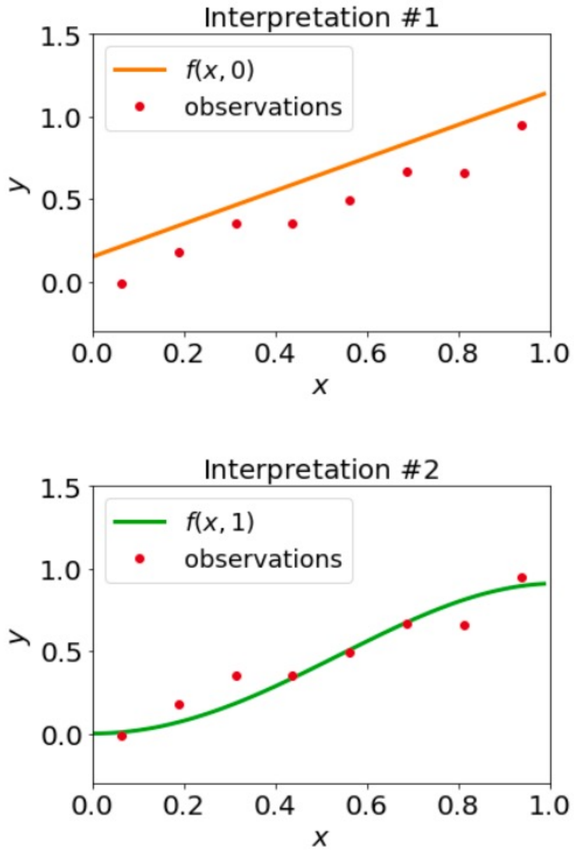
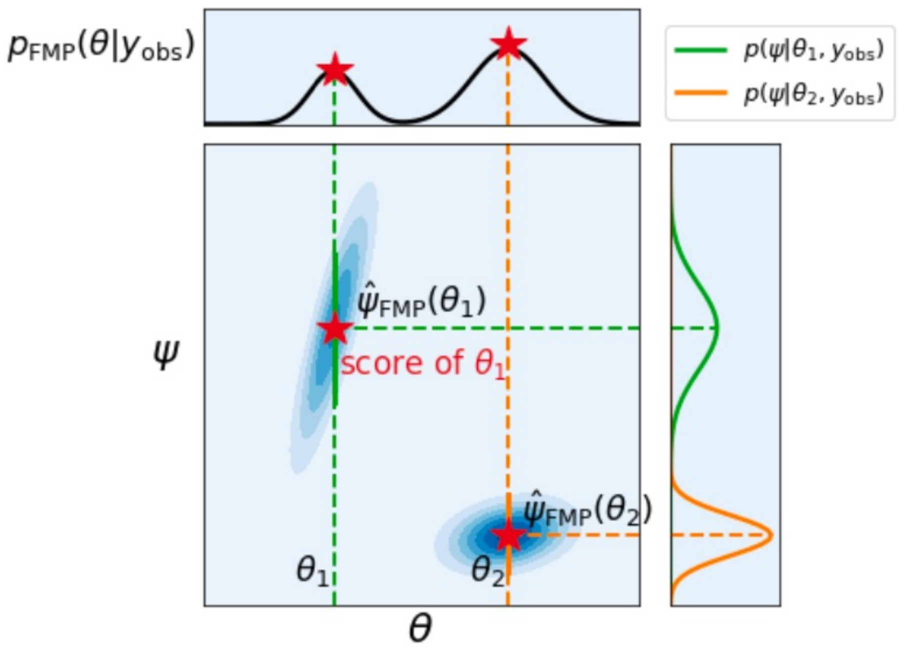
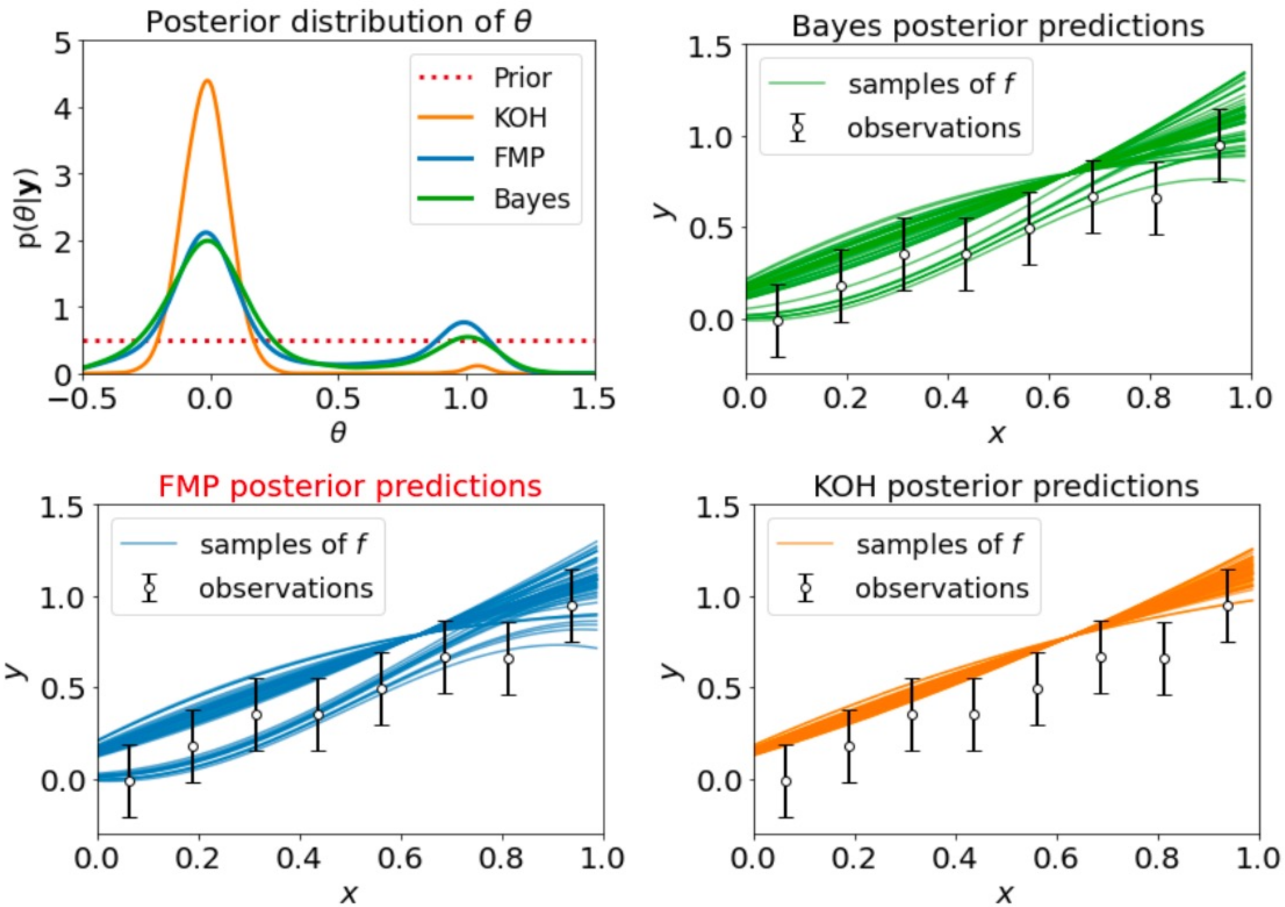




- KOH calibration misses half of the probability mass, and underestimates variance (*false certainty*).
- FMP calibration accounts for both interpretations, but might misestimate their relative importance → **proposal of additional resampling step**.

Illustrative Example

Setup: squared exponential kernel for z_θ, uniform priors, $\sigma_\epsilon = 0.1$ learnt.



- Accounting for all explanations of the data allows for more conservativity on the parameter and model predictions.

Surrogate-based speedup of FMP calibration

Take uniform priors for simplicity, note $\Gamma_{\psi} = \mathbf{C}_{\psi} + \sigma_{\epsilon}^2 \mathbf{I}_n$.

$$L(\boldsymbol{\theta}, \boldsymbol{\psi}) = -\log\det(\Gamma_{\psi}) - (\mathbf{y}_{\text{obs}} - \mathbf{f}_{\boldsymbol{\theta}})^T (\Gamma_{\psi})^{-1} (\mathbf{y}_{\text{obs}} - \mathbf{f}_{\boldsymbol{\theta}}). \tag{16}$$

For each MCMC step

Optimisation		**Substitution**
Find: $\widehat{\boldsymbol{\psi}}_{\text{FMP}}(\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\psi}} L(\boldsymbol{\theta}, \boldsymbol{\psi})$	$\longrightarrow$	Calculate: $L(\boldsymbol{\theta}, \widehat{\boldsymbol{\psi}}_{\text{FMP}}(\boldsymbol{\theta}))$
(multiple evaluations of L)		(single evaluation of L)

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(single evaluation of L)

3 sources of numerical cost:

- $\mathbf{f}_{\boldsymbol{\theta}}$ is an evaluation of the computer model.
- Inversion of Γ_ψ, increases with the number of observations: $\mathcal{O}(n^3)$.
- Multiple evaluations for optimisation (problem-dependent).

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Two strategies + Algorithm for Adaptive Sampling:

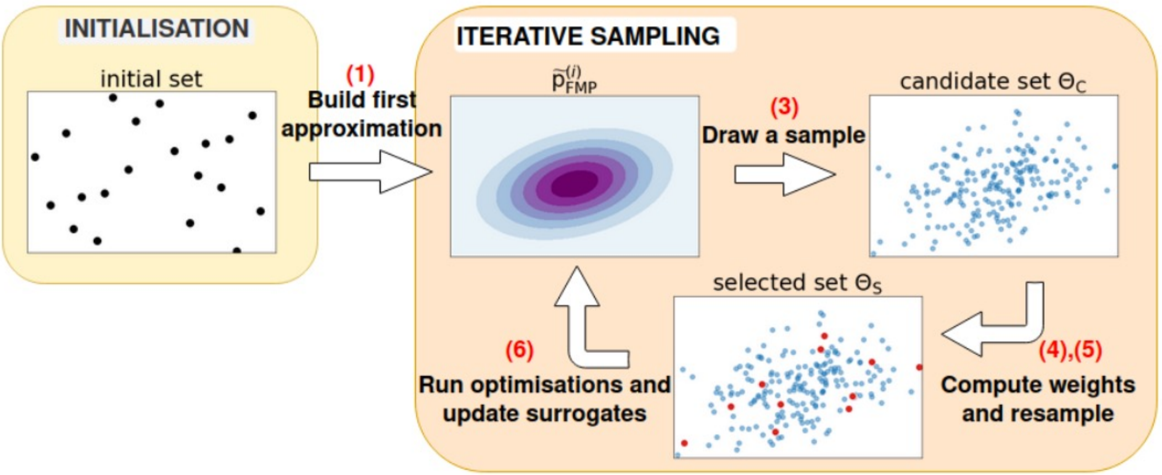
- (LL) Build a surrogate $\widetilde{L}(\boldsymbol{\theta})$ of the function $L(\widehat{\psi}_{\text{FMP}}(\boldsymbol{\theta}), \boldsymbol{\theta})$ (Optimization becomes unnecessary. Need to evaluate once $\widetilde{L}(\boldsymbol{\theta})$).
- (HP) Build surrogates of $\widehat{\psi}_{\text{FMP}}$, noted $\widetilde{\psi}$ (Evaluating $\widetilde{\psi}(\boldsymbol{\theta})$ once, $L(\boldsymbol{\theta}, \widetilde{\psi}(\boldsymbol{\theta}))$ must be computed, requiring to invert once covariance matrix of observations).

Algorithm for adaptive sampling

1: Initialisation: Build initial surrogates on a space-filling design.
2: **while** budget not exceeded **do**
3: Draw the *candidate set* Θ_C from $p^{(i)}_{FMP}$ with MCMC.
4: Compute a weight for each point of Θ_C

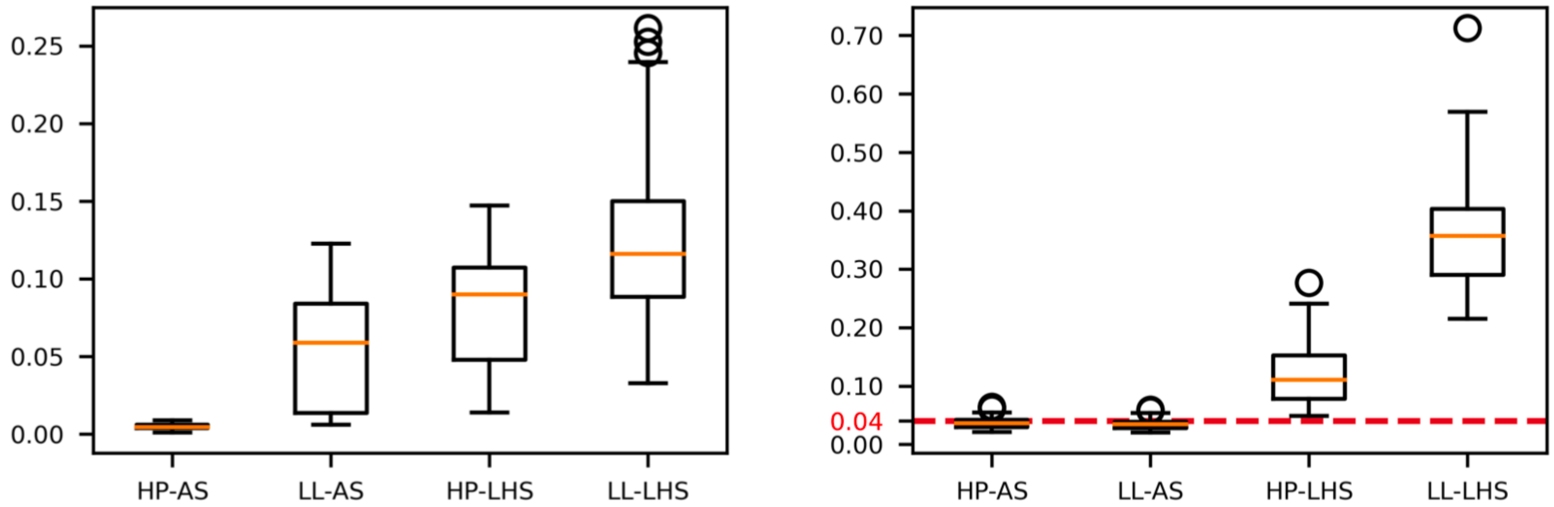
$$\omega^{(i)}(\boldsymbol{\theta}) = \begin{cases} \mathrm{Var}\,[\widetilde{L}^{(i)}(\boldsymbol{\theta})] & \text{for LL-AS,} \\ \mathrm{Var}\,[L(\widetilde{\boldsymbol{\psi}}^{(i)}(\boldsymbol{\theta}), \boldsymbol{\theta})] & \text{for HP-AS.} \end{cases} \qquad (17)$$

5: Resample from Θ_C, with weights ω, to obtain the *selected set* Θ_S.
6: Compute the training data on Θ_S, add the data to the training set, and update the surrogates.
7: **end while**



Algorithm for adaptive sampling

G-function: 6D input $\mathbf{x} \in [0,1]^6$ and 6D parameter $\boldsymbol{\theta} \in [0,1]^6$



(a) Error on MAP value

(b) Relative error on covariance matrix

Figure: 30 repetitions of each strategy at $n_{\max} = 800$. Orange lines represent the median error, red dashed line is the level of uncertainty on the covariance due to MCMC sampling.

- AS strategies outperform LHS, strategies based on HP surrogates also outperform those based on log-LL surrogates.
- Relative error: $||\mathbf{C}_{\text{post}} - \mathbf{C}_{\text{post,FMP}}||_F / ||\mathbf{C}_{\text{post,FMP}}||_F$, with $\mathbf{C}_{\text{post,FMP}}$ matrix obtained from FMP calibration, and $||\cdot||_F$ Frobenius norm.
- Maximum precision level attainable for the given length of MCMC reached for both AS strategies.

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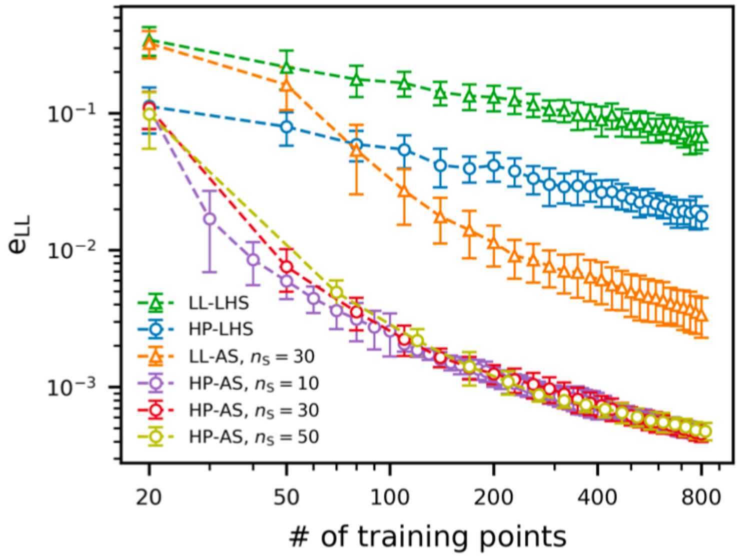


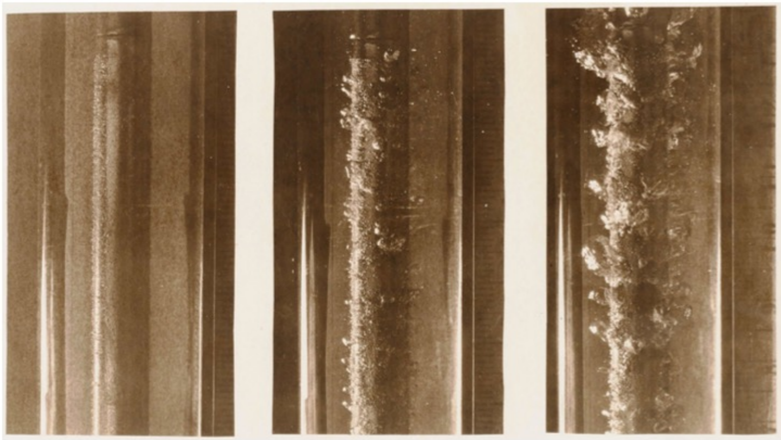
$$e_{LL}^2 = \begin{cases} \dfrac{\sum_{\boldsymbol{\theta}\in\Theta_r}(\widetilde{L}(\boldsymbol{\theta}) - L(\widehat{\boldsymbol{\psi}}_{\mathrm{FMP}}(\boldsymbol{\theta}),\boldsymbol{\theta}))^2}{\sum_{\boldsymbol{\theta}\in\Theta_r}(L(\widehat{\boldsymbol{\psi}}_{\mathrm{FMP}}(\boldsymbol{\theta}),\boldsymbol{\theta}))^2} & \text{for LL-AS and LL-LHS,} \\ \dfrac{\sum_{\boldsymbol{\theta}\in\Theta_r}(L(\widetilde{\boldsymbol{\psi}}(\boldsymbol{\theta}),\boldsymbol{\theta}) - L(\widehat{\boldsymbol{\psi}}_{\mathrm{FMP}}(\boldsymbol{\theta}),\boldsymbol{\theta}))^2}{\sum_{\boldsymbol{\theta}\in\Theta_r}(L(\widehat{\boldsymbol{\psi}}_{\mathrm{FMP}}(\boldsymbol{\theta}),\boldsymbol{\theta}))^2} & \text{for HP-AS and HP-LHS.} \end{cases} \quad (18)$$

- AS strategies outperform LHS strategies, and HP strategies outperform LL strategies in terms of precision.
- With low number of training points, adding fewer points to training set is more precise. As surrogates become more accurate, precision is mainly driven by total number of training points.

Calibration of a Boiling model

MIT Boiling model (**kommajosyula2020**): Prediction of heat flux from solid wall to liquid in various boiling regimes.
Inputs: pressure, velocity, temperatures, geometry, and wall superheat ΔT_{sup}.

Kennel experiments (**kennel1949**): Boiling of liquids in a thin glass tube with a central heating element in the shape of a cylinder.



(a) Kennel experiments, in three boiling regimes. Source: **kennel1949**.

Total: 13 experiments with various pressures, flow rates, input temperatures and heater sizes. Measurements of wall temperature are obtained, as a function of the heating power.

Calibration of a Boiling model

Calibration parameters:

- **The static contact angle** between the liquid and the wall θ_c.
- An empirical model for the **bubble departure diameter** D_d:

$$D_\mathrm{d} = 18.9 \times 10^{-6} \times \left(\frac{\rho_\mathrm{f} - \rho_\mathrm{g}}{\rho_\mathrm{g}} \right)^{0.27} \times (Ja_\mathrm{sup})^{0.75} \times (1 + Ja_\mathrm{sub})^{-0.3} \times v^{-0.26}. \quad (19)$$

with Ja_sup the Jakob number, v the liquid velocity.

Calibration of a Boiling model

Calibration parameters:

- **The static contact angle** between the liquid and the wall θ_1.
- An empirical model for the **bubble departure diameter** D_d:

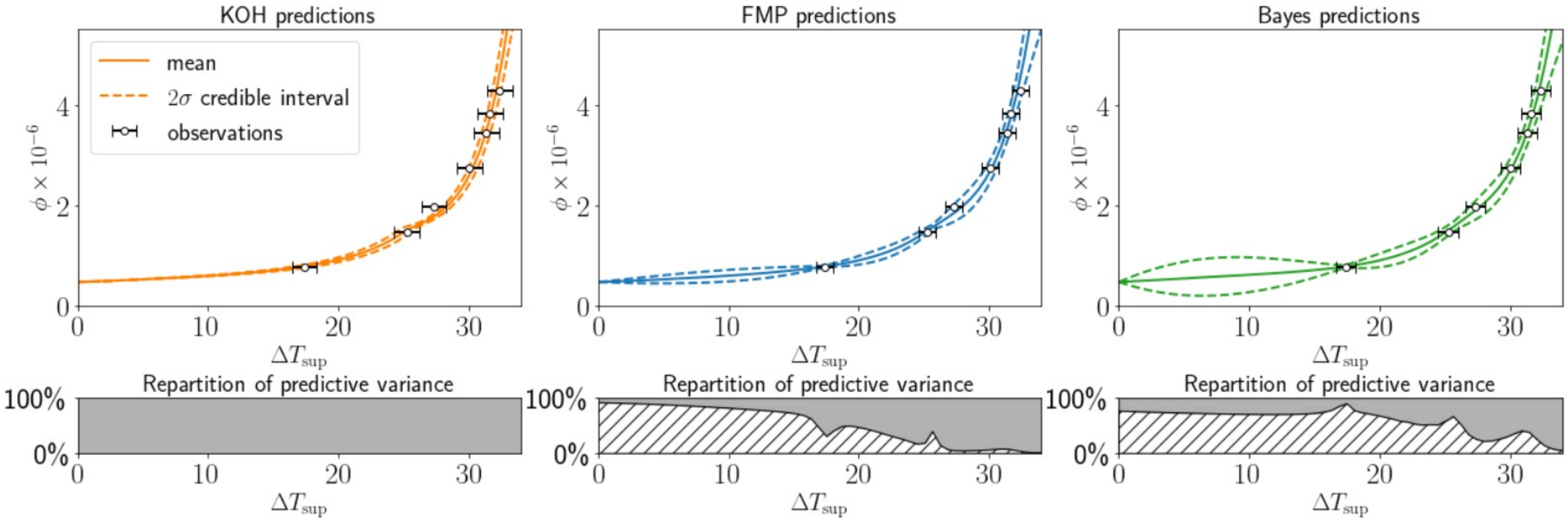
$$D_\mathrm{d} = \theta_2 \times \left(\frac{\rho_\mathrm{f} - \rho_\mathrm{g}}{\rho_\mathrm{g}}\right)^{0.27} \times (Ja_\mathrm{sup})^{\theta_3} \times (1 + Ja_\mathrm{sub})^{-0.3} \times v^{-0.26}. \tag{19}$$

with Ja_sup the Jakob number, v the liquid velocity.

Prior distributions of parameters are derived from their initial values:

	θ_1	θ_2	θ_3
Prior	$\mathcal{N}_t(40, (12)^2)$	$\mathcal{N}_t(18.9 \times 10^{-6}, (5.7 \times 10^{-6})^2)$	$\mathcal{N}_t(.75, (.225)^2)$
Support	$[0, 90]$	$]0, \infty]$	$[0, \infty]$

Calibration of a Boiling model



- KOH: zero model error σ, all the discrepancies to measurement uncertainty. Unsatisfactory, especially at low values of ΔT_{sup}.
- Credible intervals of corrected prediction in FMP and Bayes larger than for KOH, especially at low values of ΔT_{sup} (where no obs available).
- Predictive variance split into the model and residual contributions.
- All approaches agree on the dominance of the model predictions variance for the high range of ΔT_{sup} values.

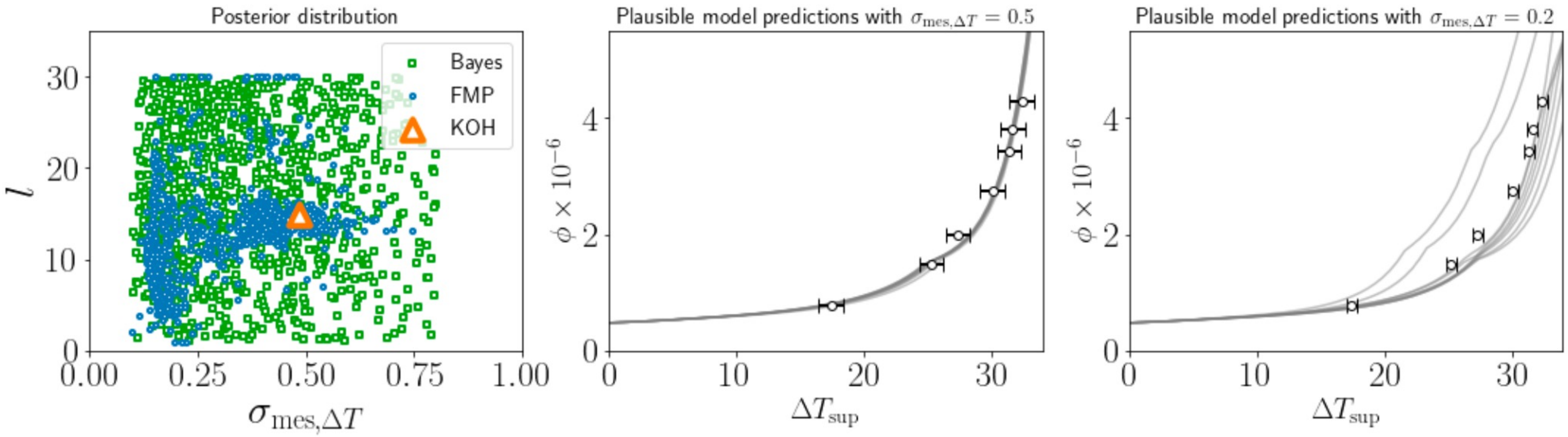
Calibration of a Boiling model

Posterior samples in $\sigma_{\text{mes},\Delta T}$ and l plane: Bayes samples cover full support of the prior; FMP samples fall primarily in two distinct interpretations of observations): high measurement error with zero model error or a combination of both. KOH estimator falls into the former.

FMP model predictions corresponding to two regions:

- With measurement error only, plausible model predictions pass through all observations, tight dispersions.
- With non-zero model error, some model predictions come close to most observations, but others are further away, following observations' trend.

FMP and Bayes methods achieve the goal of considering alternative interpretations of the observations.



Conclusions and perspectives

- New estimator of model error, Full Maximum a Posteriori (FMP), within calibration.
- Surrogate-based strategies to accelerate FMP estimation.
- In the MITB model, FMP provides results similar to Full Bayes calibration, with cost divided by 20.
- Application of the proposed methodology to problems featuring the use of complex CFD (Neptune-CFD)

Conclusions and perspectives

Perspectives:

- Include numerical error and/or surrogate error of the computer code in the calibration framework.
- Leverage the estimated model error to characterize the predictive capability of models.
- Enrich Bayesian Model Selection / Bayesian Model Averaging procedures with the inferred model error.
- Relax the hypothesis of independence between model discrepancy HP and model parameters.

References

Journal articles

- N. Leoni, P.M. Congedo, O. Le Maître and M.G. Rodio (2023). ”Bayesian Calibration with Adaptive Model Discrepancy”. Accepted for publication in International Journal for Uncertainty Quantification.
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