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Bayesian Calibration of Computer Models with Modern Gaussian Process Emulators

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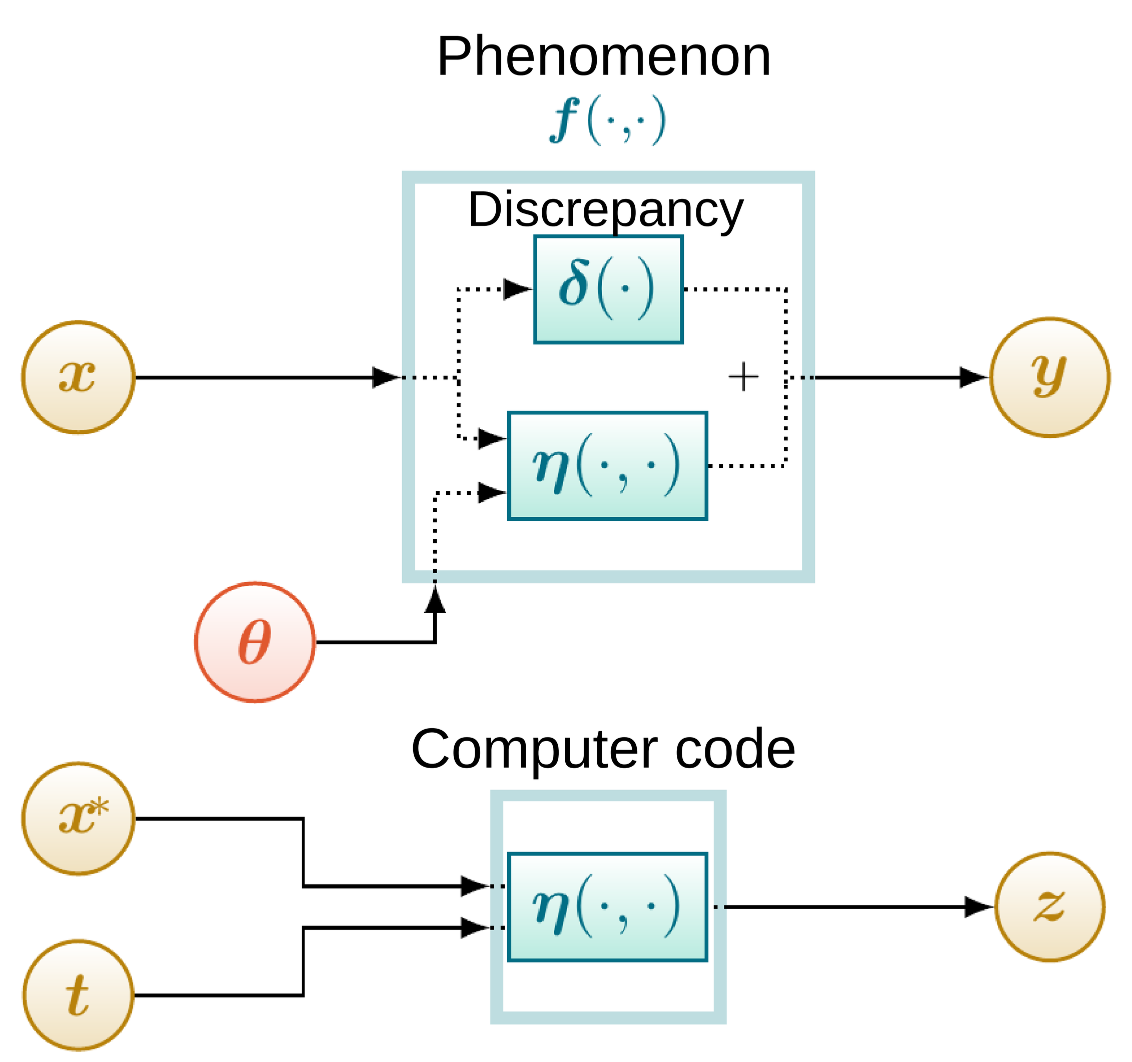
1. Context

- Uncertainty analysis of a phenomenon $\boldsymbol{f}$
- Approximation by an expensive code $\boldsymbol{\eta}$
- Infer non-observable parameters $\boldsymbol{\theta}$
- Data: - real observations Y : $p(\boldsymbol{y}_i \,|\boldsymbol{f}\,(\boldsymbol{x}_i))$
  - computer runs Z : $p(\boldsymbol{z}_j \,|\boldsymbol{\eta}(\boldsymbol{x}_j,\ \boldsymbol{t}_j))$

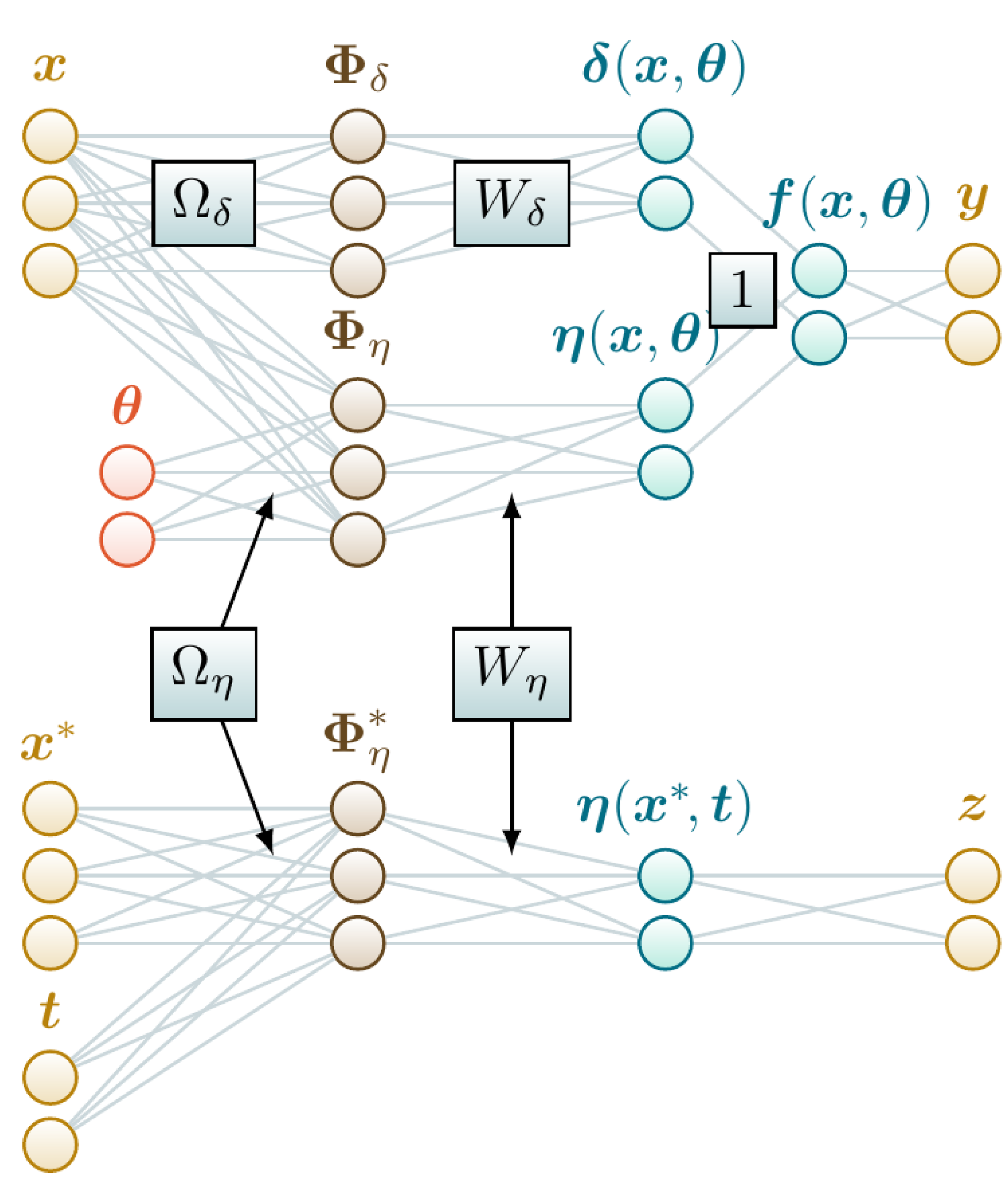
2. Framework



3. Random features approximation

$$\boldsymbol{\eta}(\boldsymbol{x},\boldsymbol{\theta}) = \Phi_{\eta}(\Omega_{\eta}^{(1)}\boldsymbol{x} + \Omega_{\eta}^{(2)}\boldsymbol{\theta})^{\top} W_{\eta}$$

where Φ_{η} is an element-wise activation function and W and Ω's are random matrices.



4. Variational inference

A tractable lower bound of the log-likelihood can be derived:

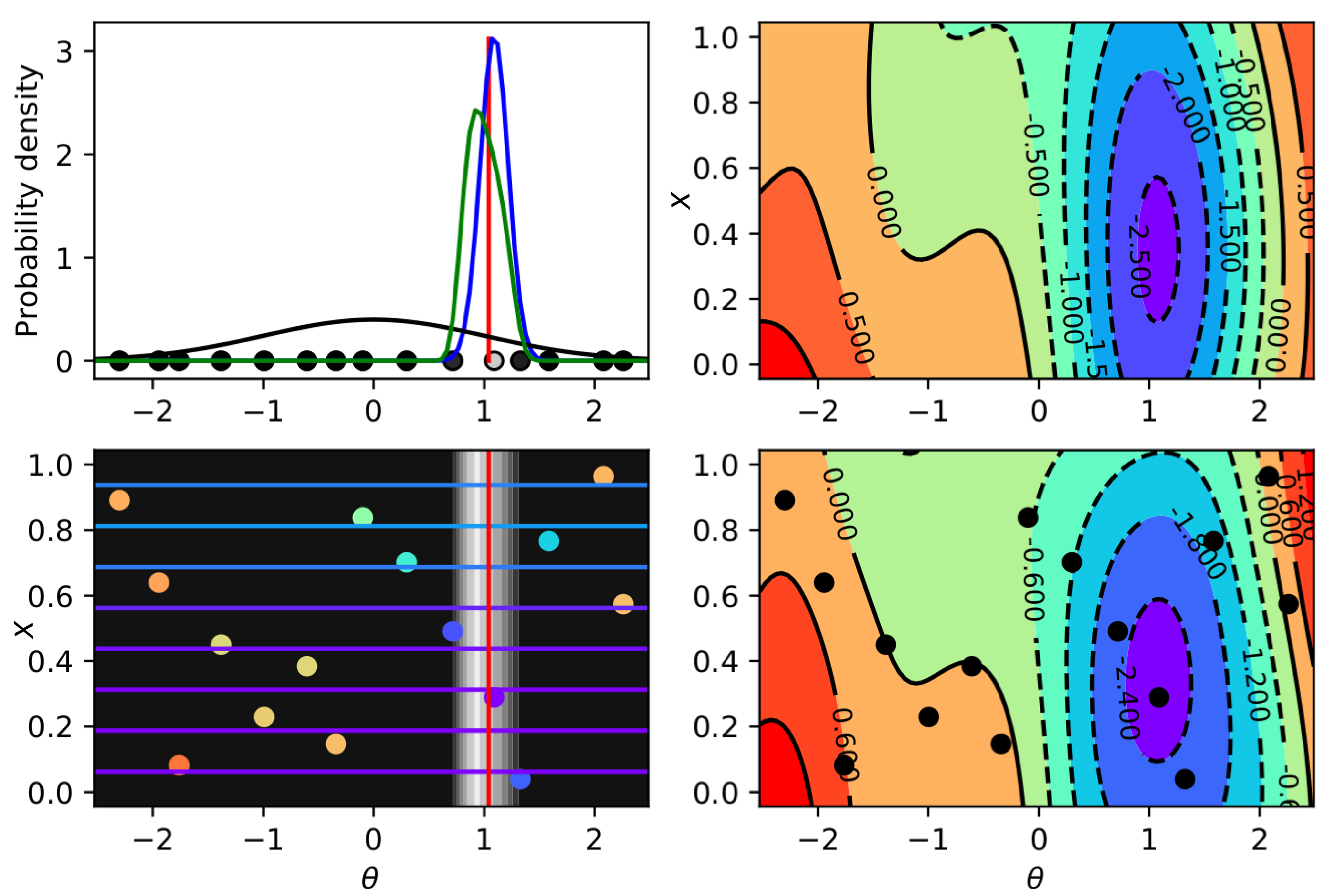
$$\mathcal{L} \geq \mathcal{E} - \mathrm{KL},$$

- $\mathcal{E} = \mathbb{E}_{q(W,\boldsymbol{\theta})}(\ln(p(Y,Z|X,X^*,T,\psi,\Omega,W_{\eta},W_{\delta},\boldsymbol{\theta})))$
- $\mathrm{KL} = \mathrm{D}_{\mathrm{KL}}(q(W_{\eta},W_{\delta},\boldsymbol{\theta})||p(W_{\eta})p(W_{\delta})p(\boldsymbol{\theta}))$
- $q(W,\boldsymbol{\theta})$ approximate the posterior $p(W_{\eta},W_{\delta},\boldsymbol{\theta}|\,Y,Z,X,X^*,T,\Omega,\psi)$
- ψ GP hyperparameters of η and δ

5. Numerical experiments

1. Simulated test case

- One variable inputs
- One calibration input
- 15 computer runs
- 8 observations
- Data is sampled form the prior distribution



2. Test case in life science

- One variable inputs
- 3 calibration input
- 200 computer runs
- 19 observations
- Data from measures of current through ion channels of cells

x 10^3	L^2	Projected	Variational	KOH	Robust
CPU time, s	0.02	3.79	0.32	3.25	0.36
L^2 residuals	1.31	-	-	-	-
MSE	-	3.19	2.05	5.21	2.06

6. Conclusion

- Low-rank GP approximation
- Stochastic variational inference

→ Infer GPs and calibration input with sound quantification of uncertainty

→ Experiment shows a flexible framework for calibration.

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