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Misspecification uncertainty in deterministic surrogate models

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Surrogate models approximate the action of expensive scientific calculations, saving time, energy and cost. Surrogate model parameters are typically determined by minimising the negative log likelihood, or empirical loss. However, as the loss ignores model misspecification, Bayesian parameter uncertainties are largely epistemic and thus severe underestimates, vanishing in the large-data (over-parametrised) limit. A "true" Bayesian regression scheme should minimise the generalisation error, for which the expected loss is a Gibbs-Bogoliubov-Jensen upper bound. Whilst typically intractable, for the special case of deterministic calculations (no aleatoric uncertainty), we derive a condition any minimiser of the generalisation error must obey and design a simple ansatz which can be variational minimised[1]. The final result gives provably superior generalisation ability over Bayesian regression, and is extremely efficient in both training and evaluation for high dimensional linear models, giving accurate prediction and very useful bounding of test errors. Importantly, model prediction errors are directly related to model parameter uncertainties, essential to capture the correlations present when propagating uncertainty through multi-scale simulations[2].

[1] https://arxiv.org/abs/2402.01810v3 (with Danny Perez, LANL)
[2] https://arxiv.org/abs/2407.02414 (with Ivan Maliyov and Petr Grigorev, CINaM/CNRS)

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