Posterior and Computational Uncertainty in Gaussian Processes

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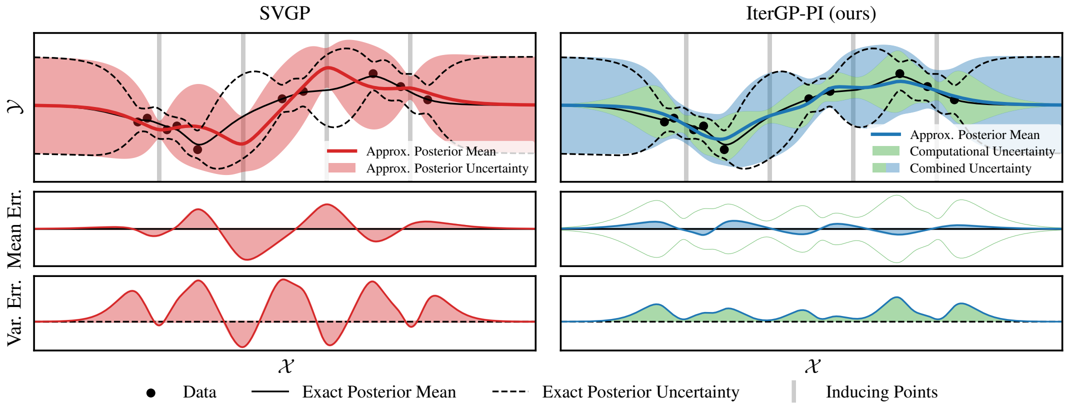
Computation-Aware Gaussian Process Inference

Limited data induces uncertainty. So does limited computation!

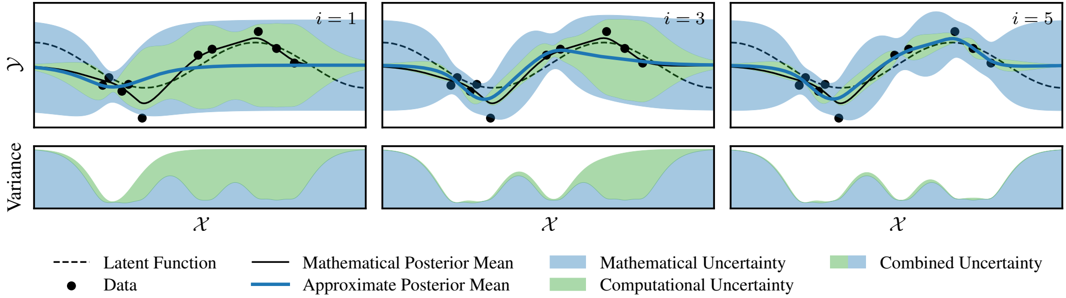


Goal: Gaussian process approximation with trustworthy uncertainty quantification.

Idea: Quantify approximation error probabilistically and propagate to posterior.

Theoretical Analysis

The combined uncertainty is a tight worst case bound on the relative error to the latent function.



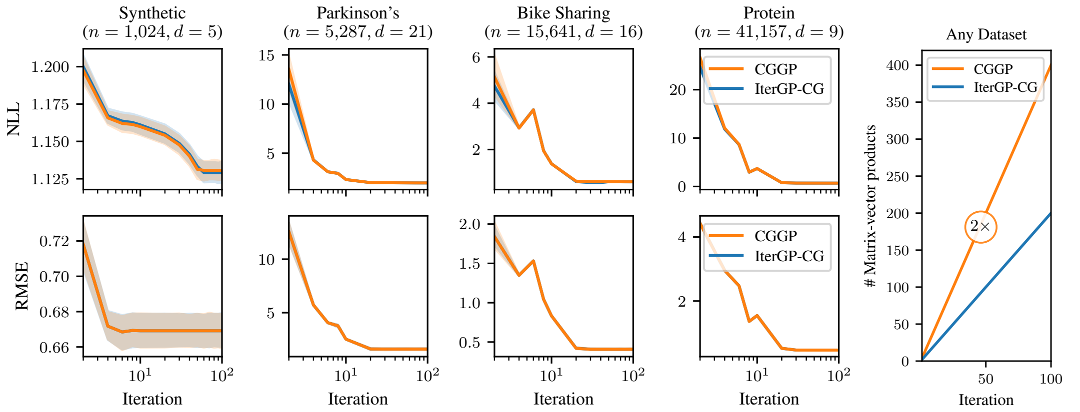
Gaussian process: $\frac{\text{Latent Function} - \text{Math. Posterior Mean}}{\|\text{Latent Function}\|} \leq$ Posterior Pred. Std. Deviation ●

IterGP (ours): $\frac{\text{Latent Function} - \text{Approx. Posterior Mean}}{\|\text{Latent Function}\|} \leq$ Combined Std. Deviation ● + ●

Exact uncertainty quantification in quadratic time!

Experiments

IterGP reduces the necessary computations for CG-based GP inference.



(a) Generalization on synthetic and UCI benchmark datasets.

(b) Comp. Cost

Figure: Generalization of CGGP and its closest IterGP analog.

Experiments

Quantifying computational uncertainty improves generalization of inducing point methods.

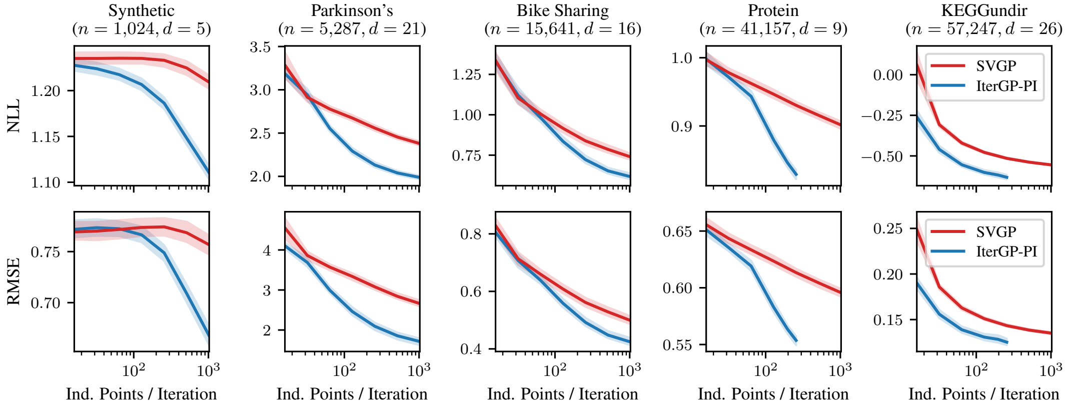


Figure: Generalization of SVGP and its closest IterGP analog.

Summary

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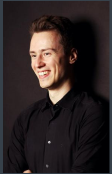
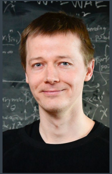
- IterGP: new class of GP approximations which implicitly quantify computational uncertainty.
- IterGP instances extend classic methods (Cholesky, CG, Nyström, . . .).
- Strong theoretical guarantees.
- Modeling computational uncertainty either saves computation or improves generalization.

Paper arXiv `https://arxiv.org/abs/2107.00243`

Implementation `https://github.com/JonathanWenger/itergp`




References I