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Recommendations for Baselines and Benchmarking Approximate Gaussian Processes

approximations.

Contributions

- **Concrete recommendations** for how approximate GP methods should be assessed
- A recommended training procedure for the SGPR method of Titsias (2009)
- We characterise and illustrate **two approximation regimes** for SGPR
- An experimental procedure for comparing approximate GP methods

Recommendations

- → Approximation quality. Assess the quality of the approximation to the exact GP, for both hyperparameter selections and posterior quality.
- → Recommended procedure. For a new method, a recommended training procedure should be given, and assessed for 1) various compute budgets, 2) how much compute is needed for desired performance
- → Dataset suitability. Compare to mean prediction and linear model to avoid trivial solutions and that the dataset is not too simple
- → Near-exact regime. Compare the compute required to achieve near-exactness
- → Non-exact regime. Compare how many datasets methods can achieve near-exactness on
- → Timed performance. Run each method for an extended amount of time, comparing at multiple time points

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Sebastian W. Ober, David R. Burt, Artem Artemev, Mark van der Wilk Motivation: approximate GP methods are often compared in a wide range of settings, making it difficult to determine what works best. Our goal: provide a training procedure that ensures that sparse GPs are a strong baseline and an experimental procedure for comparing Gaussian process

Near-Exact vs. Non-Sparse Regimes for SGPR egression example (N=200, M=15) Tightness of bounds → In the **near-exact regime**, — lower bound 0.70 inducing points upper bound an approximation can get full GP - - marg. lik. ____ close to the exact GP: 2 0.55 0.50 • Compare the compute required Number of inducina points • For SGPR, few inducing points are needed Regression example (N=200, M=100) Tightness of bounds → For non-sparse datasets: • ~N inducing points are data needed for exact Inducing points lower bound -- marg, lik performance Regression input :

- One cause is *model* misspecification

Timed Performance Evaluation

Training procedure:

- \rightarrow Iterate:
 - Choose inducing points using procedure from Foster et al. (2009)/Burt et al. (2020)
 - Learn hyperparameters with *fixed* inducing points

Results:

- \rightarrow For elevators, both methods perform near-exactly, with SGPR being faster
- \rightarrow kin40k is non-sparse, so that the Iterative GP performs better

Bounds (nats) 0.50 + tors 14939 $0.45 \cdot$ 0.40-5000Nel 0.351000Time (s) Time (s)Bounds (nats) NLPD (nats) 25000----- $\begin{array}{l} kin40k\\ N=36000 \end{array}$ -250005001000500Time (s) Time (s)





