Bayesian Optimization using Deep Gaussian Processes

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Objectives

My thesis focuses on the use Deep Gaussian Processes for Bayesian Optimization with Expected Improvement, where the main objectives are:

- Assess the quality of Expectation Propagation as inference for regression of DGP samples.
- Test performance of AEP-EI DGPs on benchmark Bayesian Optimization problems.

Bayesian Optimization

Interested in finding minima of black-box functions where evaluation is expensive, noisy and gradient information is not available. Two components:

- **Regression** of objective function using standard *Gaussian Processes* (GPs) to yield predictive distribution $P(y|\mathbf{x}, \mathcal{D}_n) = \mathcal{N}(y|\mu(\mathbf{x}), \sigma^2(\mathbf{x}))$.
- **Data collection strategy** by maximizing *Expected Improvement* (EI) acquisition function $\alpha_{EI}(\mathbf{x}) = \mathbf{E}_{P(y|\mathbf{x},\mathcal{D}_n)}(\max(0, \mu_{min} - y))$.

Although robust and analytically tractable, the expressiveness of standard GPs is limited by the choice of kernel $\mathcal{K}(\cdot, \cdot)$ (e.g.: SE, Matern).

Limitations of GP Regression

In Bayesian Optimization problems often length-scales vary as a function of space requiring:

- Covariance function design, which only guarantees local smoothing with a fixed length-scale.
- Sophisticated kernel design in higher dimensions.
- Input and output warping [1].
- Leverage multiple correlated outputs.

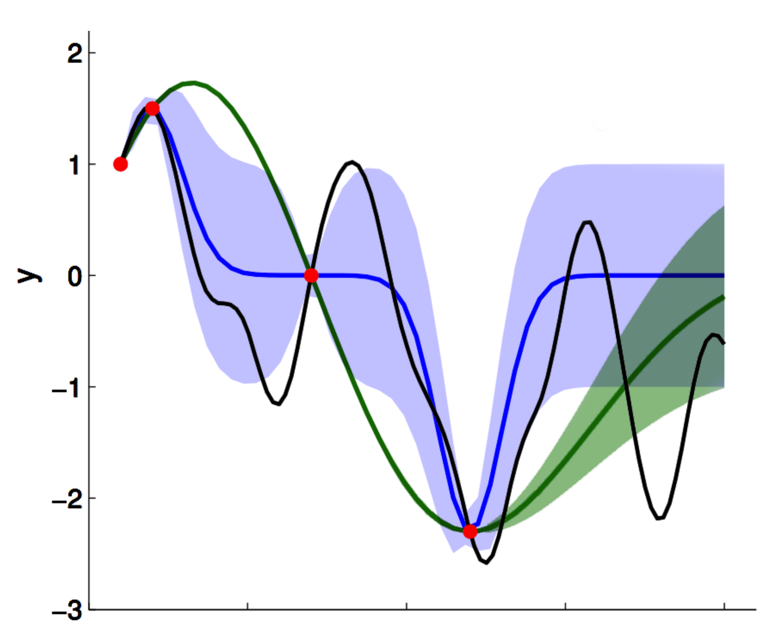
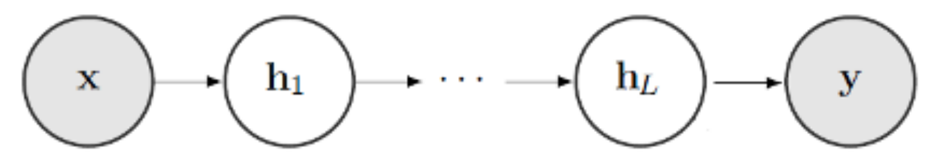


Figure: GP regression with two different kernel functions

Deep Gaussian Processes



Deep Gaussian Processes (DGPs) [2] are a multi-layer hierarchical generalisation of standard GPs. Given inputs and observation pairs $(\mathbf{x}_n, y_n)_{n=1}^N$:

$$p(f_l|\theta_l) = \mathcal{GP}(f_l; \mathbf{0}, \mathbf{K}_l) \quad (1)$$

$$p(\mathbf{h}_l|f_l, \mathbf{h}_{l-1}, \sigma_l^2) = \prod_n \mathcal{N}(h_{l,n}; f_l(h_{l-1,n}), \sigma_l^2) \quad (2)$$

$$p(\mathbf{y}|f_L, \mathbf{h}_{L-1}, \sigma_L^2) = \prod_n \mathcal{N}(y_n; f_L(h_{L-1,n}), \sigma_L^2) \quad (3)$$

with hidden layers $\mathbf{h}_l$ for $l = 1, \ldots, L$.

Technical Challenges

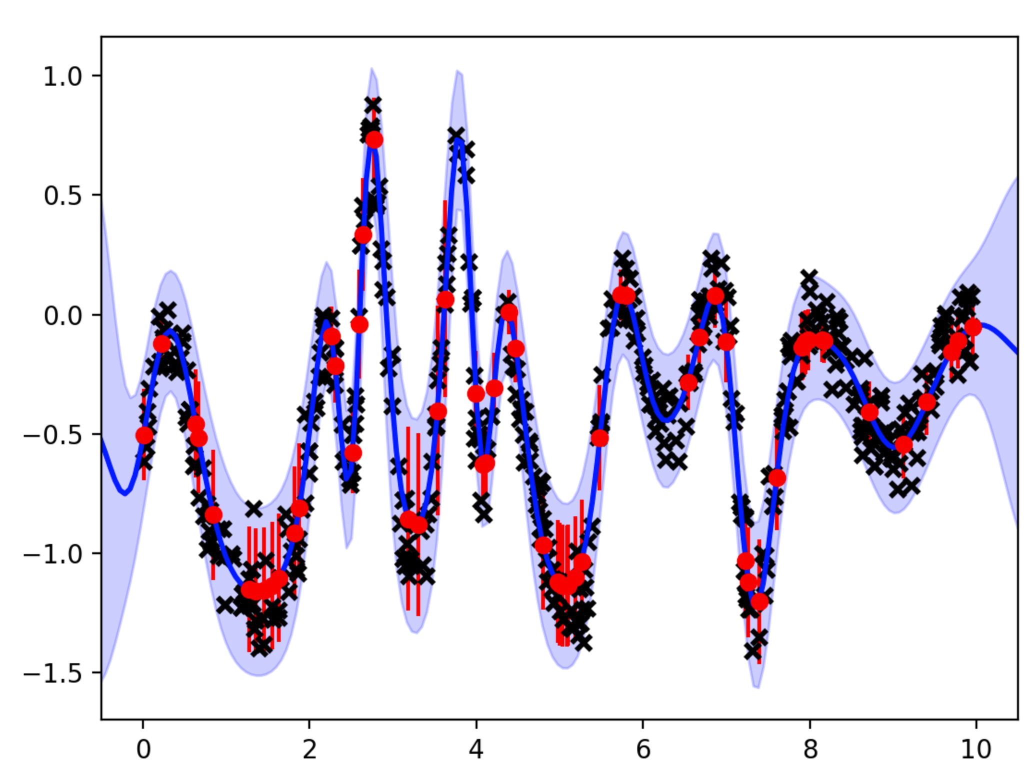
In practice, the DGP objective, the marginal likelihood $p(y|\mathbf{x}, \alpha)$, is intractable and regression has a high computational cost, $\mathcal{O}(LN^3)$. The following approximation scheme was proposed in [3]:

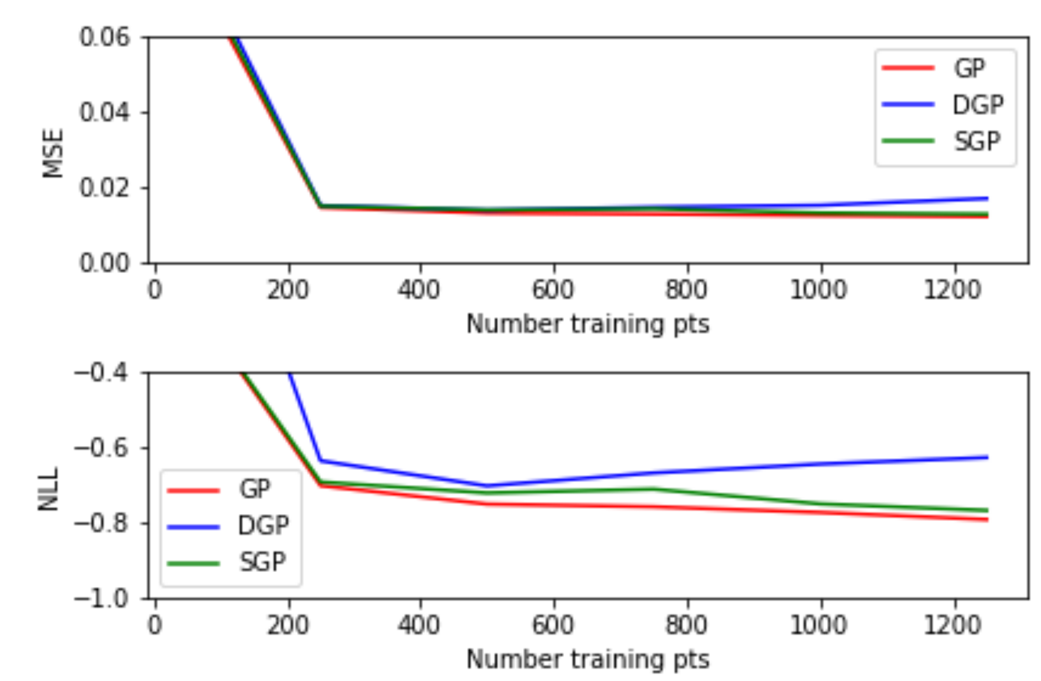
- *FITC* based pseudo-point sparse approximations, lowering the cost to $\mathcal{O}(LNM^2)$ where M is the number of pseudo points induced.
- Approximate inference for objective using approximate *Expectation Propagation* (AEP).
- *Probabilistic Backpropagation Algorithm* for training.

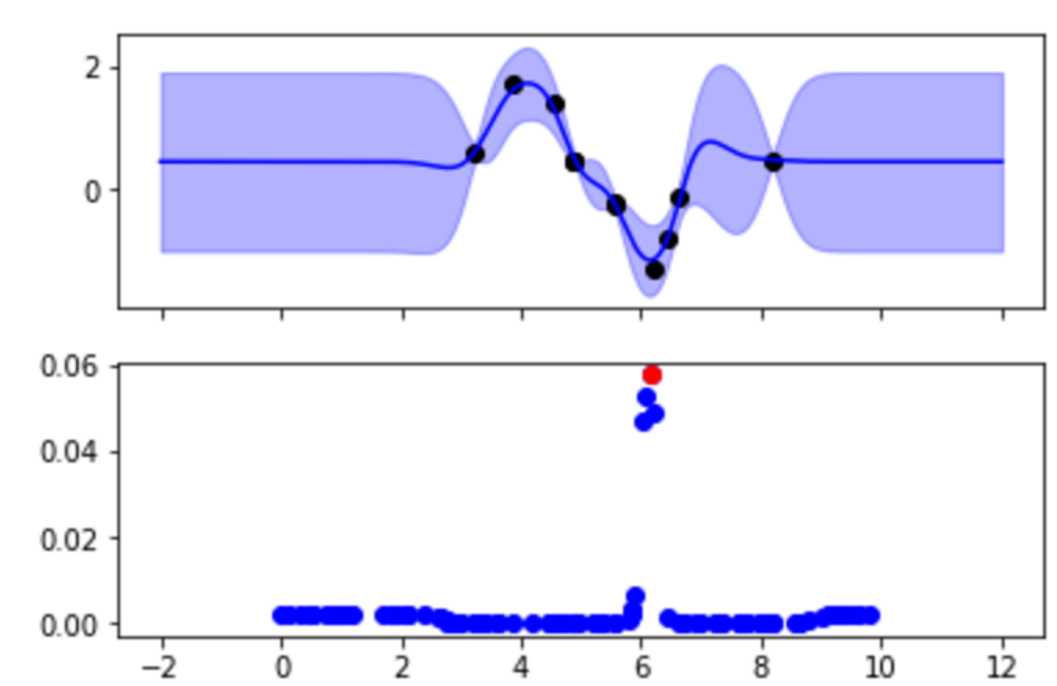
Experimental Results

Perform regression on multiple one-hidden-layer one-dimensional DGP samples to assess quality of Approximate EP inference scheme:

- AEP-DGP MSE and NLL scores compared to Full standard GPs and Sparse GPs. (Top-right)
- AEP-DGP fit to test data from DGP sample. (Bottom-left)
- Bayesian Optimization example for a DGP sample, using EI optimized by max pooling. (Bottom-right)







Alternative Methods

- *Bayesian Neural Networks* [4] require Monte Carlo methods making EI intractable.
- Rich and complex *Covariance Functions* require bayesian handling of hyperparameters to prevent overfitting.

Discussion

- DGPs present a flexible, more analytic generative model, making EI tractable.
- Hierarchical structure of DGPs allows for automatic input and output warping as well as non-parametric kernel design.
- DGPs are able to find correlations between multiple outputs and estimate expensive objectives based on cheaper ones.

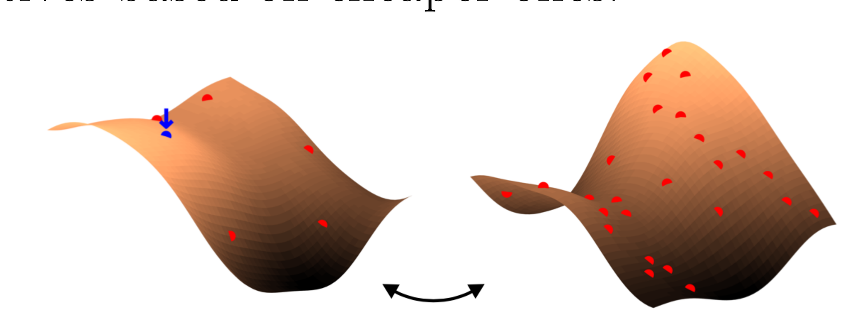


Figure: Expensive surface (right) and cheap surface (left) with multiple evaluations.

Future Work

- Investigate Sequential Monte Carlo based inference for DGPs in small-size Bayesian Optimization regression problems.

References

[1] Nando de Freitas Bobak Shahriari, Ryan P. Adams. Taking the human out of the loop: A review of bayesian optimization (2016).

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[3] Yingzhen Li JosÃl Miguel HernÃąndez-Lobato Richard E. Turner Thang D. Bui, Daniel HernÃąndez-Lobato. Deep gaussian processes for regression using approximate expectation propagation (2016).

[4] Falkner Frank Hutter Jost Tobias, Klein Stefan. Bayesian optimization with robust bnns.