# Fantasizing with Dual GPs in Bayesian Optimization and Active Learning

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## TL;DR

- Our dual conditioning efficiently updates variational parameters of a sparse GP in sequential/streaming settings.
- Unifying previous methods based on dual variables, we approximate the full-data posterior without revisiting previous batches.
- Our method works well in sequential decision making, particularly in batch acquisition of new data.

## Background

### Bayesian optimization (BO) and active learning (AL)

- BO: black-box optimization. AL: learning a decision boundary.
- Both techniques combine an acquisition function $\boldsymbol{\alpha}(\cdot)$ and a surrogate model to encode a trade-off between exploration and exploitation.
- Standard BO/AL usually find one query points, however in high data settings it may be beneficial to find a **batch** of query points.

### Variational sparse surrogate GP model

- Sparse GP methods swap computations on the full training set $\mathbf{X}$ with a sparser set of *inducing points* $\mathbf{Z} := (\mathbf{z}_j)_{j=1}^m$, $(\mathbf{u})_j = f(\mathbf{z}_j)$, with the approximate posterior $q(\mathbf{u}; \mathbf{m}, \mathbf{V})$.
- Common approach: use the variational ELBO to learn $(\mathbf{m}, \mathbf{V})$.
- [1] show that optimal variational parameters decompose as:

$$\mathbf{m}^* \equiv \mathbf{V}^* \boldsymbol{\lambda}^* \qquad \text{and} \qquad \mathbf{V}^* \equiv [\mathbf{K}_{\mathbf{zz}}^{-1} + \boldsymbol{\Lambda}^*]^{-1}. \tag{1}$$

We therefore reparameterize our variational parameters as $\boldsymbol{\lambda}$ and $\boldsymbol{\Lambda}$.

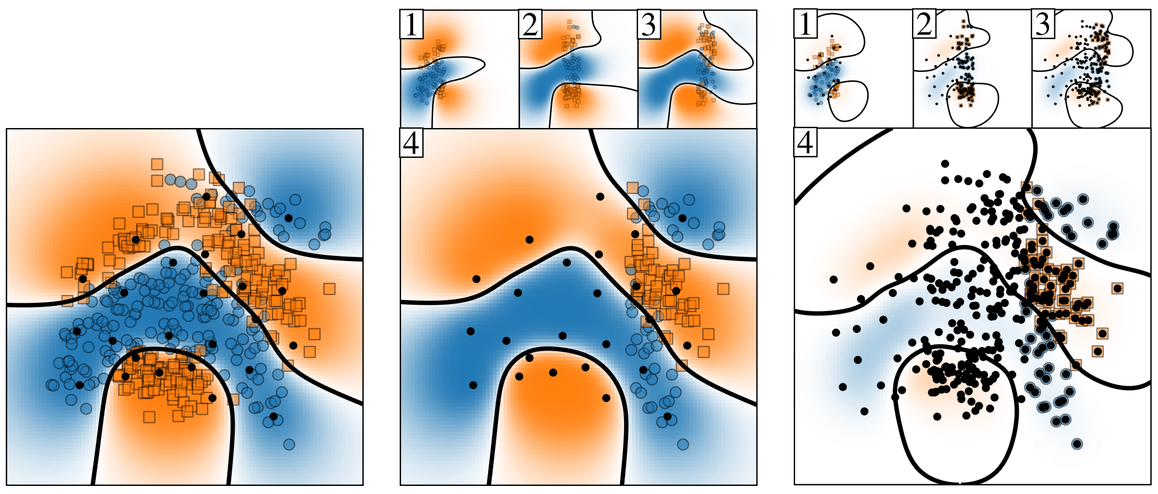
## Model & Methods

- We show how to use **dual conditioning** for batch BO/AL. We build a batch greedily by '**fantasizing**' for each point an observation value and updating the posterior [2, 3].
- Our dual conditioning updates are as follows:

$$\begin{aligned} \boldsymbol{\lambda}^*_{\text{new}} &\leftarrow \boldsymbol{\lambda}^*_{\text{old}} + \nabla_{\boldsymbol{\mu}^{(1)}} \mathbb{E}_{q_{\mathbf{u}}(\mathbf{f}_{\text{new}})}[\log p(\mathbf{y}_{\text{new}} \mid \mathbf{f}_{\text{new}})], \\ \boldsymbol{\Lambda}^*_{\text{new}} &\leftarrow \boldsymbol{\Lambda}^*_{\text{old}} + \nabla_{\boldsymbol{\mu}^{(2)}} \mathbb{E}_{q_{\mathbf{u}}(\mathbf{f}_{\text{new}})}[\log p(\mathbf{y}_{\text{new}} \mid \mathbf{f}_{\text{new}})], \end{aligned} \tag{2}$$

  where $q_{\mathbf{u}}(\cdot)$ is the posterior process and $\boldsymbol{\mu}$ are the expectation parameters of $q(\mathbf{u})$.
- The updates Eq. (2) are exact for Gaussian likelihoods and for non-Gaussian likelihoods recreate the posterior well compared to the offline solution (see Figure 1).
- Novelty of dual conditioning: does not need an optimization loop [4] or use previous data when conditioning the posterior on new information.
- We use Eq. (2) to iteratively add 'fantasized' data points from our $\boldsymbol{\alpha}(\cdot)$ to build a batch of query points.
- The method is independent of the acquisition function and can be used to perform batch BO/AL for any simple acquisition function.

## Sequential data classification




(a) Offline SVGP model (baseline) (b) Streaming dual SVGP (ours) (c) OVC (previous work by Maddox et al., 2021)

Figure 1: Sequential banana data set: our one-step updates on batches give similar solution to multiple optimization steps on full training data.

## Batch acquisition in Bayesian optimization

- We apply our batch method to the lunar landing problem where the goal is to land a rocket successfully on a specific region of a lunar surface under stochasticity.
- The acquisition function is a product of Expected Improvement of the regression model and the predictive mean of the classification model. Therefore, needing both a Gaussian and non-Gaussian surrogate model.
- Our method shows an improvement over the non-batch baseline (see Figure 2).

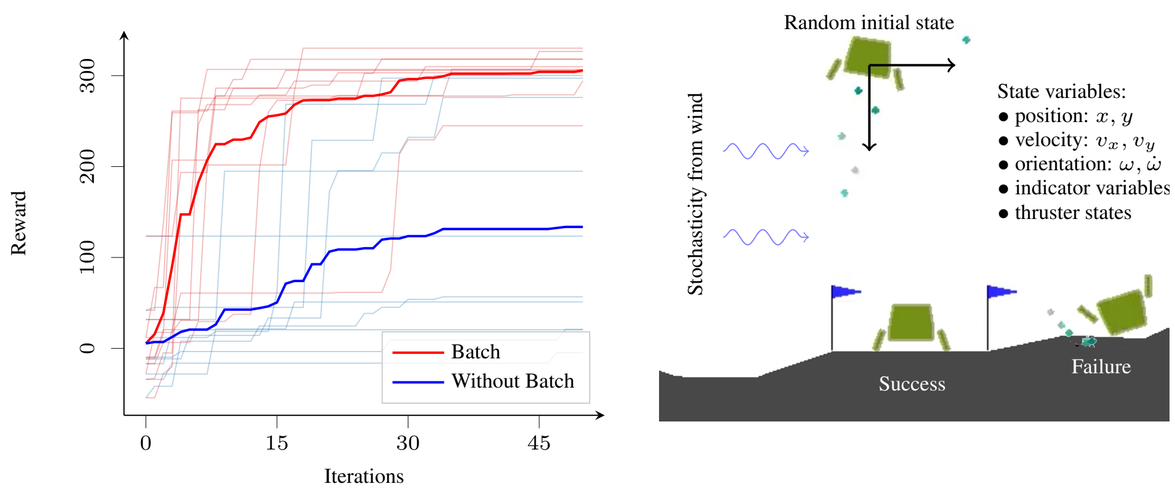



Figure 2: We test our method on lunar landing problem where we need to find optimal parameters of landing a rocket with wind stochasticity.

- In summary, we present dual conditioning, a method to condition data quickly into a sparse GP posterior. We show its usefulness for BO and AL.

## More details...

See the paper:

arxiv.org/abs/2211.01053

## References

[1] V. Adam, P. Chang, M. E. E. Khan, and A. Solin, "Dual parameterization of sparse variational Gaussian processes," *Advances in Neural Information Processing Systems*, 2021.

[2] D. Ginsbourger, R. L. Riche, and L. Carraro, "Kriging is well-suited to parallelize optimization," in *Computational intelligence in expensive optimization problems*, pp. 131–162, Springer, 2010.

[3] T. Desautels, A. Krause, and J. W. Burdick, "Parallelizing exploration-exploitation tradeoffs in Gaussian process bandit optimization," *Journal of Machine Learning Research*, 2014.

[4] W. J. Maddox, S. Stanton, and A. G. Wilson, "Conditioning sparse variational Gaussian processes for online decision-making," *Advances in Neural Information Processing Systems*, 2021.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