Bayesian Optimization of Composite Functions

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Joint work with Peter I. Frazier

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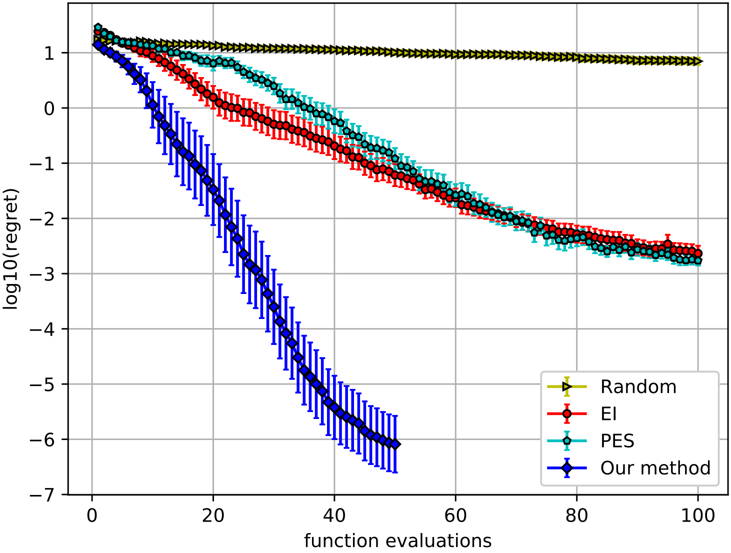


log10(regret)
function evaluations
Random
EI
PES
Our method

Problem

We consider problems of the form

$$\max_{x \in \mathcal{X}} f(x),$$

where

$$f(x) = g(h(x))$$

and

- $h : \mathcal{X} \subset \mathbb{R}^d \to \mathbb{R}^m$ is a time-consuming-to-evaluate black-box,
- $g : \mathbb{R}^m \to \mathbb{R}$ and its gradient are known in closed form and fast-to-evaluate.

Composite functions arise naturally in practice

- Hyperparameter tuning of classification algorithms:

$$g(h(x)) = -\sum_{j=1}^{m} h_j(x),$$

  where $h_j(x)$ is the classification error on the j-th class under hyperparameters x.

- Calibration of expensive simulators:

$$g(h(x)) = -\sum_{j=1}^{m} (h_j(x) - y_j)^2,$$

  where $h(x)$ is the output of the simulator under parameters x and y is a vector of observed data.

Standard BayesOpt approach

- Set a Gaussian process distribution on f.
- While evaluation budget is not exhausted:
  - Compute the posterior distribution on f given the evaluations so far, $\{(x_i, f(x_i))\}_{i=1}^{n}$,
  - Choose the next point to evaluate as the one that maximizes an acquisition function a:

$$x_{n+1} \in \text{argmax}_x a_n(x),$$

    where the subscript n indicates the dependence on the posterior distribution at time n.

Background: Expected Improvement (EI)

The most widely used acquisition function in standard BayesOpt is:

$$\mathrm{EI}_n(x) = \mathbb{E}_n\left[\{f(x) - f_n^*\}^+\right],$$

where

- f_n^* is the best observed value so far,
- $\mathbb{E}_n$ is the conditional expectation under the posterior after n evaluations.

Background: Expected Improvement (EI)

The most widely used acquisition function in standard BayesOpt is:

$$\mathrm{EI}_n(x) = \mathbb{E}_n \left[\{ f(x) - f_n^* \}^+ \right].$$

When $f(x)$ is Gaussian, EI and its derivative have a closed form which make it easy to optimize.

Our contribution

1. A **statistical approach** for modeling f that greatly improves over the standard BayesOpt approach.
2. An efficient **way to optimize the expected improvement** under this new statistical model.

Our approach

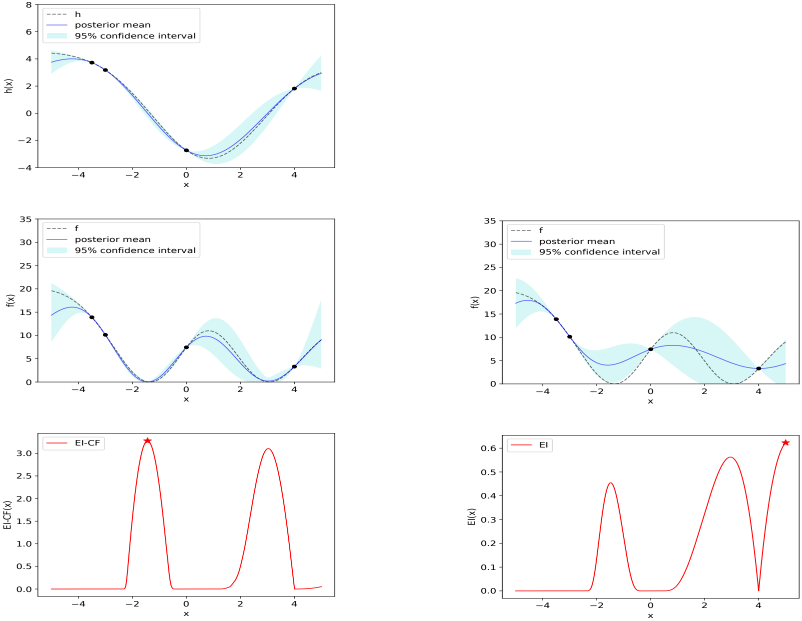
- Model h using a multi-output Gaussian process instead of f directly.
- This implies a (non-Gaussian) posterior on $f(x) = g(h(x))$.
- To decide where to sample next: compute and optimize the expected improvement under this new posterior.

Expected Improvement for Composite Functions

Our acquisition function is Expected Improvement for Composite Functions (EI-CF):

$$\text{EI-CF}_n(x) = \mathbb{E}_n\left[\{g(h(x)) - f_n^*\}^+\right],$$

where h is a GP, making $h(x)$ Gaussian.


h
posterior mean
95% confidence interval
h(x)
x
f
posterior mean
95% confidence interval
f(x)
x
f
posterior mean
95% confidence interval
f(x)
x
EI-CF
EI-CF(x)
x
EI
EI(x)
x

Challenge: maximizing $\mathrm{EI\text{-}CF}$ is hard

Expected Improvement for Composite Functions (EI-CF):

$$\mathrm{EI\text{-}CF}_n(x) = \mathbb{E}_n\left[\{g(h(x)) - f_n^*\}^+\right].$$

Challenge:

- When h is a GP and g is nonlinear, $f(x) = g(h(x))$ is **not Gaussian**.
- $\mathrm{EI\text{-}CF}$ does not have a closed form, making it hard to optimize.

Our approach to maximize EI-CF

- Construct an unbiased estimator of $\nabla \text{EI-CF}_n(x)$ using the reparametrization trick and infinitesimal perturbation analysis.

- Use this estimator within multi-start stochastic gradient ascent to find an approximate solution of

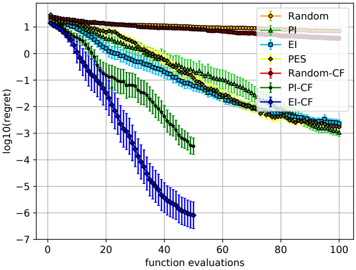
$$\text{argmax}_x \text{EI-CF}_n(x).$$

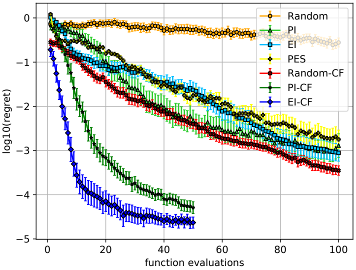
Asymptotic consistency

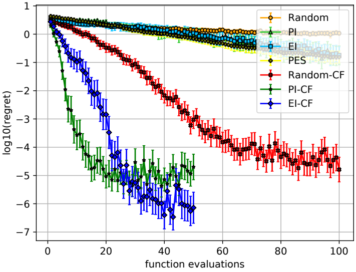
Theorem.

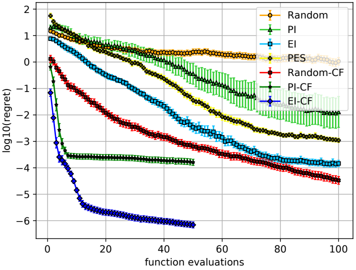
Under suitable regularity conditions, $\mathrm{EI\text{-}CF}$ is asymptotically consistent, i.e., it finds the true global optimum as the number of evaluations goes to infinity.

Numerical experiments









Conclusion

- Exploiting composite objectives can improve BayesOpt performance by 3-6 orders of magnitude.
- Come to our poster: Wed 6:30-9pm Pacific Ballroom #237.
- Check out our code: `https://github.com/RaulAstudillo06/BOCF`