New One-Step Bayes-Optimal Algorithms for Global Optimization: Parallel Computing and Common Random Numbers

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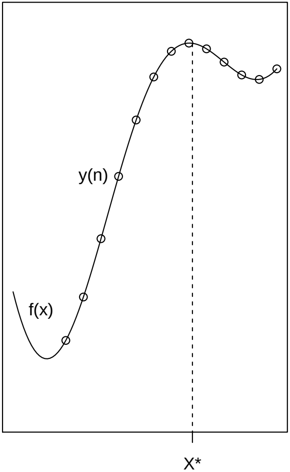
Derivative-Free Black-box Global Optimization



- Objective function $f : \mathbb{R}^d \mapsto \mathbb{R}$, continuous but not concave.
- Feasible set $A \subseteq \mathbb{R}^d$.
- Our goal is to solve

$$\max_{x \in A} f(x)$$

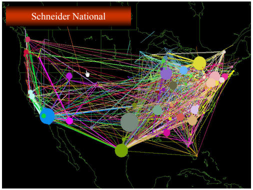
- Assumptions: f is time-consuming to evaluate (hours or days), and derivative information is unavailable.

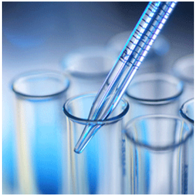
This is joint work with Scott C. Clark (Cornell PhD student).

Bayesian Global Optimization is a class of methods for Derivative-Free Black-Box Global Optimization

- One class of methods for derivative-free black-box global optimization is the class of **Bayesian Global Optimization (BGO)** methods.
- In these methods, we place a **Bayesian prior distribution** on the objective function f. (This is typically a Gaussian process prior).
- Ideally, we would find an algorithm with optimal average-case performance under this prior.
- We will settle for an algorithm with good average-case performance.
- (There are many other types of DFO methods. We do not discuss these in this talk.)

BGO is useful for optimizing computational models and physical experiments





- BGO is often used for optimizing large-scale computational models.
  - Example: Design of grafts to be used in heart surgery. [Yang et al., 2010]
  - Example: Calibration of a simulation-based logistics model. [Frazier et al., 2009b].
- BGO can also be used for optimization problems where "evaluating the objective function" means running a physical experiment
  - Example: Optimizing the concentrations of chemicals used to manufacture a material.
  - (Typically, physical experiments are noisy. We do not consider noise in this talk.)

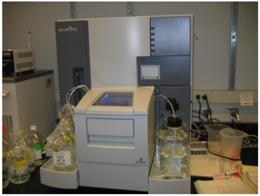
Almost all existing BGO methods are sequential

- Early work: [Kushner, 1964, Mockus et al., 1978, Mockus, 1989]
- Convergence analysis: [Calvin, 1997, Calvin and Zilinskas, 2002, Vazquez and Bect, 2010].
- Perhaps the most well-known method is Efficient Global Optimization (EGO) [Schonlau, 1997, Jones et al., 1998], which uses the notion of expected improvement.
- Recently many metheds have been developed that allow noise: [Calvin and Zilinskas, 2005, Villemonteix et al., 2009, Frazier et al., 2009a, Huang et al., 2006]

These methods are all fully sequential (one function evaluation at a time).

How can we extent BGO to multiple simultaneous function evaluations?

Cornell Tardis Cluster



BIAcore machine

- What if we can perform multiple function evaluations simultaneously?
- This is the case with parallel computing, and in many experimental settings (particularly in biology).
- We explore an idea that follows naturally from a decision-theoretic analysis.
- This idea was previously suggested by [Ginsbourger et al., 2007].

We generalize to multiple function evaluations using a decision-theoretic approach

- We've evaluated $\vec{x}^{(1)}, \dots, \vec{x}^{(n)}$, and observed $f(\vec{x}^{(1)}), \dots, f(\vec{x}^{(n)})$.
- Once sampling stops, we will select the best point evaluated so far.
- **What would be the Bayes-optimal way to choose the set of points $\vec{x}_1, \dots, \vec{x}_q$ to evaluate next?**
- In general, the optimal points are given by the solution to a dynamic program. (Difficult to solve)
- When this is the last stage of measurements, the dynamic program becomes a more straightforward optimization problem.

Generalizing EI to multiple function evaluations

- We've evaluated $\vec{x}^{(1)}, \ldots, \vec{x}^{(n)}$, and observed $f(\vec{x}^{(1)}), \ldots, f(\vec{x}^{(n)})$.
- Let $f_n^* = \max_{m=1,\ldots,n} f(\vec{x}_m)$ be the best value observed so far.
- If we measure at new points $\vec{x}_1, \ldots, \vec{x}_q$, and if that is our last stage of measurements, then the expected value of our solution is

$$\mathbb{E}_n \left[\max\left(f_n^*, \max_{i=1,\ldots,q} f(\vec{x}_i) \right) \right]$$

- This can be rewritten as $\mathrm{EI}_n(\vec{x}_1, \ldots, \vec{x}_q) + f_n^*$ where

$$\mathrm{EI}_n(\vec{x}_1, \ldots, \vec{x}_q) = \mathbb{E}_n \left[\left(\max_{i=1,\ldots,q} f(\vec{x}_i) - f_n^* \right)^+ \right]$$

  is given the name **q-EI** (and also "multipoints expected improvement") by [Ginsbourger et al., 2007].

q-EI gives the single-stage Bayes-optimal set of evaluations

- If we have one stage of function evaulations left to take, and must take our final solution from the set of points that have been evaluated, then evaluating

$$\arg\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}_n(\vec{x}_1,\ldots,\vec{x}_q)$$

  is **Bayes optimal**, i.e., optimal with respect to average case performance under posterior.
- If we have more than one stage left to go, it is a heuristic.

q-EI has no general closed form expression

$\mathrm{EI}_n(\vec{x}_1, \ldots, \vec{x}_q) = \mathbb{E}_n\left[\left(\max_{i=1,\ldots,q} f(\vec{x}_i) - f_n^*\right)^+\right]$

- When $q = 1$ (no parallelism), this reduces to the expected improvement of [Jones et al., 1998], which has a closed form.
- When $q = 2$, [Ginsbourger et al., 2007] provides an expression in terms of bivariate normal cdfs.
- When $q > 2$, there is no analytic expression.
  [Ginsbourger et al., 2007] proposes estimation through Monte Carlo.

q-EI is hard to optimize

- From [Ginsbourger, 2009], "*directly optimizing the q-EI becomes extremely expensive as q and d (the dimension of inputs) grow.*"
- Rather than actually solving $\arg\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$ when $q > 2$, [Ginsbourger et al., 2007] proposes other heuristic schemes.

Our Contribution

- Our contribution is an efficient method for solving

$$\arg\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$$

- This transforms the Bayes optimal function evaluation plan, previously considered to be a purely conceptual algorithm, into something implementable.

Our approach to solving $\arg\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$

1. Construct an unbiased estimater of

$$\nabla \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$$

   using infinitessimal perturbation analysis (IPA).

2. Use multistart stochastic gradient ascent to find an approximate solution to $\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$.

We construct an estimator of the gradient

- Using sufficient conditions described on the next slide, we switch ∇ and expectation to obtain our unbiased estimator of the gradient,

$$\begin{aligned}\nabla \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q) &= \nabla \mathbb{E}_n\left[\left(\max \vec{\mu}_n(\vec{x}_1,\ldots,\vec{x}_q) + C_n(\vec{x}_1,\ldots,\vec{x}_q)\vec{Z} - f_n^*\right)^+\right] \\ &= \mathbb{E}_n\left[g(\vec{x}_1,\ldots,\vec{x}_q,\vec{Z})\right],\end{aligned}$$

  where

$$g(\vec{x}_1,\ldots,\vec{x}_q,\vec{Z}) = \nabla\left(\max \vec{\mu}_n(\vec{x}_1,\ldots,\vec{x}_q) + C_n(\vec{x}_1,\ldots,\vec{x}_q)\vec{Z} - f_n^*\right)^+$$

  when this gradient exists, and 0 otherwise.
- $g(\vec{x}_1,\ldots,\vec{x}_q,\vec{Z})$ can be computed using results from [Smith, 1995] on differentiation of the Cholesky decomposition.

Our gradient estimator is unbiased, given sufficient conditions

Theorem

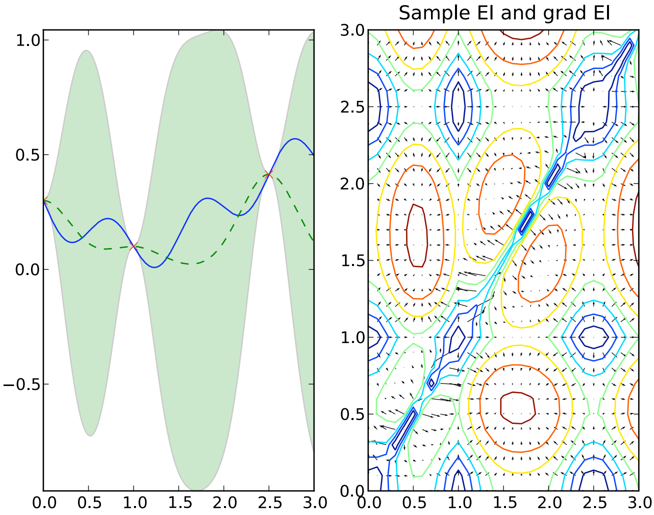
If the following conditions hold

- $\vec{\mu}_n(\vec{x}_1,\ldots,\vec{x}_q)$ *and* $\Sigma_n(\vec{x}_1,\ldots,\vec{x}_q)$ *are continuously differentiable in a neighborhood of* $\vec{x}_1,\ldots,\vec{x}_q$
- $\vec{x}_i \neq \vec{x}_j$ *for all* $i \neq j$*. (Don't propose measuring the same point twice)*
- $\vec{x}_i \neq x^{(j)}$ *for all* i,j*. (Don't measure a previously measured points)*
- $P_n(f(x') \neq f(x)) = 1$ *for all* $x' \neq x$ *and all* $x \notin \{\vec{x}^{(1)},\ldots,\vec{x}^{(n)}\}$ *(Our model is not degenerate)*

then

$$\nabla \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q) = \mathbb{E}_n\left[g(\vec{x}_1,\ldots,\vec{x}_q,\vec{Z})\right].$$

Example of Estimated Gradient

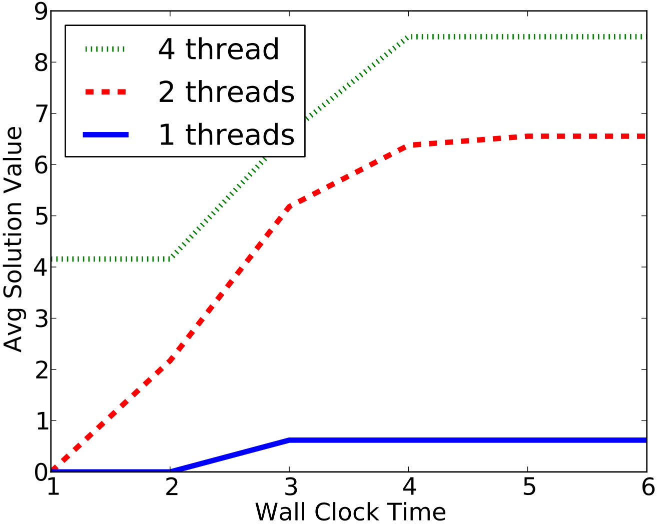


We can handle asynchronous function evaluations

- As previously described, if there are no function evaluations currently in progress, we solve
$$\max_{\vec{x}_1,\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$$
to get the set to run next.
- If there are function evaluations already in progress, say $\vec{x}_1,\ldots,\vec{x}_k$, we take these as given and optimize the rest $\vec{x}_{k+1},\ldots,\vec{x}_q$.

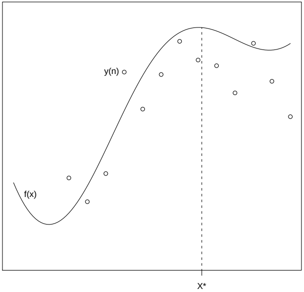
$$\max_{\vec{x}_{k+1},\ldots,\vec{x}_q} \mathrm{EI}(\vec{x}_1,\ldots,\vec{x}_q)$$

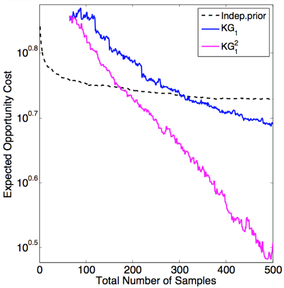
Initial Results



Other Work: Stochastic Global Optimization Using Common Random Numbers

Maximize a noisy non-concave function in $\mathbb{R}^d$. Use common random numbers to reduce the variance of comparisons.

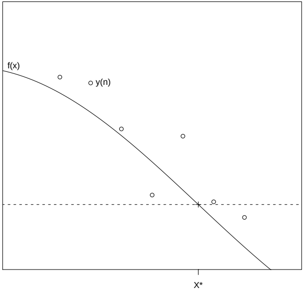


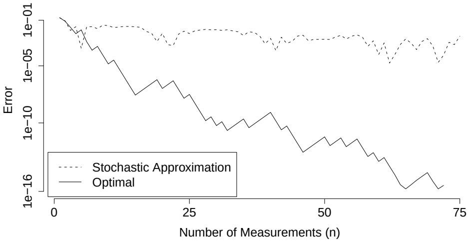


- P.I. Frazier, J. Xie, and S.E. Chick, "Bayesian Optimization via Simulation with Correlated Sampling and Correlated Prior Beliefs," Winter Simulation Conference, 2011.
- J. Xie, P.I. Frazier and S.E. Chick, "Large-Scale Bayesian Optimization via Simulation with Common Random Numbers," in preparation.

Other Work: Stochastic Root Finding

Find the root of a monotone function whose values can only be measured with noise. Use as few function evaluations as possible.

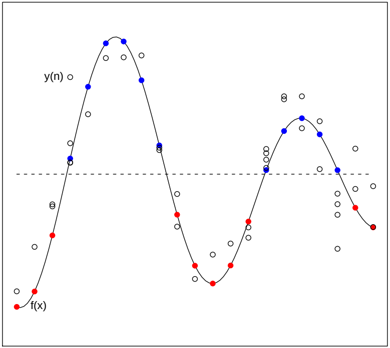


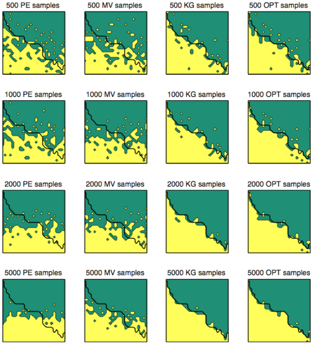


- R. Waeber, P.I. Frazier and S.G. Henderson, "Bisection Search with Noisy Responses." in review at SIAM Journal on Control and Optimization.
- R. Waeber, P.I. Frazier, and S.G. Henderson, "A Bayesian Approach to Stochastic Root-Finding," Winter Simulation Conference, 2011. Winner of the Best Student Paper (OR/MS focused).

Other Work: Finding Level Sets

Identify those points whose value $f(x)$ is above a threshold. Use as few function evaluations as possible.

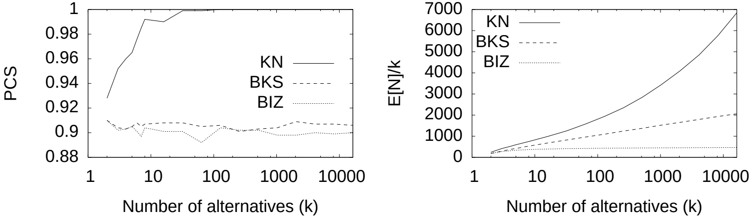




- J. Xie and P.I. Frazier, "Sequential Bayes-Optimal Policies for Multiple Comparisons with a Control." in revision for Operations Research. Finalist, INFORMS Junior Faculty Interest Group (JFIG) Paper Competition, 2011.

Other Work: Ranking & Selection

Find the alternative in a finite discrete set with the largest sampling mean. Do so with a guarantee on probability of correct selection, while taking as few samples as possible.



We provide the first fully sequential elimination procedure with tight bounds on probability of correct selection.

- P.I. Frazier, "A Fully Sequential Elimination Procedure for Indifference-Zone Ranking and Selection with Tight Bounds on Probability of Correct Selection." in revision for Operations Research.

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Backup

The Gradient Estimator

- We can rewrite our gradient estimator $g(\vec{x}_1, \ldots, \vec{x}_q, \vec{Z})$ more clearly.
- Let e_* be the unit vector corresponding to the maximal strictly positive component of

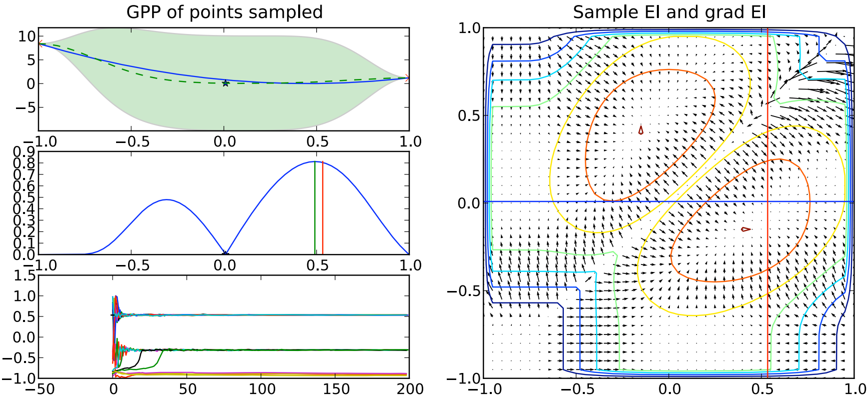
$$\vec{\mu}_n(\vec{x}_1, \ldots, \vec{x}_q) + C_n(\vec{x}_1, \ldots, \vec{x}_q)\vec{Z} - f_n^*,$$

  or 0 if all components are non-negative.
- Then,

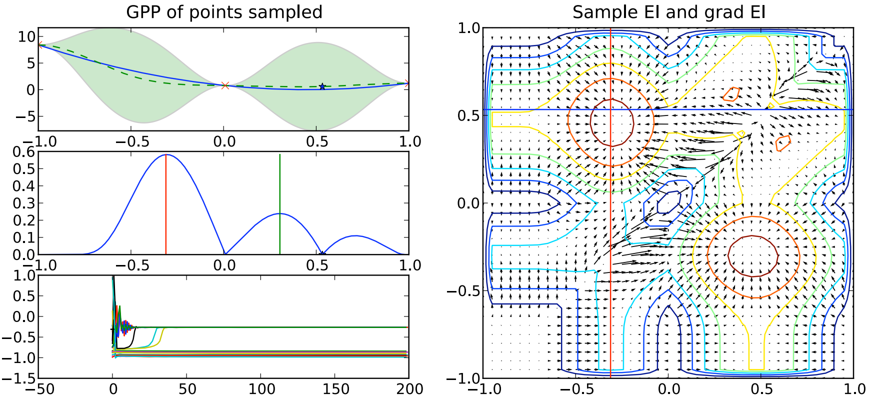
$$g(\vec{x}_1, \ldots, \vec{x}_q, \vec{Z}) = \nabla \left[e_* \vec{\mu}_n(\vec{x}_1, \ldots, \vec{x}_q) + e_* C_n(\vec{x}_1, \ldots, \vec{x}_q)\vec{Z} \right]$$

- $g(\vec{x}_1, \ldots, \vec{x}_q, Z)$ can be computed using results from [Smith, 1995] on differentiation of the Cholesky decomposition.

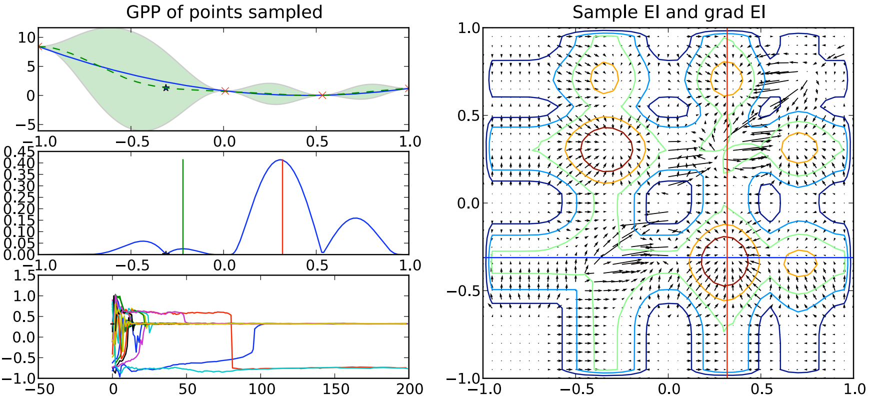
Animation



Animation



Animation


GPP of points sampled
10
5
0
−5
−1.0
−0.5
0.0
0.5
1.0
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1.5
0.5
−0.5
−50
50
100
150
200
Sample EI and grad EI

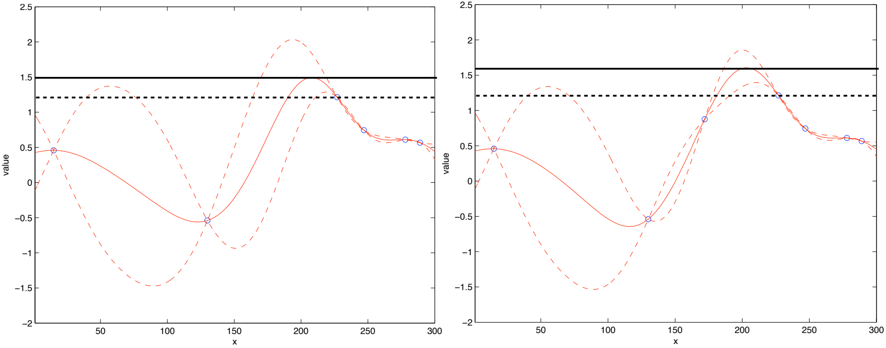
Best estimated overall value might be at an unmeasured point

- The improvement considered by EI is:

$$[f(x) - f_n^*]^+ = \max(f(x), f_n^*) - f_n^* = f_{n+1}^* - f_n^*$$

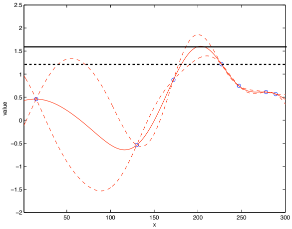
where $f_n^* = \max_{m \leq n} f(x_m)$ is the best point we've measured by time n.

- But the point with the best estimated value might not be a point we've measured.



We can measure improvement w.r.t. the best overall value

$$\text{Replace } f_n^* = \max_{m \leq n} f(x_m) = \max_{m \leq n} \mu_n(x_m) \text{ with } \mu_n^* = \max_{x \in A} \mu_n(x).$$



- The corresponding improvement is $\mu_{n+1}^* - \mu_n^*$.
- The corresponding value for taking a sample is

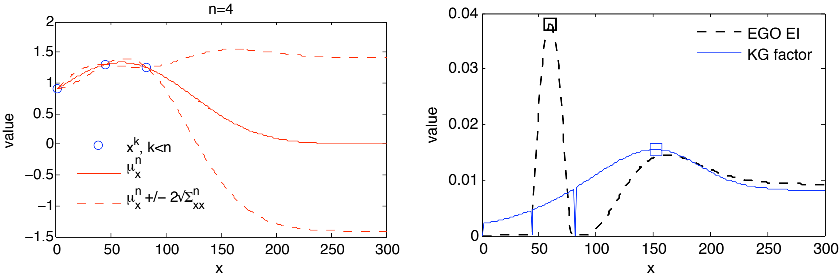
$$\mathbb{E}_n \left[\mu_{n+1}^* - \mu_n^* \mid x_{n+1} = x \right].$$

- The policy that measures at the x with the largest such value is called the **knowledge-gradient with correlated beliefs** (KGCB) policy.

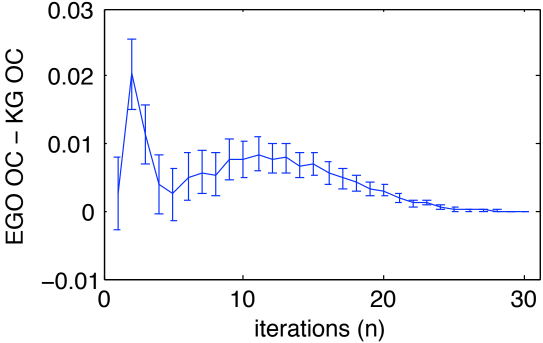
Knowledge-Gradient with Correlated Beliefs (KGCB)

- Call this modified expected improvement the knowledge-gradient (KG) factor
$$\mathrm{KG}_n(x) = \mathbb{E}_n\left[\mu^*_{n+1} - \mu^*_n \mid x_{n+1} = x\right].$$
- The KGCB policy measures at the point with the largest KG factor.

$$x_{n+1} \in \arg\max_x \mathrm{KG}_n(x).$$



KGCB Requires Fewer Function Evaluations than EGO, but More Computation



- Graph shows the difference in expected solution quality between KGCB and EGO, on noise-free problems.
- KGCB needs fewer function evaluations to find a good solution, but more computation to decide where to evaluate.