Acquisition fn $\alpha(x)$

- Depends on past info (implicit)
- Sample location $x$

$\alpha(x)$ in simple EI case is

$$\mathbb{E}\left[(f(x) - f_*)_+\right]$$

random piece, 1D Gaussian
Compute integral in "closed form"

Want to optimize via gradient descent

General: $\alpha(x) = \mathbb{E}[g(x)]$

$$\nabla \alpha(x) = \mathbb{E}[\nabla g(x)]$$

(with enough reg.)

$$\hat{\alpha}(x) = \frac{1}{N} \sum_{i=1}^{N} g(x; \xi_i)$$

random draws

$$\nabla \hat{\alpha}(x) = \frac{1}{N} \sum_{i=1}^{N} \nabla g(x; \xi_i)$$

Rollout acquisition

$$\alpha(x) = \mathbb{E}_{\substack{g \sim \text{posterior} \\ \text{GP}}}\left[\min_{\text{traj. } x_t}\left(g(x_t)\right) - g(\hat{x})\right]_+$$

where $\hat{x}$ is the best known sample point (before this)

Trajectory (for $g$)

$x_0 = x$ (starting point $\alpha(x)$)

$x_{k+1} = \underset{x}{\operatorname{argmax}}\; EI(x \mid \text{prior data up thru } k)$

$$\underbrace{x \quad \ldots \quad x_{-2} \quad x_{-1}}_{\substack{\text{stuff} \\ \text{I've seen} \\ \text{(know fn vals)}}} \quad \overset{?}{x_0} \quad \underbrace{x_1 \quad x_2 \quad \ldots \quad x_r}_{\substack{\text{fantasized samples} \\ \text{(guess values via} \\ \text{a draw)}}}$$

$f$ unknown fn, assumed drawn from GP

Have sampled
$x_{-m}, \ldots, x_{-1}$ & got
$y_{-m}, \ldots, y_{-1}$, $y_j = f(x_j)$

Posterior dist $\mathcal{G}$, gaussian proc conditioned on samples at $x_{-m}, \ldots, x_{-1}$

$$\alpha(x \mid g) = \max_{x_1, \ldots, x_r} [g(x_k) - y_*]_+$$

$x_1, \ldots, x_r$ depend on $g$ & hist
define by

$$x_{k+1} = \underset{x}{\operatorname{argmax}}\, EI(x \mid \text{samples through } x_k)$$

$$\alpha(x) = \mathbb{E}_{g \sim \mathcal{G}} [\alpha(x \mid g)]$$

$$\approx \hat{\alpha}(x) = \frac{1}{N} \sum_{i=1}^{N} \alpha(x \mid g^i), \quad g^i \sim \mathcal{G} \text{ are draws}$$

To est derivs,

$$\nabla \hat{\alpha}(x) = \frac{1}{N} \sum_{i=1}^{N} \nabla \alpha(x \mid g^i)$$

Assume $x_b$ is unique best pt on trajectory for $x_0 = x$ & fn $g^i$
Then we want

$$\nabla_x [g(x_b) - y_*]$$

$$x_{k+1} = \underset{x}{\operatorname{argmax}}\ EI(x \mid x_{-m}, \ldots x_k, y_{-m}, \ldots y_k, g)$$

Stationarity: $x_{k+1}$ solves

$$\nabla_x EI(x \mid x_{-m}, \ldots, x_k, g) = 0$$

Solution to this is an implicitly defined function)

$$x_{k+1}(x_{-m}, \ldots, x_k, g)$$

Get:

$$\nabla^2 EI(x_{k+1} \mid \ldots)\, \delta x_{k+1} + \underbrace{\sum_{j=-m}^{k} \frac{\partial}{\partial x_j} EI(x_k \mid x_{-m}, \ldots, x_k, g)\, \frac{\delta x_k}{?}}_{=0}$$

Algebra! And we have

$$\delta x_b = \frac{\partial x_b}{\partial x_0 = x}$$

$$\nabla \alpha(x \mid g) = g'(x_b) \frac{\partial x_b}{\partial x_0}$$