Expected Improvement

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June 6, 2021

These notes are based on "A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning" by Eric Brochu et al. In Brochu's tutorial one way expected improvement is defined is

$$EI(\mathbf{x}) = \begin{cases} (\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi)\Phi(Z) + \sigma(\mathbf{x})\phi(Z) & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \tag{1}$$

where

$$Z = \begin{cases} \frac{\mu(\mathbf{x}) - f(\mathbf{x}^+) - \xi}{\sigma(\mathbf{x})} & \text{if } \sigma(\mathbf{x}) > 0 \\ 0 & \text{if } \sigma(\mathbf{x}) = 0 \end{cases} \tag{2}$$

Here ξ is a parameter which trades off between the algorithms tendency to explore or exploit and its recommended value is $\xi = 0.01$. Additionally, $\mathbf{x}$ is a data point and $f(\mathbf{x}^+)$ is the current optimal value of function f at the current optimal point $\mathbf{x}^+$ in the set of observed or training points $\mathbf{X}'$.

A key point which I initially missed is that $\mu(\mathbf{x})$ and $\sigma(\mathbf{x})$ are the mean and standard deviation of the Gaussian Process prediction for the objective function $f(\mathbf{x})$. This Gaussian Process's covariance kernel is the Radial Basis function (RBF) with length scale $l = 2$ defined as

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{||\mathbf{x} - \mathbf{x}'||}{2l^2}\right) \tag{3}$$

and the Gaussian Process is defined as

$$GP(m(\mathbf{x}), K(\mathbf{x}, \mathbf{x}')) \tag{4}$$

where under the assumption that $f(\mathbf{x})$ can be model as a Gaussian Process

$$m(\mathbf{x}) = \mathbb{E}[f(\mathbf{x})] \tag{5}$$

$$K(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}') - m(\mathbf{x}'))] \tag{6}$$

The conditional mean of the Gaussian Process and by assumption $f(\mathbf{x})$ given $\mathbf{x}$, $\mathbf{X}'$, and $\mathbf{y}'$ is

$$\mathbb{E}[f(\mathbf{x})|\mathbf{X}', \mathbf{y}', \mathbf{x}] = K(\mathbf{X}', \mathbf{x})[K(\mathbf{X}', \mathbf{X}') + \sigma_n^2\mathbf{I}]^{-1}\mathbf{y}' \tag{7}$$

given training data and labels $(\mathbf{X}', \mathbf{y}')$. Similarly the conditional covariance of $f(\mathbf{x})$ is

$$Cov[f(\mathbf{x})|\mathbf{X}', \mathbf{x}] = K(\mathbf{x}, \mathbf{x}) - K(\mathbf{x}, \mathbf{X}')[K(\mathbf{X}', \mathbf{X}') + \sigma_n^2\mathbf{I}]^{-1}K(\mathbf{X}', \mathbf{x}) \tag{8}$$

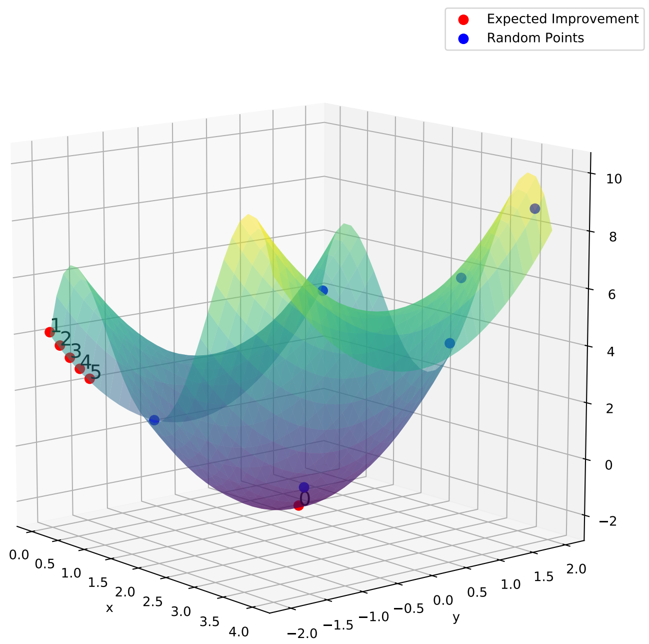
which if $\mathbf{x}$ is a single point reduces to the conditional variance.

Choosing a initial sample point $\mathbf{x}_0$ and subsequent points using the expected improvement algorithm as $\mathbf{x}^* = \text{argmax}_{\mathbf{x} \in \mathbf{D}}(EI(\mathbf{x}))$ in an attempt to maximize objective function Equation (9) where $\mathbf{D}$ is the set of potential points.

$$f(x, y) = -x(x-1)(x-3)(x-4) + x + y^2 \tag{9}$$

The results for 6 samples given initial points $(0.414, 0)$ and $(2, 0)$ with $\xi = 0.01$ are shown in Figure 1 relative to a random sample of 6 points where $|\mathbf{D}| = 900$. In this example the success of the expected improvement sampling scheme appears sensitive to initial sampling point and I have found it can also be sensitive to the value of ξ.

The code implementing this expected improvement sampling scheme and Figure 1 can be found at: `https://github.com/sophist0/expected_improvement`



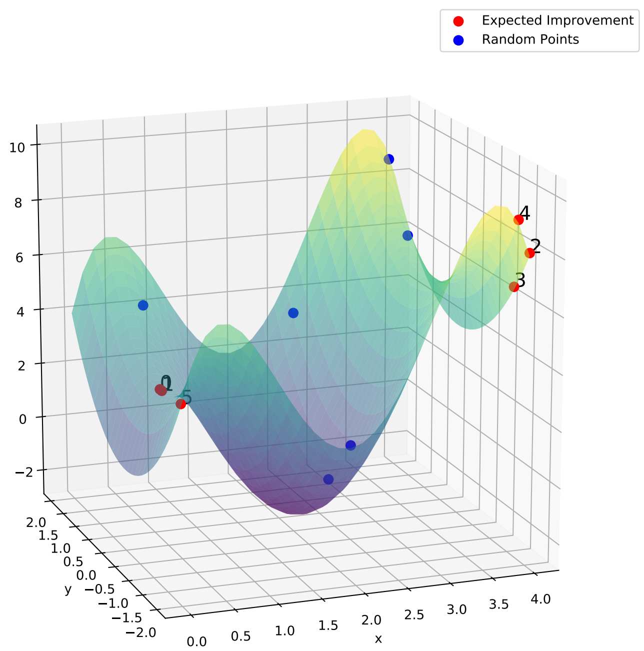


Figure 1: **Top:** Initial sample point $(0.414, 0)$, **Bottom:** Initial sample point $(2, 0)$. In both figures the numbers indicate the order of the samples.