Suppose we have computed n samples $y_j = f(x^j)$. We collect the sample points into $X = \begin{bmatrix} x^1 & x^2 & \dots & x^n \end{bmatrix}$ and the values into $y = \begin{bmatrix} y_1 & y_2 & \dots & y_n \end{bmatrix}^T$. When necessary to avoid ambiguity, we denote these as X^n and y^n, using the superscript to denote the number of data points. We denote any kernel hyperparameters by θ.

An s-step EI *rollout* policy involves choosing x^{n+1} based on the anticipated behavior of the EI algorithm starting from x^{n+1} and proceeding for s steps. That is, we consider the iteration

$$x^{k+1} = \text{argmax}_x \, \alpha(x|X^k, y^k, f^{+k}, \theta^k)$$

where θ^k denotes the kernel hyperparameters chosen at step k. A typical approach might involve running the trajectory forward for s steps with sample values drawn according to the current GP model, and looking at the best point found in s steps for several such runs. One could also consider a non-Monte-Carlo based quadrature approach.

Gradient information is particularly useful in this computation, but it requires that we be able to differentiate the whole (anticipated) sequence. That is, we might suppose that $\hat{f}$ is a draw of the GP, conditioned on the data from the first n samples, and then try to compute the derivative with respect to the proposed sample point x^{n+1} of the maximum of $\hat{f}(x^k)$ for k from 1 to $n+s$. Of course, this requires some algebra to set up.

We begin by differentiating α. Let $\nabla\alpha$ and H_α refer to the gradient and the Hessian with respect to the first slot (the x variable). Then differentiating the basic iteration gives us at step k that

$$H_\alpha \delta x^{k+1} + \sum_{j=1}^{k} \left(\frac{\partial \nabla\alpha}{\partial x^j} \delta x^j + \frac{\partial \nabla\alpha}{\partial y_j} \delta y_j \right) + \frac{\partial \nabla\alpha}{\partial f^{+k}} \delta f^{+k} + \frac{\partial \nabla\alpha}{\partial \theta^k} \delta\theta^k = 0.$$

Given the "fantasized" sample $\hat{f}$, we have

$$\delta y_j = \hat{f}'(x^j) \delta x^j$$

and if $b[k]$ denotes the index of the best point found up to step j, then $f^{+k} = y_{b[k]}$ and (assuming no ties)

$$\delta f^{+k} = \delta y_{b[k]}.$$

If the hyperparameters θ are determined by maximum likelihood estimation with the (log) likelihood function $\ell(\theta|X, y)$, we can again use implicit differentiation to obtain $\delta\theta^k$:

$$\frac{\partial^2 \ell}{\partial \theta^2} \delta\theta^k + \left(\sum_{j=1}^{k} \frac{\partial^2 \ell}{\partial \theta \partial x^j} \delta x^j + \frac{\partial^2 \ell}{\partial \theta \partial y_j} \delta y^j \right) = 0.$$