Lecture 23: Bayesian global optimization

Professor Ilias Bilionis

Expected improvement - No observation noise

PREDICTIVE
SCIENCE LABORATORY

Derivation of expected improvement

$x_{1:n} = (x_1, \dots, x_n)$; $y_{1:n} = (y_1, \dots, y_n)$; $\sigma = 0$

$f(\cdot) \sim GP(m(\cdot), c(\cdot,\cdot)) \Rightarrow$ posterior point predictive distribution

$$p(y \mid x, x_{1:n}, y_{1:n}) = N(y \mid m_n^*(x), \sigma_n^{*2}(x))$$

Current best observed output: $\bar{y}_n = \max_{1 \le i \le n} y_i$

Assume make hypothetical obs. (x, y):

Improvement: $I(x, \underset{?}{y}) = \begin{cases} 0, & y \le \bar{y}_n \\ y - \bar{y}_n \end{cases} = \max\{0, y - \bar{y}_n\}$

Exp. Improvement: $EI(x) = \mathbb{E}[I(x,y) \mid x, x_{1:n}, y_{1:n}]$

$$= \int_{-\infty}^{+\infty} \boxed{I(x,y)}\, p(y \mid x, x_{1:n}, y_{1:n})\, dy$$

$$= (m_n^*(x) - \bar{y}_n)\, \Phi\left(\frac{m_n^*(x) - \bar{y}_n}{\sigma_n^*(x)}\right) + \sigma_n^*(x)\, \phi\left(\frac{m_n^*(x) - \bar{y}_n}{\sigma_n^*(x)}\right)$$

Exploitation

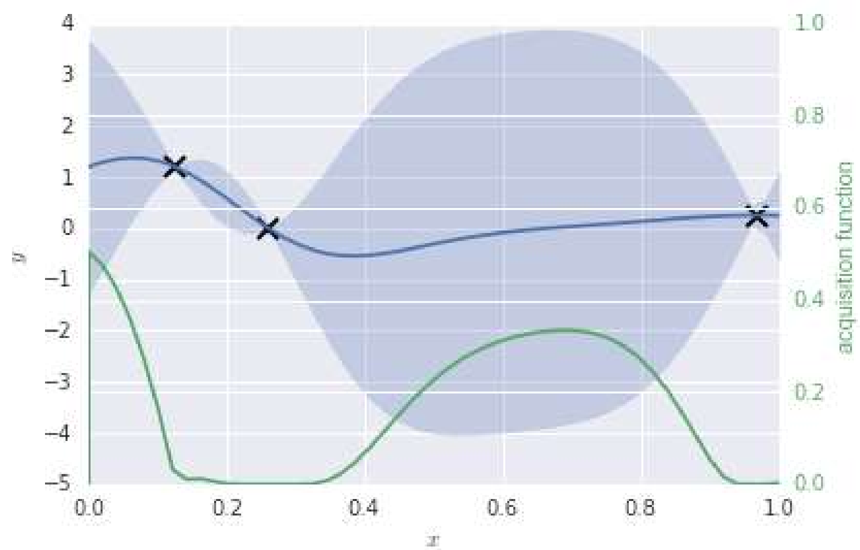
Exploration

CDF $N(0,1)$

pdf $N(0,1)$

PREDICTIVE
SCIENCE LABORATORY

Expected Improvement



Automatic exploration vs exploitation…

PREDICTIVE
SCIENCE LABORATORY