Lecture 23: Bayesian global optimization

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Probability of improvement - No observation noise

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Derivation of the probability of improvement

assume noiseless

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

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

$$p(y|x, x_{1:n}, y_{1:n}) = N(y|m_n^*(x), \sigma_n^{*2}(x)) \quad {+0}$$

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

controllable parameter

$$a(x) = p(y > \bar{y}_n + \psi | x, x_{1:n}, y_{1:n}) = \int_{\bar{y}_n + \psi}^{+\infty} p(y|x, x_{1:n}, y_{1:n})\, dy$$

transform variables

$$\dots = \left[\begin{array}{l} y|x, x_{1:n}, y_{1:n} \sim N(\dots) \\ z = \frac{y - m_n^*(x)}{\sigma_n^*(x)} \sim N(0,1) \end{array} \right] = p\left(z > \frac{\bar{y}_n + \psi - m_n^*(x)}{\sigma_n^*(x)}\right)$$

$$= 1 - \Phi\left(\frac{\bar{y}_n + \psi - m_n^*(x)}{\sigma_n^*(x)}\right)$$

CDF of $N(0,1)$

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

$\hookrightarrow$ by symmetry

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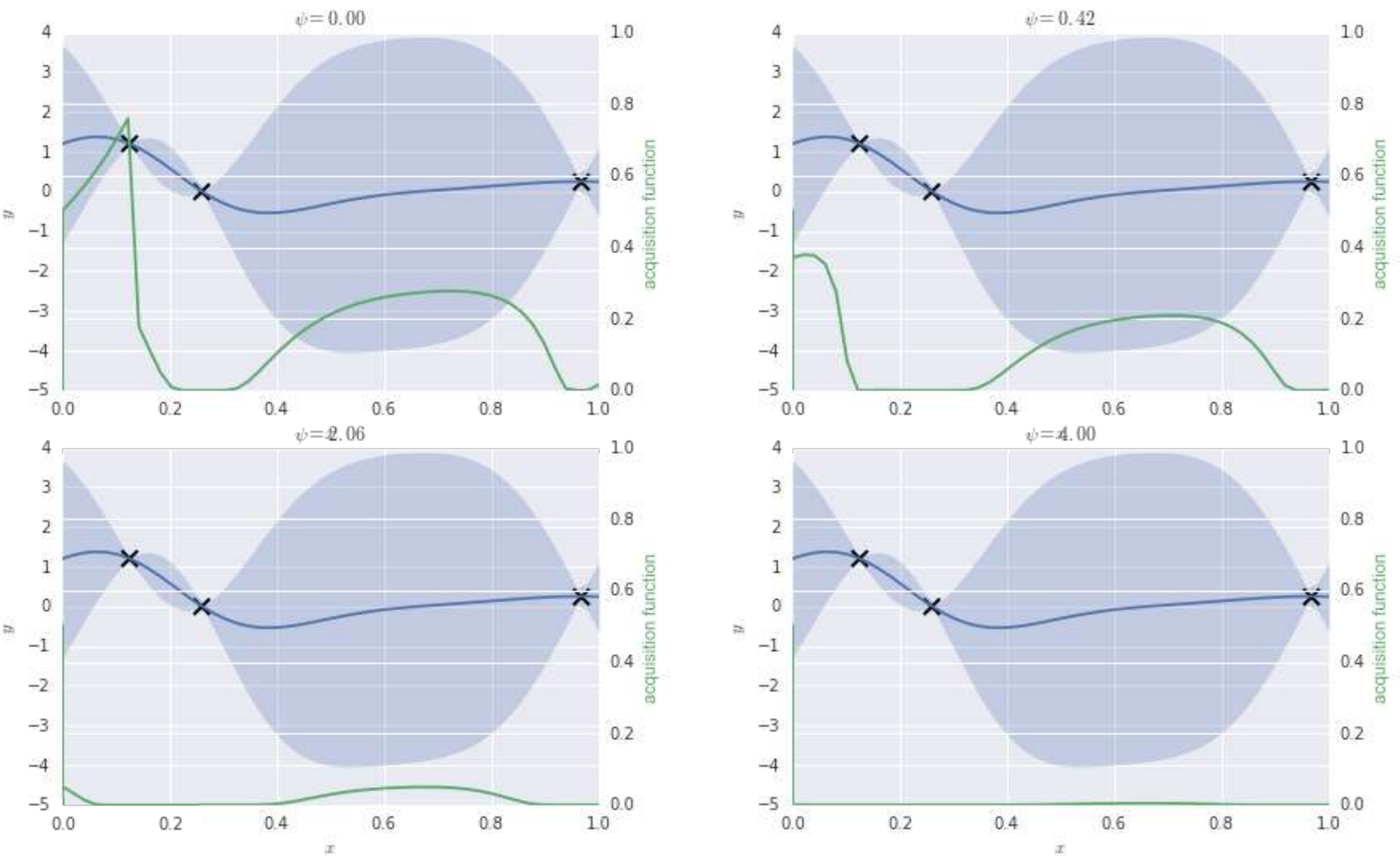
Probability of Improvement



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Probability of Improvement - Why not use it?

- Large value of ψ -> exploration.
- Small value of ψ -> exploitation.
- But how to you pick it?