Train In Data

Acquisition Functions

Acquisition Functions

- Guides the search for the optimum
- The acquisition function is high when the prediction is high (**exploitation**) or the uncertainty is high (**exploration**)

Acquisition Functions

- The acquisition function is high when the prediction is high (**exploitation**) or the uncertainty is high (**exploration**)

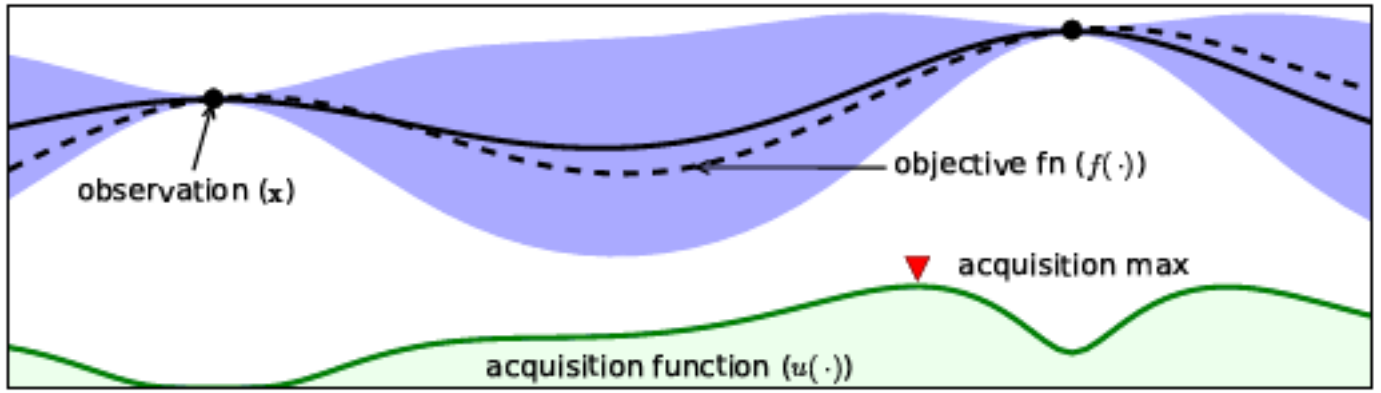
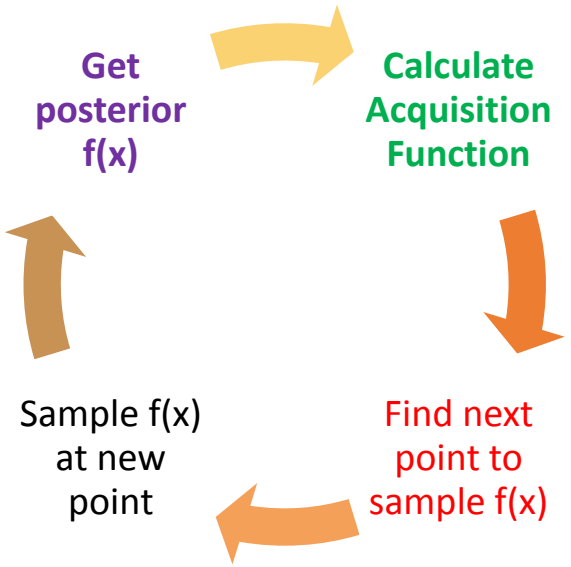


Image taken from Bochu, Cora, de Freitas, 2010

Acquisition Functions

- Guides the search for the optimum



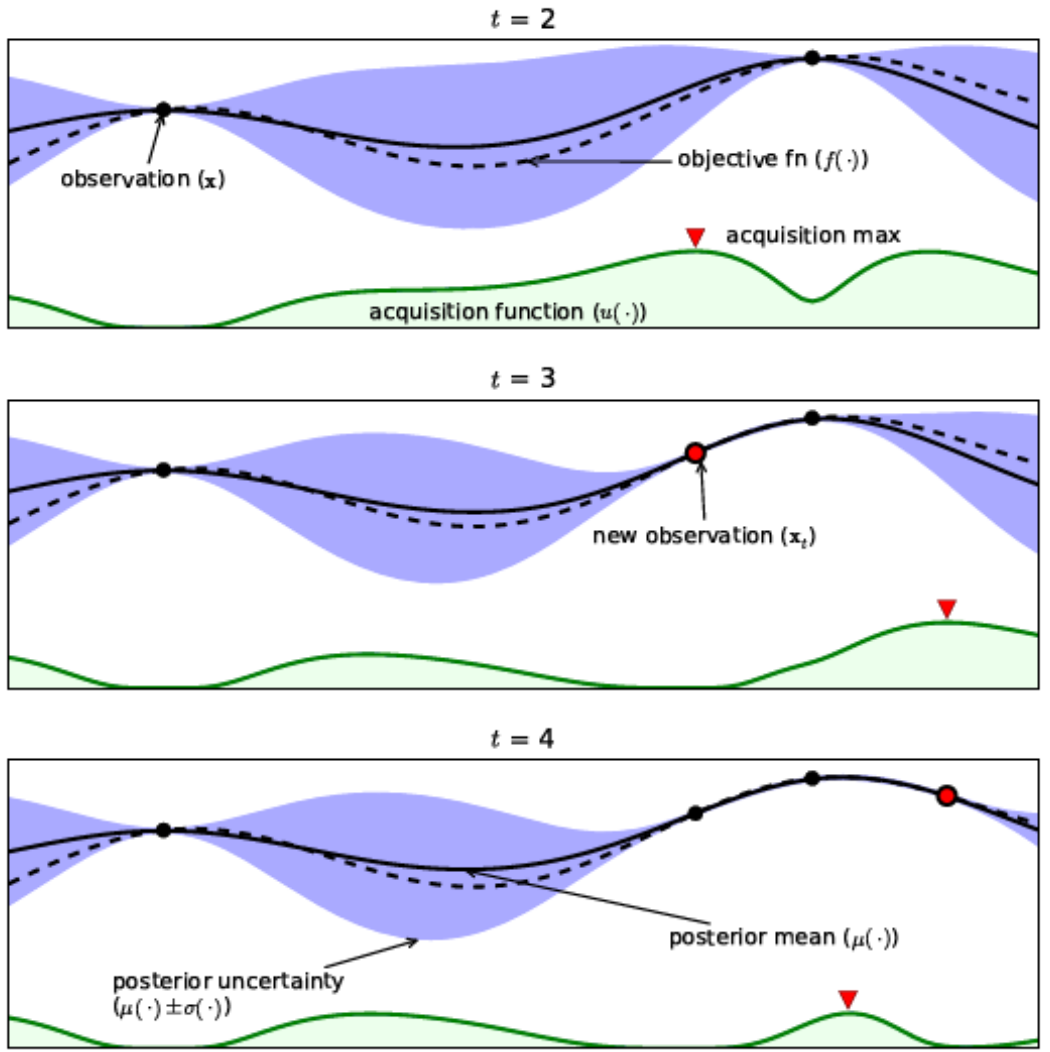


Image taken from Bochu, Cora, de Freitas, 2010

Acquisition Functions

- Probability of Improvement (PI)
- Expected Improvement (EI)
- Upper (or Lower) confidence bound (UCB or LCB)

Probability of Improvement

- PI = P(f(x) > max(μ))
- Probability that the new sampled value is bigger than the highest observed value

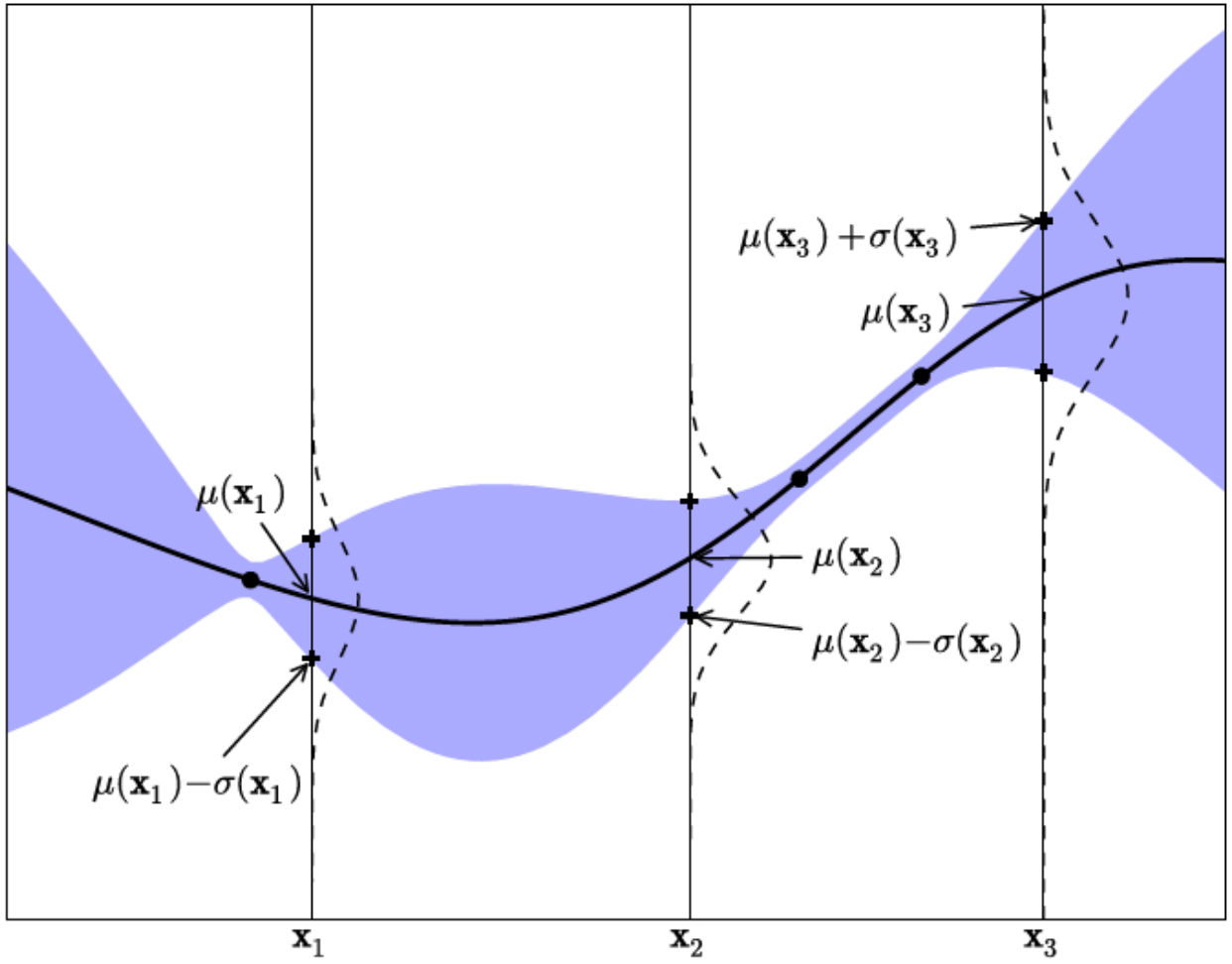


Image taken from Bochu, Cora, de Freitas, 2010

Probability of Improvement

- PI = P(f(x) > max(μ))
- Probability that the new sampled value is bigger than the highest observed value

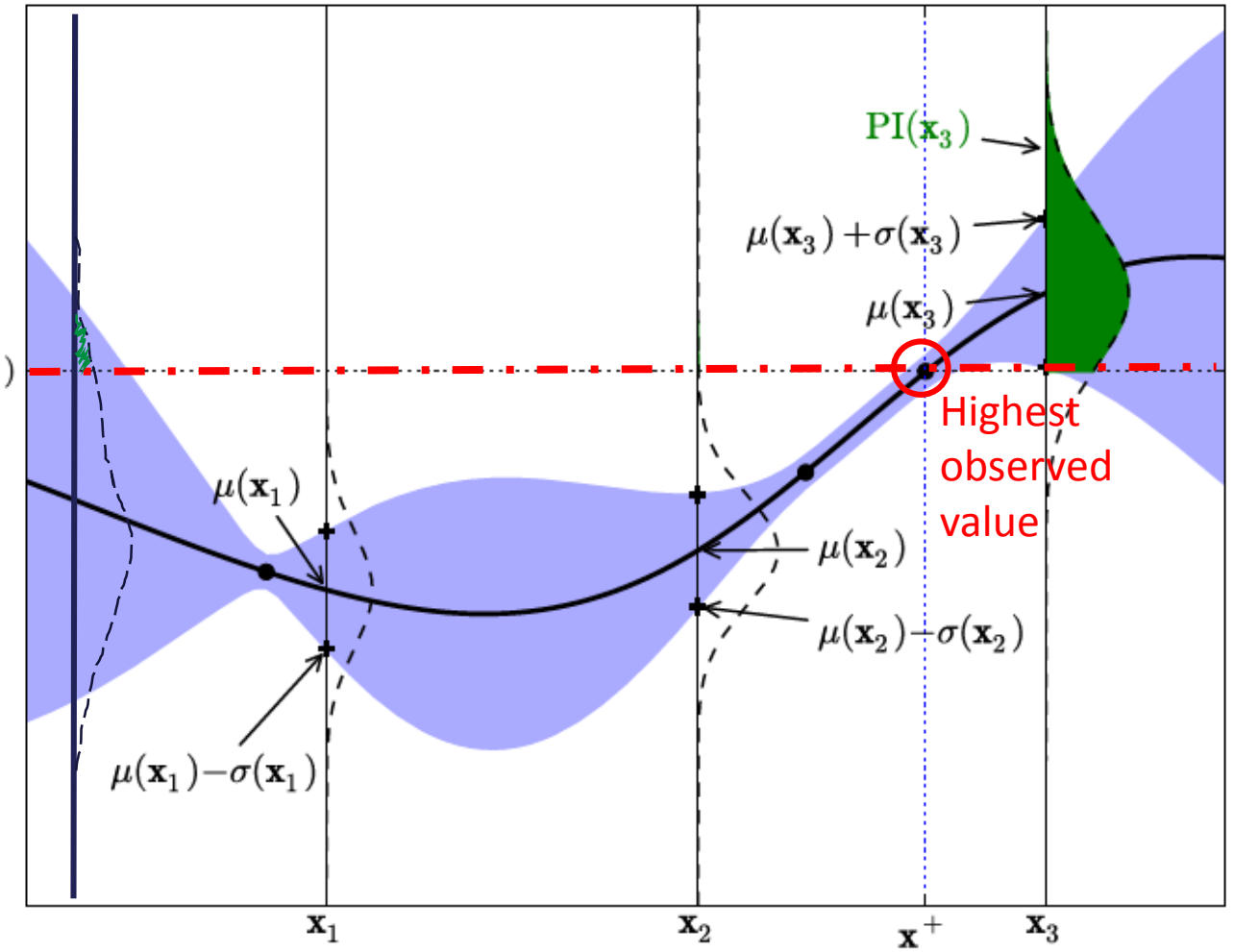


Image taken from Bochu, Cora, de Freitas, 2010

Probability of Improvement

Limitation:

- Does not contemplate how big the increase is
- If the probability of increase is high, even when the increase is small, it would sample that x_i

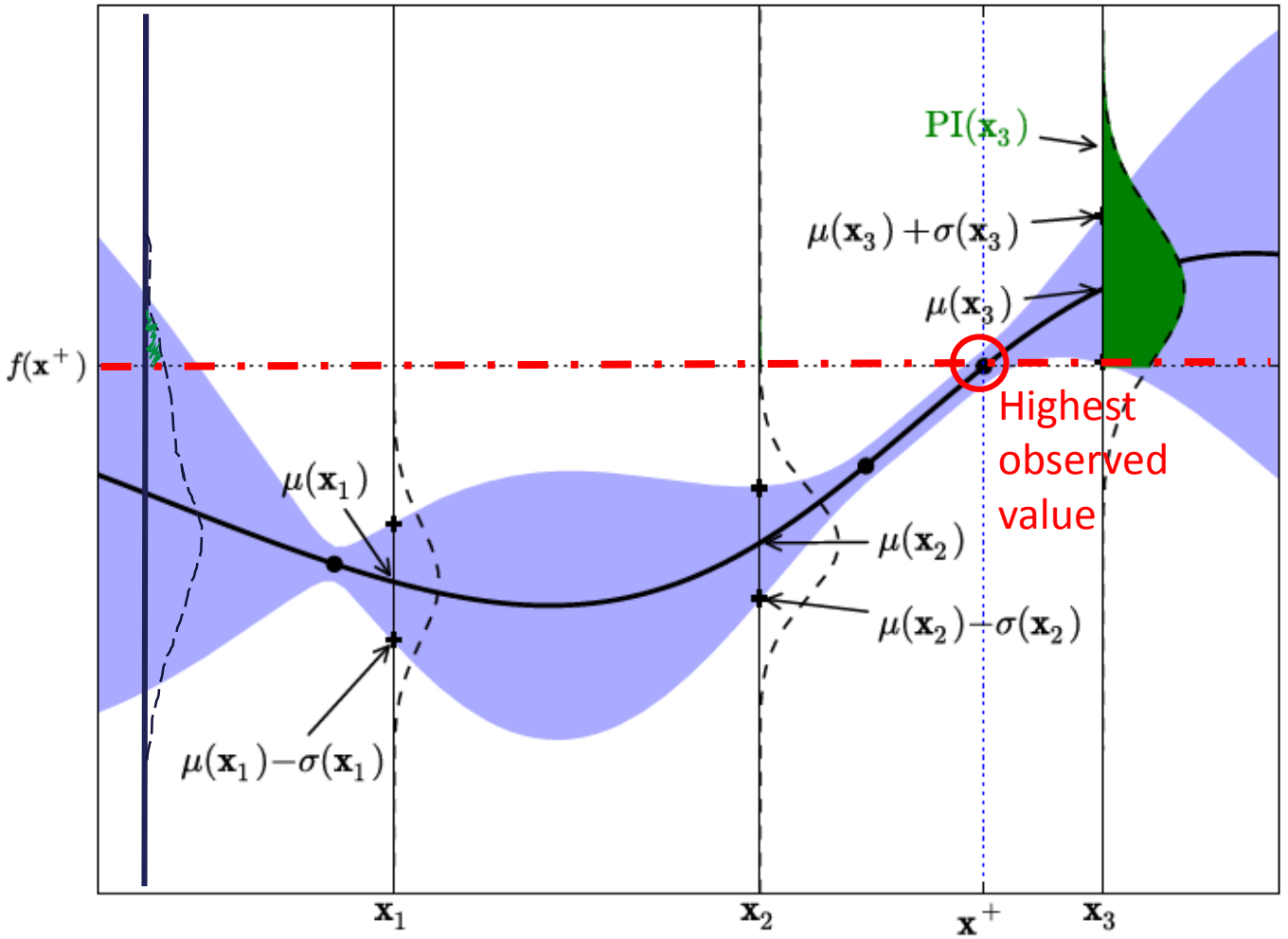


Image taken from Bochu, Cora, de Freitas, 2010

Expected Improvement

$$EI(x) = (f(x) - f(x_{best})) \times \phi \left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right) + \sigma(x) \times \varphi \left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right)$$

Expected Improvement

$$EI(x) = (f(x) - f(x_{best})) \times \phi\left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right) + \sigma(x) \times \varphi\left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right)$$

CDF: cumulative distribution of the standard normal

Certainty

PDF: probability distribution of the standard normal

Expected Improvement

$$EI(x) = (f(x) - f(x_{best})) \times \phi \left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right) + \sigma(x) \times \varphi \left(\frac{\mu(x)-\mu(x_{best})}{\sigma(x)}\right)$$

EI is big if:

The absolute improvement is big

The certainty on the improvement is big

The uncertainty (variance) is big

Lower confidence bound

- LCB(x) = $\mu(x) - \alpha\,\sigma(x)$
- UCB(x) = $\mu(x) + \alpha\,\sigma(x)$

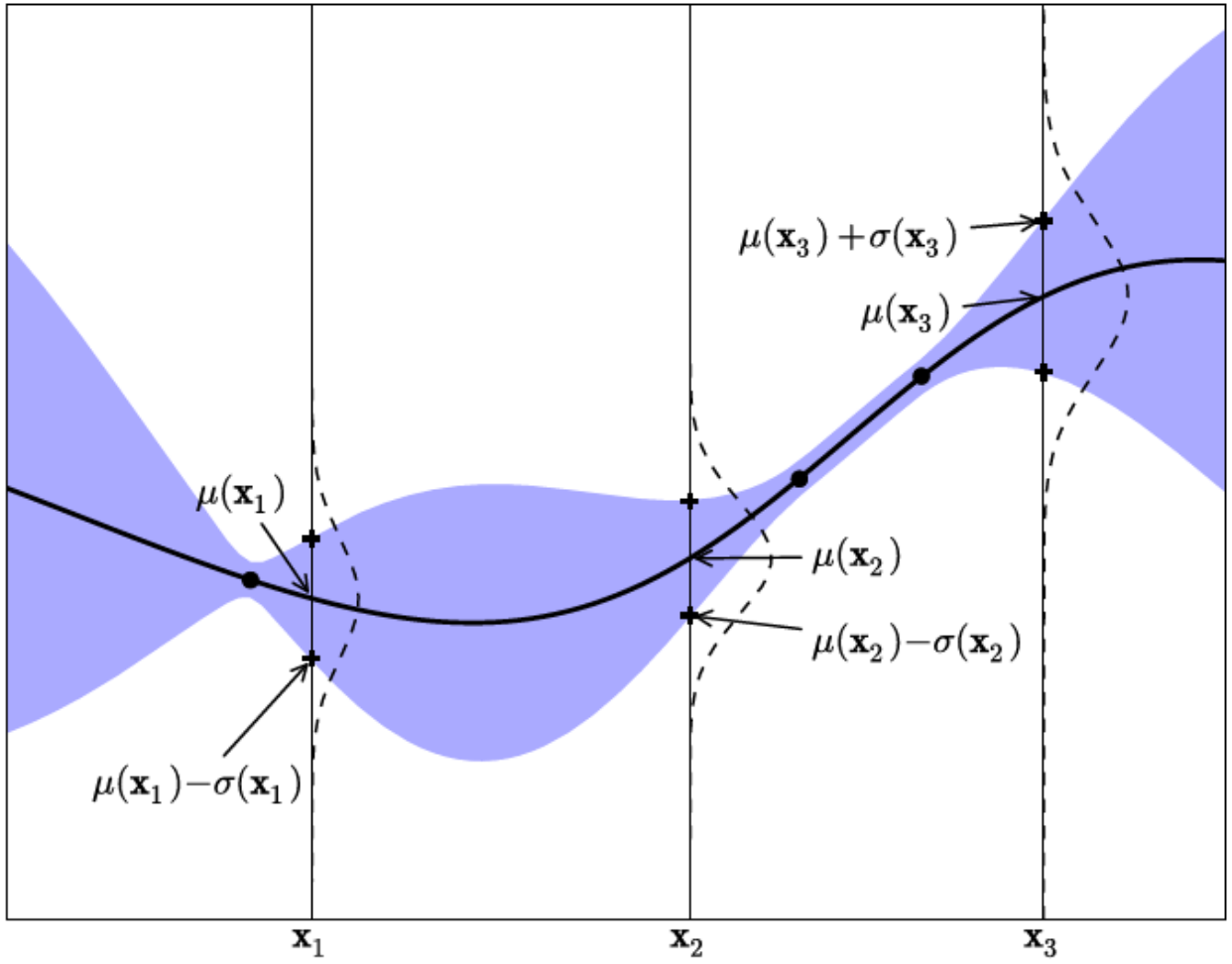


Image taken from Bochu, Cora, de Freitas, 2010

Lower confidence bound

- LCB(x) = $\mu(x) - \alpha\, \sigma(x)$
- UCB(x) = $\mu(x) + \alpha\, \sigma(x)$

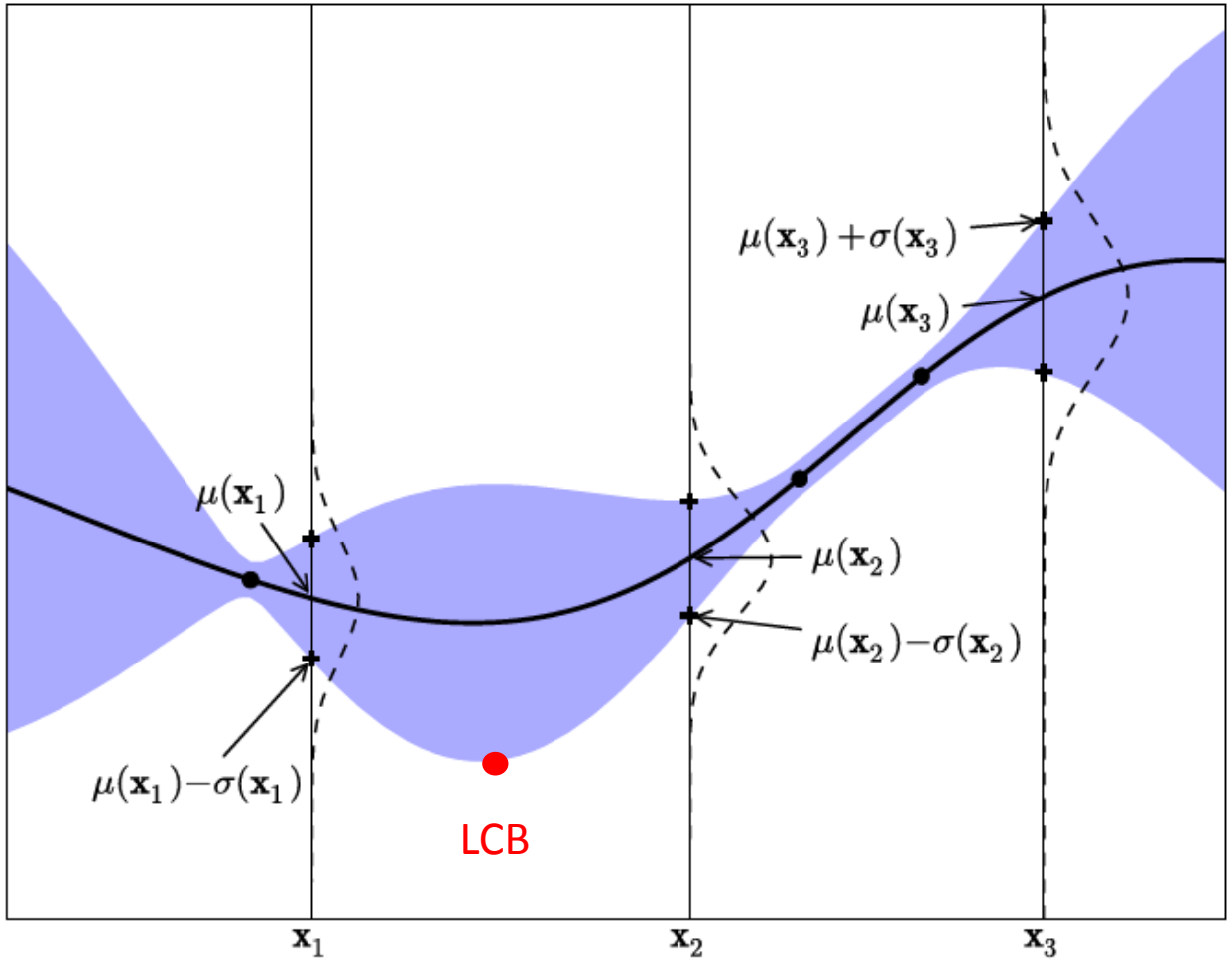


Image taken from Bochu, Cora, de Freitas, 2010

Upper confidence bound

- LCB(x) = $\mu(x) - \alpha\,\sigma(x)$
- UCB(x) = $\mu(x) + \alpha\,\sigma(x)$

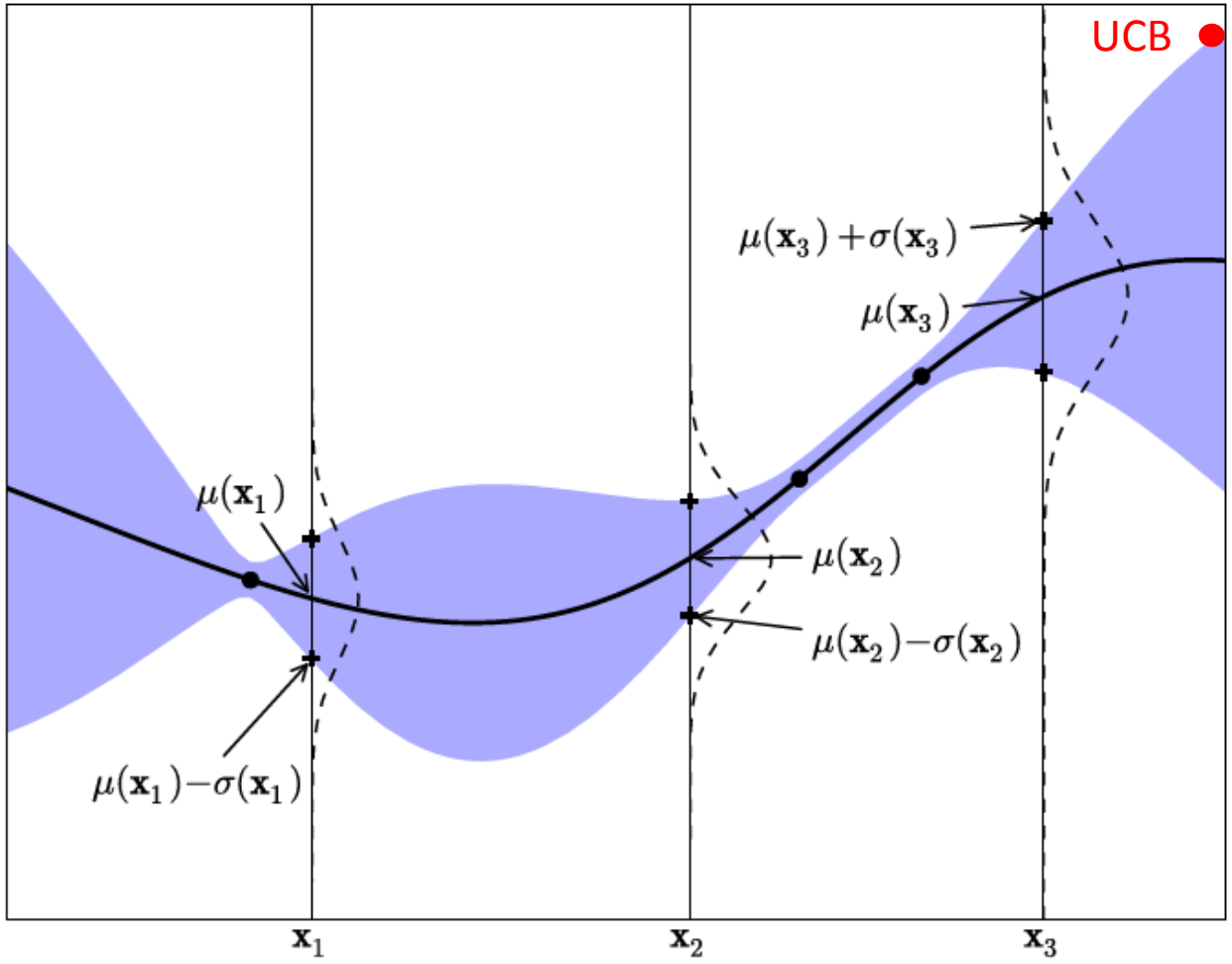


Image taken from Bochu, Cora, de Freitas, 2010

Comparison

- PI is high where P(f(x) > max(μ)) is high
- EI is high where improvement is high with high certainty and variance is high
- UCB is high when variance is high

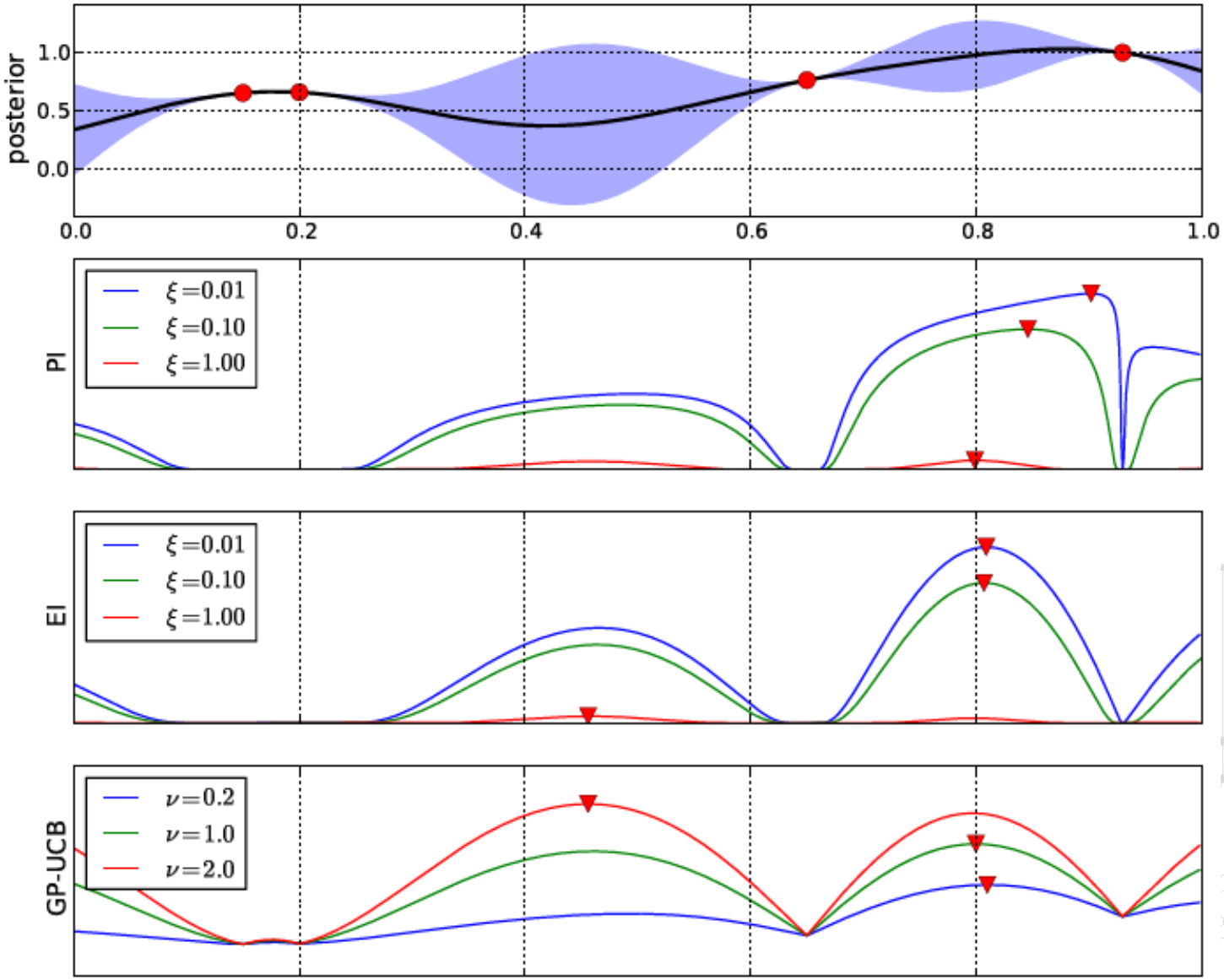


Image taken from Bochu, Cora, de Freitas, 2010

Train In Data

THANK YOU

www.trainindata.com