Lecture 23: Bayesian global optimization

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Quantifying epistemic uncertainty in the location and value of maximum

PREDICTIVE SCIENCE LABORATORY

Derivation of epistemic uncertainty on location and value of maximum

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

$$\rightarrow f(\cdot) \sim GP(m(\cdot), c(\cdot, \cdot)) \Rightarrow f(\cdot) \mid x_{1:n}, y_{1:n} \sim GP(m_n^*(\cdot), c_n^*(\cdot, \cdot))$$

post. state of knowledge about functions

$$\hat{X} = \underset{x}{\arg\max} f(x) \quad \text{r.v.}$$

$$\hat{F} = f(\hat{X}) \quad \text{r.v.}$$

$$p(\hat{x}, \hat{f} \mid x_{1:n}, y_{1:n}) = \int \delta(\hat{x} - \underset{x}{\arg\max} f(x)) \delta(\hat{f} - \underset{x}{\max} f(x)) p(f(\cdot) \mid x_{1:n}, y_{1:n}) df(\cdot)$$

$$x_1^*, \ldots, x_{n^*}^* \ , \quad \hat{X}_{n^*} = \underset{1 \leq i \leq n^*}{\arg\max} f(x_i^*)$$

$$\hat{F}_{n^*} = f(\hat{X}_{n^*})$$

Example: Epistemic Uncertainty in Maximum and Its Location