

Lecture 23: Bayesian global optimization

Professor Ilias Bilonis

**Quantifying epistemic uncertainty in
the location and value of maximum**

Derivation of epistemic uncertainty on location and value of maximum

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

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

posterior GP

Post. state of knowledge about functions

stochastic process

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

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

$$p(\hat{X}, \hat{F} | x_{1:n}, y_{1:n}) = \int \delta(\hat{X} - \arg \max_x f(x)) \delta(\hat{F} - \max_x f(x)) p(f(\cdot) | x_{1:n}, y_{1:n}) df(\cdot)$$

discretize

$$x_1^*, \dots, x_n^*, \quad \hat{X}_{n^*} = \arg \max_{1 \leq i \leq n^*} f(x_i^*)$$

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

Example: Epistemic Uncertainty in Maximum and Its Location

Done by sampling from the posterior Gaussian Process

