

Constrained BO Definition

$$x^* = \arg \max_{x \in \mathcal{X}} f(x) \quad \text{s.t.} \quad c_k(x) \leq 0, \quad k = 1, \dots, K.$$

Both the objective $f(x)$ and the constraints $c_k(x)$ are modeled as independent Gaussian Processes (GPs). At iteration n , their posteriors are described by their respective means and variances:

$\mu_y^n(x), \sigma_y^n(x)$ for the objective, and $\mu_{c_k}^n(x), \sigma_{c_k}^n(x)$ for each constraint.

Probability of Feasibility (PF)

The **probability of feasibility** for a candidate design x is defined as the probability that all constraints are satisfied under the current GP models:

$$\text{PF}^n(x) = \prod_{k=1}^K P(c_k(x) \leq 0) = \prod_{k=1}^K \Phi\left(-\frac{\mu_{c_k}^n(x)}{\sigma_{c_k}^n(x)}\right),$$

The **penalized posterior mean**— the GP mean of the objective scaled by the probability of feasibility:

$$x_r^n = \arg \max_{x \in \mathcal{X}} \mu_y^n(x) \text{PF}^n(x).$$