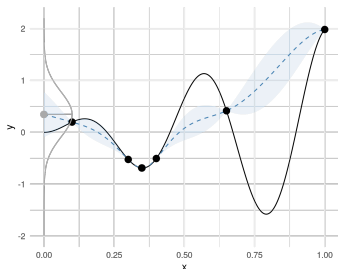


Optimization in Machine Learning

Bayesian Optimization: Posterior Uncertainty and Acquisition Functions I



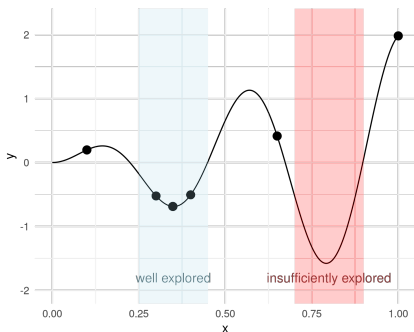
Learning goals

- Bayesian surrogate modeling
- Acquisition functions
- Lower confidence bound

BAYESIAN SURROGATE MODELING

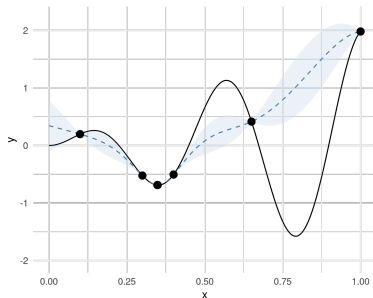
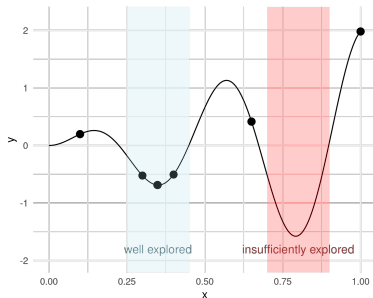
Goal:

Find trade-off between **exploration** (areas we have not visited yet) and **exploitation** (search around good design points)



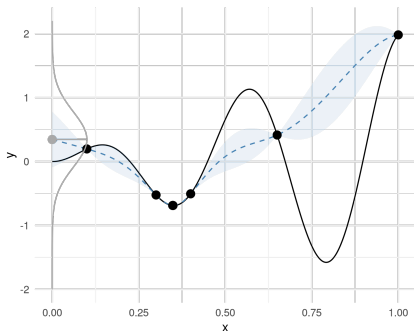
BAYESIAN SURROGATE MODELING

- **Idea:** Use a **Bayesian approach** to build SM that yields estimates for the posterior mean $\hat{f}(\mathbf{x})$ and the posterior variance $\hat{s}^2(\mathbf{x})$
- $\hat{s}^2(\mathbf{x})$ expresses “confidence”/“certainty” in prediction



BAYESIAN SURROGATE MODELING

- Denote by $Y \mid \mathbf{x}, \mathcal{D}^{[t]}$ the (conditional) RV associated with the posterior predictive distribution of a new point \mathbf{x} under a SM; will abbreviate it as $Y(\mathbf{x})$
- Most prominent choice for a SM is a **Gaussian process**, here $Y(\mathbf{x}) \sim \mathcal{N}(\hat{f}(\mathbf{x}), \hat{s}^2(\mathbf{x}))$

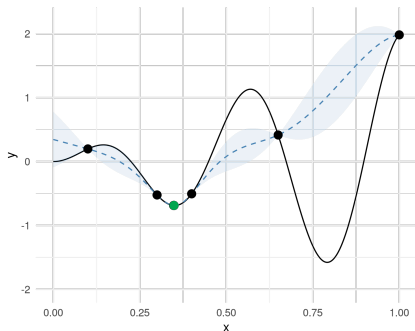


For now we assume an interpolating SM; $\hat{f}(\mathbf{x}) = f(\mathbf{x})$ and $\hat{s}(\mathbf{x}) = 0$ for training points

ACQUISITION FUNCTIONS

To sequentially propose new points based on the SM, we make use of so-called acquisition functions $a : \mathcal{S} \rightarrow \mathbb{R}$

Let $f_{\min} := \min \{f(\mathbf{x}^{[1]}), \dots, f(\mathbf{x}^{[t]})\}$ denote the best observed value so far (visualized in green - we will need this later!)



In the examples before we simply used the posterior mean $a(\mathbf{x}) = \hat{f}(\mathbf{x})$ as acquisition function - ignoring uncertainty

LOWER CONFIDENCE BOUND

Goal: Find $\mathbf{x}^{[t+1]}$ that minimizes the **Lower Confidence Bound** (LCB):

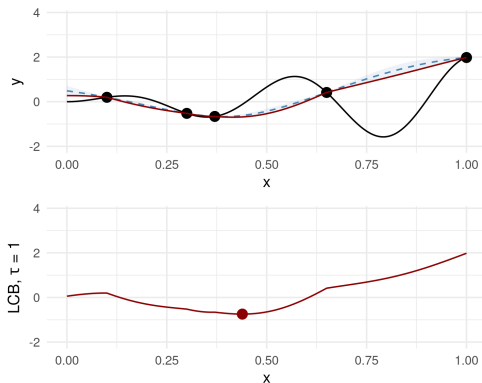
$$a_{\text{LCB}}(\mathbf{x}) = \hat{f}(\mathbf{x}) - \tau \hat{s}(\mathbf{x})$$

where $\tau > 0$ is a constant that controls the “mean vs. uncertainty” trade-off

The LCB is conceptually very simple and does **not** rely on distributional assumptions of the posterior predictive distribution under a SM

LOWER CONFIDENCE BOUND

$$\tau = 1$$

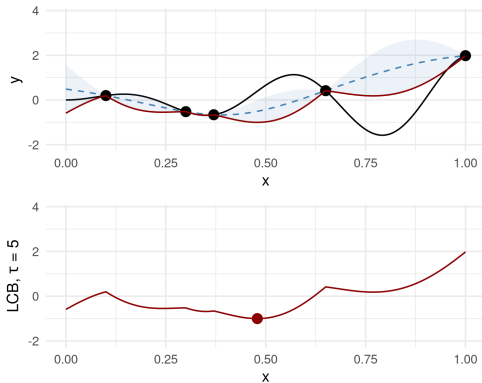


Top: Design points and SM showing $\hat{f}(x)$ (blue) and $\hat{f}(x) - \tau \hat{s}(x)$ (red)

Bottom: the red point depicts $\arg \min_{x \in \mathcal{S}} a_{LCB}(x)$

LOWER CONFIDENCE BOUND

$$\tau = 5$$



LOWER CONFIDENCE BOUND

$\tau = 10$

