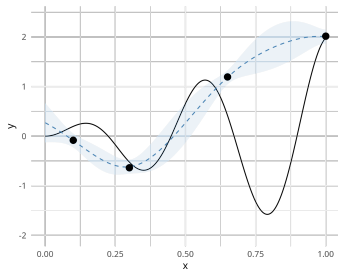


Optimization in Machine Learning

Bayesian Optimization

Noisy Bayesian Optimization



Learning goals

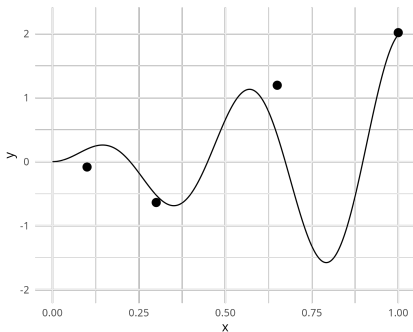
- Noisy surrogate modeling
- Noisy acquisition functions
- Final best point

NOISY EVALUATIONS

In many real-life applications, we cannot access the true function values $f(\mathbf{x})$ but only a **noisy** version thereof

$$f(\mathbf{x}) + \epsilon(\mathbf{x})$$

For the sake of simplicity, we assume $\epsilon(\mathbf{x}) \sim \mathcal{N}(0, \sigma_\epsilon^2)$ for now



NOISY EVALUATIONS

In many real-life applications, we cannot access the true function values $f(\mathbf{x})$ but only a **noisy** version thereof

$$f(\mathbf{x}) + \epsilon(\mathbf{x})$$

For the sake of simplicity, we assume $\epsilon(\mathbf{x}) \sim \mathcal{N}(0, \sigma_\epsilon^2)$ for now



Examples:

- HPO (due to non-deterministic learning algorithm and/or resampling technique)
- Oil drilling optimization (an oil sample is only an estimate)
- Robot gait optimization (velocity of a run of a robot is an estimate of true velocity)

NOISY EVALUATIONS

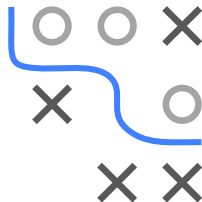
This raises the following problems:

- **Surrogate modeling:** So far we used an interpolating GP that is based on noise-free observations; as a consequence, the variance is modeled as 0

$$s^2(\mathbf{x}^{[i]}) = 0$$

for design points $(\mathbf{x}^{[i]}, y^{[i]}) \in \mathcal{D}^{[t]}$. This is problematic.

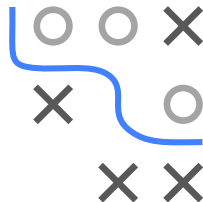
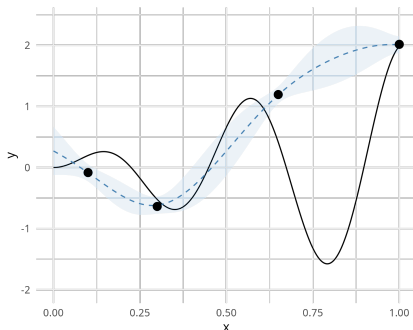
- **Acquisition functions:** Most acquisition functions are based on the best observed value f_{\min} so far. If evaluations are noisy, we do not know this value (it is a random variable).
- **Final best point:** The design point evaluated best is not necessarily the true best point in design (overestimation).



SURROGATE MODEL

In case of noisy evaluations, a nugget-effect GP (GP regression) should be used instead of an interpolating GP.

The posterior predictive distribution for a new test point $\mathbf{x} \in \mathcal{S}$ under a GP assuming homoscedastic noise (σ_ϵ^2) is:



$$Y(\mathbf{x}) \mid \mathbf{x}, \mathcal{D}^{[t]} \sim \mathcal{N}(\hat{f}(\mathbf{x}), \hat{s}^2(\mathbf{x}))$$

with

$$\begin{aligned}\hat{f}(\mathbf{x}) &= k(\mathbf{x})^\top (\mathbf{K} + \sigma_\epsilon^2 \mathbf{I}_t)^{-1} \mathbf{y} \\ \hat{s}^2(\mathbf{x}) &= k(\mathbf{x}, \mathbf{x}) - k(\mathbf{x})^\top (\mathbf{K} + \sigma_\epsilon^2 \mathbf{I}_t)^{-1} k(\mathbf{x})\end{aligned}$$

NOISY ACQUISITION FUNCTIONS: AEI

Augmented Expected Improvement (*Huang et al., 2006*)

$$a_{\text{AEI}}(\mathbf{x}) = a_{\text{EI}_{f_{\min_*}}}(\mathbf{x}) \left(1 - \frac{\sigma_\epsilon}{\sqrt{\hat{S}^2(\mathbf{x}) + \sigma_\epsilon^2}} \right).$$

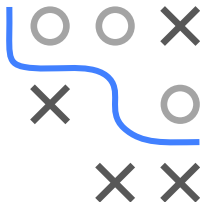
Here, $a_{\text{EI}_{f_{\min_*}}}$ denotes the **Expected Improvement with Plugin**.

It uses the **effective best solution** as a plugin for the (unknown) best observed value f_{\min}

$$f_{\min_*} = \min_{\mathbf{x} \in \{\mathbf{x}^{[1]}, \dots, \mathbf{x}^{[t]}\}} \hat{f}(\mathbf{x}) + c\hat{S}(\mathbf{x}),$$

where $c > 0$ is a constant that controls the risk aversion.

σ_ϵ^2 is the nugget-effect as estimated by the GP regression.



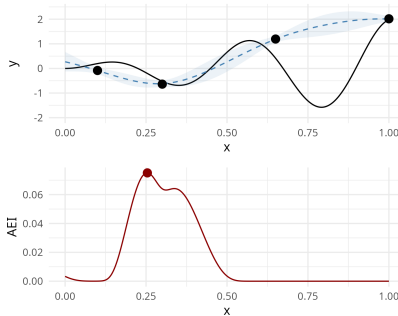
NOISY ACQUISITION FUNCTIONS: AEI / 2

In addition, it takes into account the nugget-effect σ_ϵ^2 by a penalty term:

$$\left(1 - \frac{\sigma_\epsilon}{\sqrt{\hat{s}^2(\mathbf{x}) + \sigma_\epsilon^2}}\right)$$

The penalty is justified to “account for the diminishing return of additional replicates as the predictions become more accurate”
(*Huang et al., 2006*)

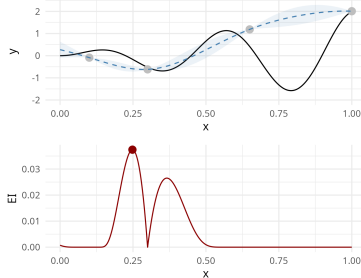
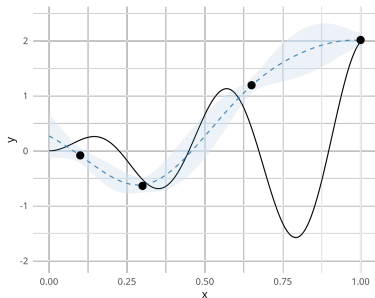
- Designs with small predictive variance $\hat{s}^2(\mathbf{x})$ are penalized in favor of more exploration.
- If $\sigma_\epsilon^2 = 0$ (noise-free), the AEI corresponds to the EI with plugin.



REINTERPOLATION

Algorithm Reinterpolation Procedure

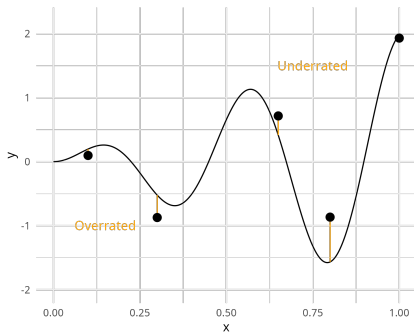
- 1: Build a nugget-effect GP model based on noisy evaluations
- 2: Compute predictions for all points in the design $\hat{f}(\mathbf{x}^{[1]}), \dots, \hat{f}(\mathbf{x}^{[l]})$
- 3: Train an interpolating GP on $\left\{ \left(\mathbf{x}^{[1]}, \hat{f}(\mathbf{x}^{[1]}) \right), \dots, \left(\mathbf{x}^{[l]}, \hat{f}(\mathbf{x}^{[l]}) \right) \right\}$
- 4: Based on the interpolating model, obtain a new candidate using a noise-free acquisition function



IDENTIFICATION OF FINAL BEST POINT

Another problem is the identification of a final best point:

- Assume that all evaluations are noisy
- The probability is high that **by chance**
 - bad points get overrated
 - good points get overlooked



IDENTIFICATION OF FINAL BEST POINT / 2

Possibilities to reduce the risk of falsely returning a bad point:

- Return the best predicted point: $\arg \min_{\mathbf{x} \in \{\mathbf{x}^{[1]}, \dots, \mathbf{x}^{[t]}\}} \hat{f}(\mathbf{x})$
- Repeated evaluations of the final point: infer guarantees about final point (however if final point is “bad” unclear how to find a better one)
- Repeated evaluations of all design points: reduce noise during optimization and risk of falsely returning a bad point
- More advanced replication strategies, e.g. incumbent strategies: also re-evaluate the “incumbent” in each iteration

