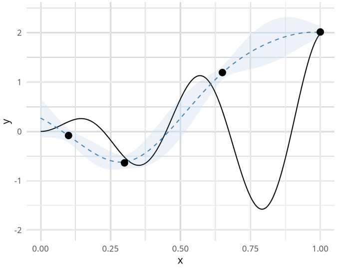
Optimization in Machine Learning

Bayesian Optimization
Noisy Bayesian Optimization



Learning goals

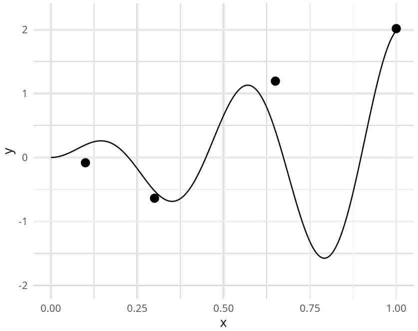
- Noisy surrogate modeling
- Noisy acquisition functions
- Final best point

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 $\epsilon(\mathbf{x}) \sim \mathcal{N}\left(0, \sigma_\epsilon^2\right)$ for now



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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

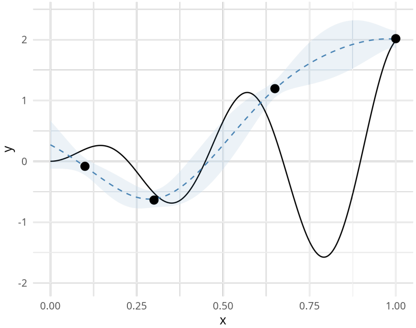
This raises the following problems:

- **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:



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

with

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

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 $f_{\min}$

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

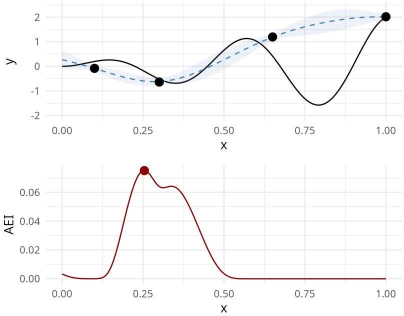
where $c > 0$ is a constant that controls the risk aversion.

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:

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



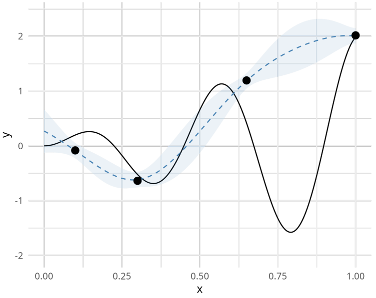
The penalty is justified to "account for the diminishing return of additional replicates as the predictions become more accurate" (*Huang et al., 2006*)

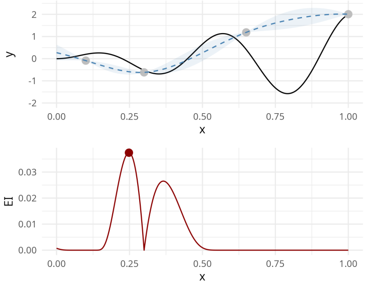
- Designs with small predictive variance $\hat{s}^2(\mathbf{x})$ are penalized in favor of more exploration.
- If $\sigma_\epsilon^2 = 0$ (noise-free), the AEI corresponds to the EI with plugin.

REINTERPOLATION

Clean noise from the model and then apply a general acquisition function (EI, PI, LCB, ...)

The RP suggests to build **two models**: a nugget-effect GP (regression model; left) and then, on the predictions from the first model (grey), an interpolating GP (right)

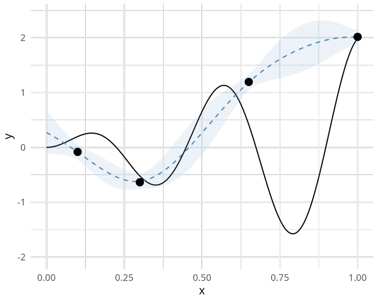


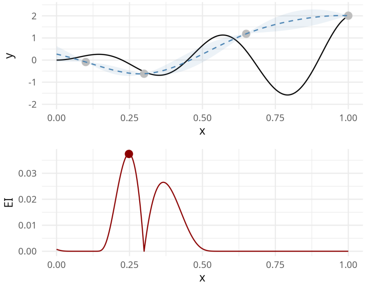


REINTERPOLATION

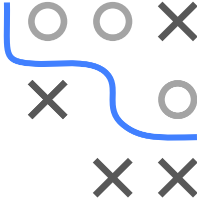
Algorithm Reinterpolation Procedure

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



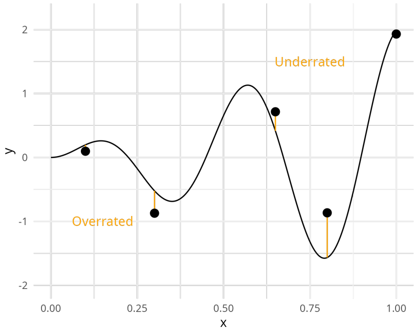


IDENTIFICATION OF FINAL BEST POINT



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