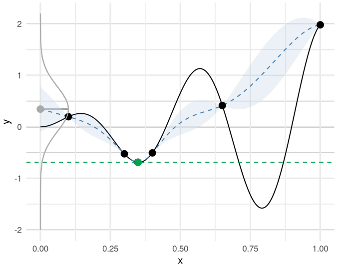
Optimization in Machine Learning

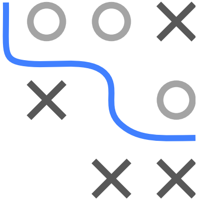
Bayesian Optimization
Posterior Uncertainty and Acquisition Functions II



Learning goals

- Probability of improvement
- Expected improvement

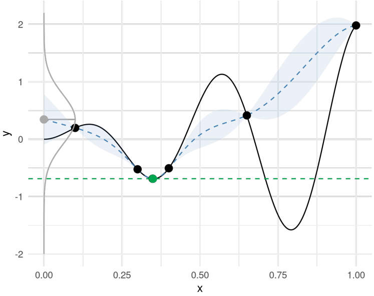
PROBABILITY OF IMPROVEMENT

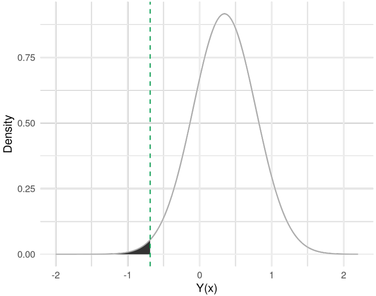


Goal: Find $\mathbf{x}^{[t+1]}$ that maximizes the **Probability of Improvement** (PI):

$$a_{\text{PI}}(\mathbf{x}) = \mathbb{P}(Y(\mathbf{x}) < f_{\min}) = \Phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right)$$

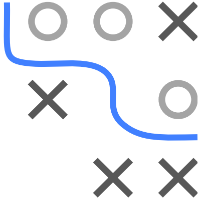
where $\Phi(\cdot)$ is the standard normal cdf (assuming Gaussian posterior)





Left: The green vertical line represents $f_{\min}$. **Right:** $a_{\text{PI}}(\mathbf{x})$ is given by the black area.

PROBABILITY OF IMPROVEMENT



Goal: Find $\mathbf{x}^{[t+1]}$ that maximizes the **Probability of Improvement** (PI):

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where $\Phi(\cdot)$ is the standard normal cdf (assuming Gaussian posterior)

Note: $a_{\text{PI}}(\mathbf{x}) = 0$ for design points $\mathbf{x}$, since

- $\hat{s}(\mathbf{x}) = 0$,
- $\hat{f}(\mathbf{x}) = f(\mathbf{x}) \geq f_{\min} \quad \Leftrightarrow \quad f_{\min} - \hat{f}(\mathbf{x}) \leq 0$.

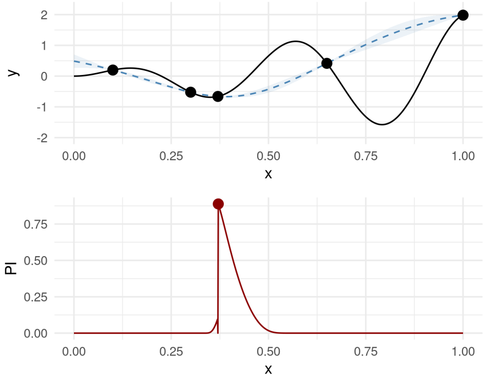
Therefore:

$$\Phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) = \Phi(-\infty) = 0$$

PROBABILITY OF IMPROVEMENT

The PI does not take the size of the improvement into account
Often it will propose points close to the current $f_{\min}$

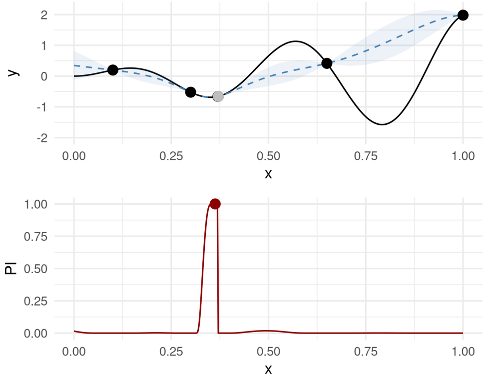
We use the PI (red line) to propose the next point ...



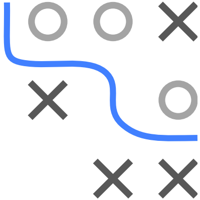
The red point depicts $\arg\max_{\mathbf{x}\in\mathcal{S}} a_{\mathrm{PI}}(\mathbf{x})$

PROBABILITY OF IMPROVEMENT / 2

... evaluate that point, refit the SM and propose the next point



(grey point = prev point from last iter)



PROBABILITY OF IMPROVEMENT

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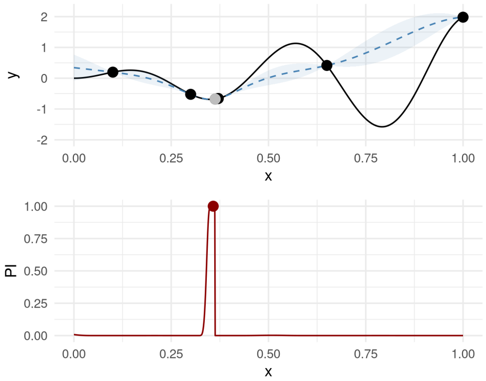
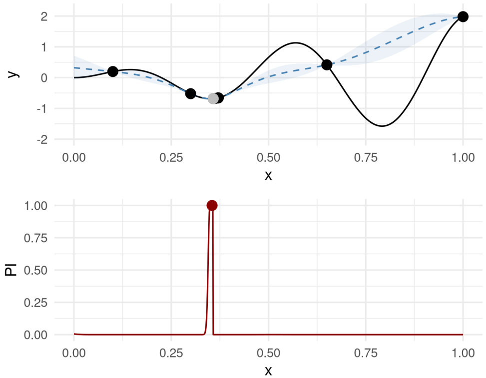


PROBABILITY OF IMPROVEMENT

In our example, using the PI results in spending plenty of time optimizing the local optimum ...



PROBABILITY OF IMPROVEMENT

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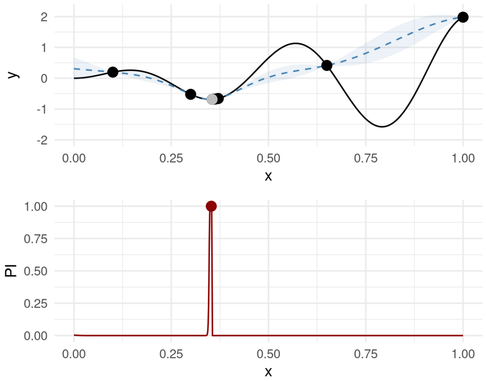

PROBABILITY OF IMPROVEMENT

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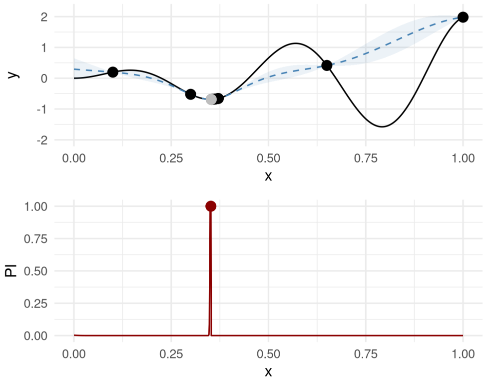

PROBABILITY OF IMPROVEMENT

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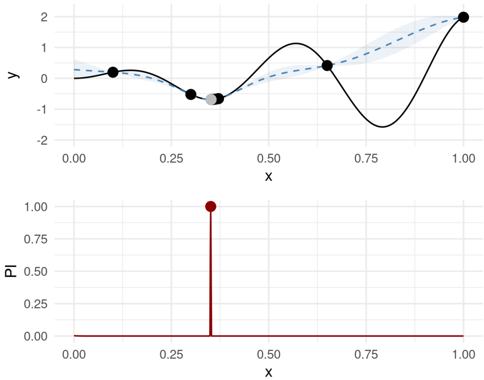
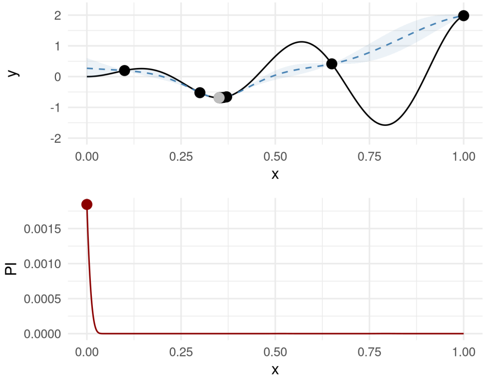
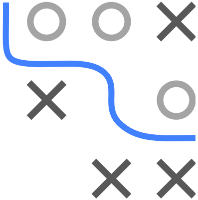


PROBABILITY OF IMPROVEMENT

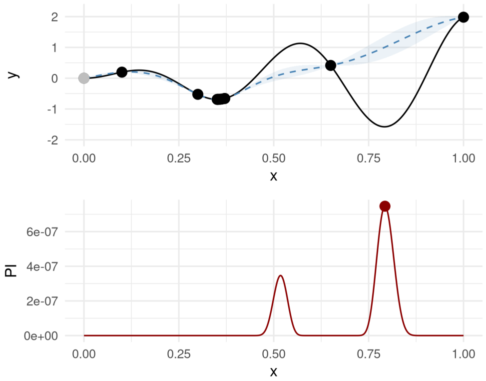
... eventually, we explore other regions ...



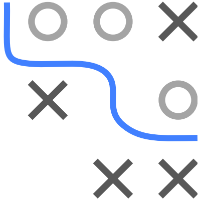


PROBABILITY OF IMPROVEMENT

...

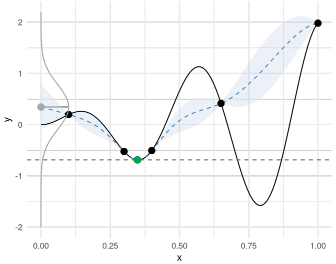


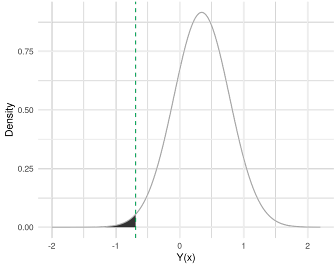
EXPECTED IMPROVEMENT



Goal: Propose $\mathbf{x}^{[t+1]}$ that maximizes the **Expected Improvement** (EI):

$$a_{\mathrm{EI}}(\mathbf{x}) \quad = \quad \mathbb{E}(\max\{f_{\min} - Y(\mathbf{x}), 0\})$$





- We now take the expectation in the tail, instead of the prob as in PI.
- Improvement is always assumed ≥ 0.

EXPECTED IMPROVEMENT

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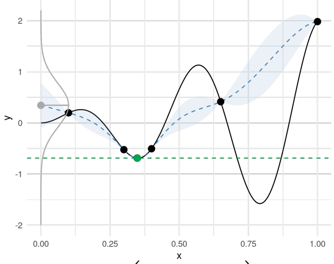
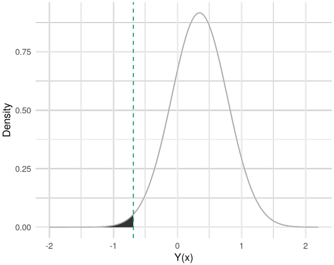




If $Y(\mathbf{x}) \sim \mathcal{N}\left(\hat{f}(\mathbf{x}), \hat{s}^2(\mathbf{x})\right)$, we can express the EI in closed-form as:

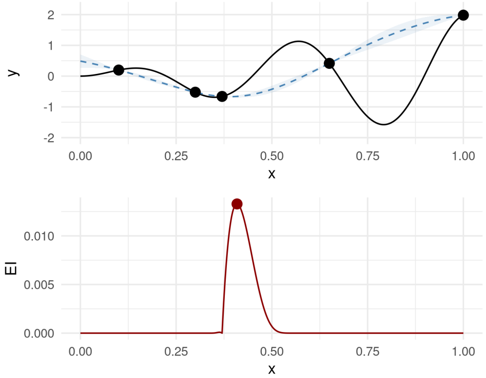
$$a_{\text{EI}}(\mathbf{x}) = (f_{\min} - \hat{f}(\mathbf{x}))\Phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right) + \hat{s}(\mathbf{x})\phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right),$$

- $a_{\text{EI}}(\mathbf{x}) = 0$ at design points $\mathbf{x}$:

$$a_{\text{EI}}(\mathbf{x}) = (f_{\min} - \hat{f}(\mathbf{x}))\underbrace{\Phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right)}_{=0,\text{ see PI}} + \underbrace{\hat{s}(\mathbf{x})}_{=0}\phi\left(\frac{f_{\min} - \hat{f}(\mathbf{x})}{\hat{s}(\mathbf{x})}\right)$$

EXPECTED IMPROVEMENT

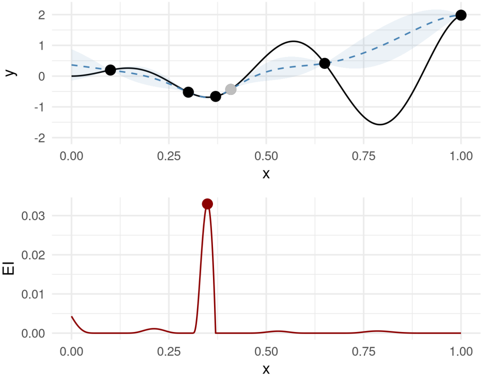
We use the EI (red line) to propose the next point ...



The red point depicts $\arg\max_{\mathbf{x}\in\mathcal{S}} a_{\text{EI}}(\mathbf{x})$

EXPECTED IMPROVEMENT / 2

... evaluate that point, refit the SM and propose the next point



(grey point = prev point from last iter)

EXPECTED IMPROVEMENT

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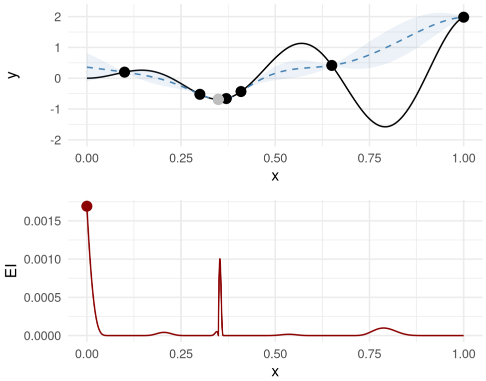

EXPECTED IMPROVEMENT

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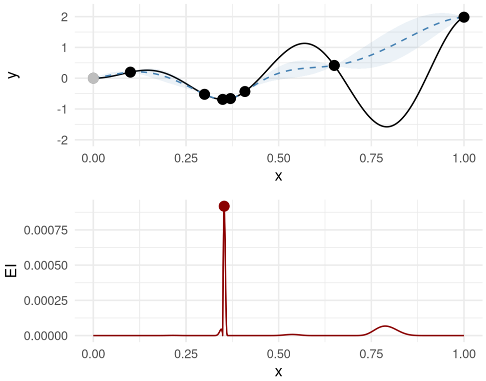

EXPECTED IMPROVEMENT

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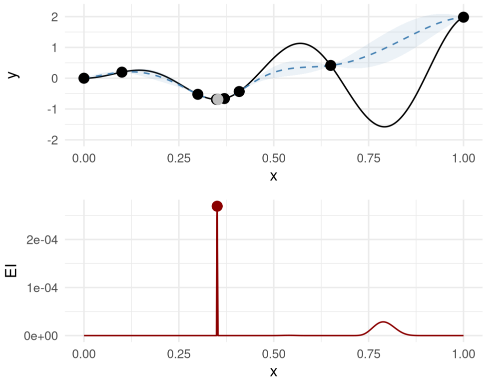
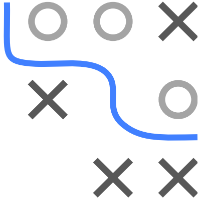
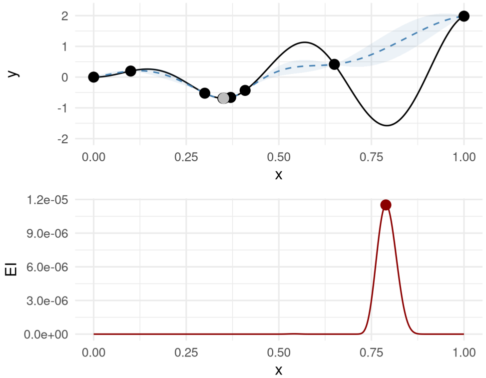




EXPECTED IMPROVEMENT

The EI is capable of exploration and quickly proposes promising points in areas we have not visited yet



Here, also a result of well-calibrated uncertainty $\hat{s}(\mathbf{x})$ of our GP.

DISCUSSION

- Under some mild conditions: BO with a GP as SM and EI is a **global optimizer**, i.e., convergence to the **global** (!) optimum is guaranteed given unlimited budget
- Cannot be proven for the PI or the LCB
- In theory, this suggests choosing the EI as ACQF
- In practice, LCB works quite well, and EI generates a very multi-modal landscape

Other ACQFs:

- Entropy based: Entropy search, predictive entropy search, max value entropy search
- Knowledge Gradient
- Thompson Sampling
- ...