Surrogate Optimization: Expected Improvement

BIOE 498/598 PJ

Spring 2022

Exploration vs. exploitation

There is a fundamental tradeoff in global optimization:

- **Exploration** searches areas of high uncertainty to find *new* regions of interest.
- **Exploitation** refines existing optima by adding points to *known* regions of interest.

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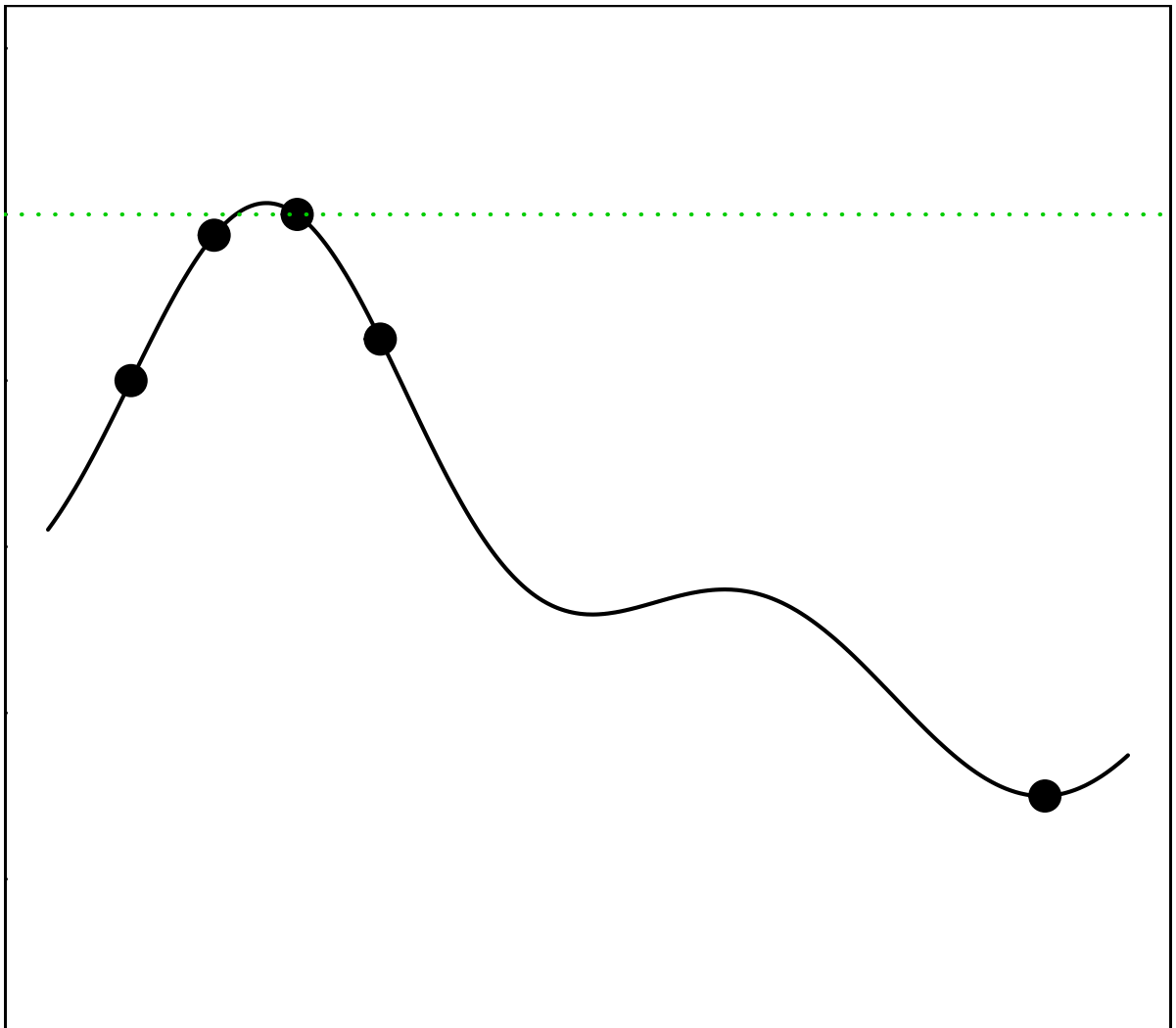
Should we explore or exploit?

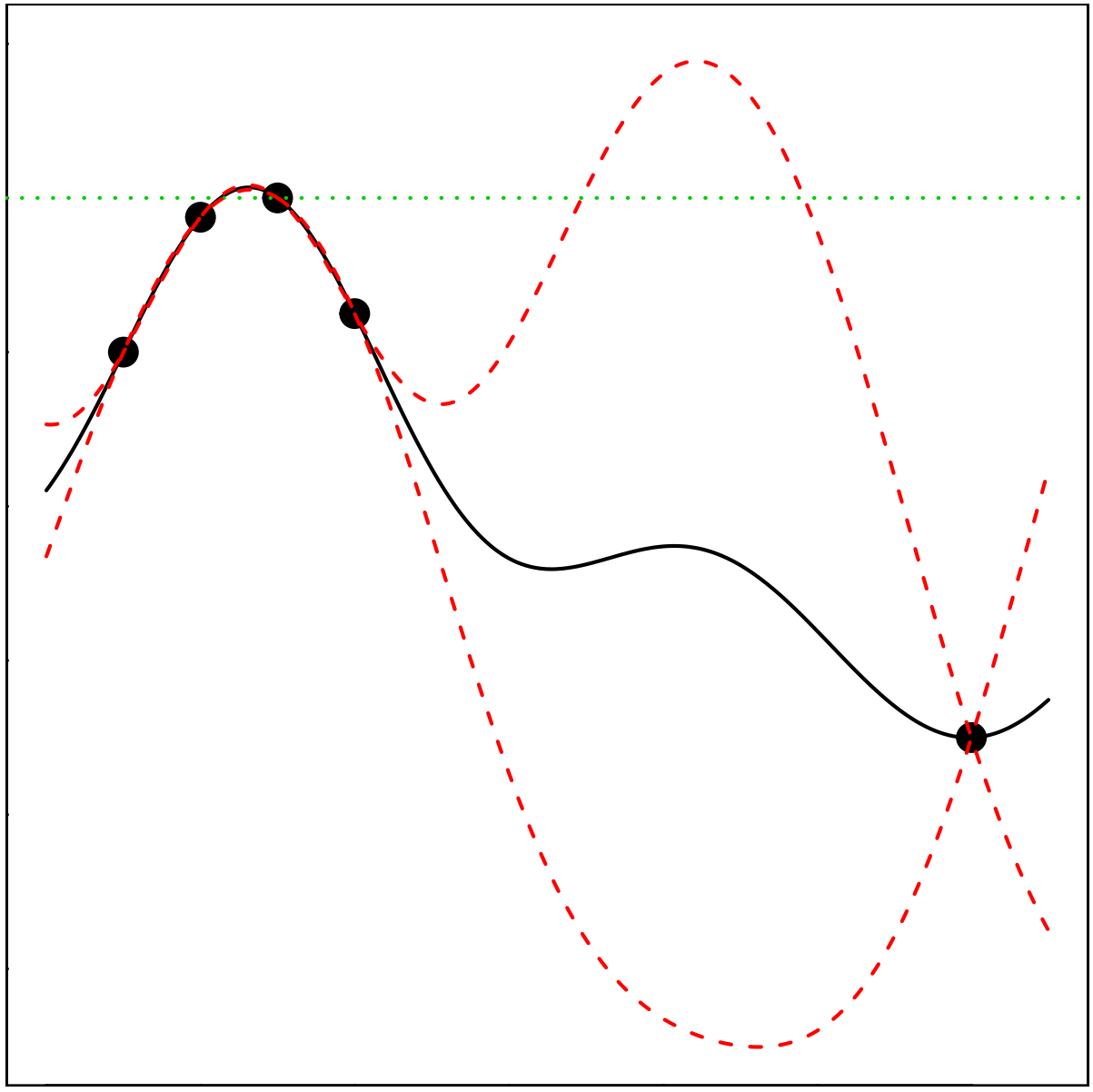
- **Both.** Good algorithms balance discovery and refinement.
- The *best* balance is an open problem. Some solutions:
  - Always explore some (small) percent of the time.
  - Explore early, exploit later.
  - Alternate between batches of exploration and exploitation.
  - **Today:** Combine exploration and exploitation into a single metric.

A 1-D example (Gramacy 2020)

```
Xn <- c(1, 2, 3, 4, 12)
yn <- c(0, 1.75, 2, 0.5, -5)
gp <- newGP(matrix(Xn, ncol=1), yn, d=10, g=1e-8)
X <- seq(0, 13, length=1000)
p <- predGP(gp, matrix(X, ncol=1), lite=TRUE)
```



What happens when we consider uncertainty?



Optimizing for objective improvement

A key insight in Bayesian optimization was the switch to *expected improvement* (Schonlau 1997).

As usual, assume we've measured n responses y_n at locations X_n. Define

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The *expected improvement* $\mathrm{EI}(x) = \mathbb{E}\{I(x)\}$ quantifies how much we expect the best objective value to increase after measuring at point x.

Expected Improvement

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We can sample $y(x)$ many times, averaging the improvement $I(x)$ for T samples:

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Even better, we can leverage that GPR predictions are multivariate normal with mean $\mu(x)$ and variance $\sigma(x)$. Let $z = (\mu(x) - y_{\max})/\sigma(x)$. Then

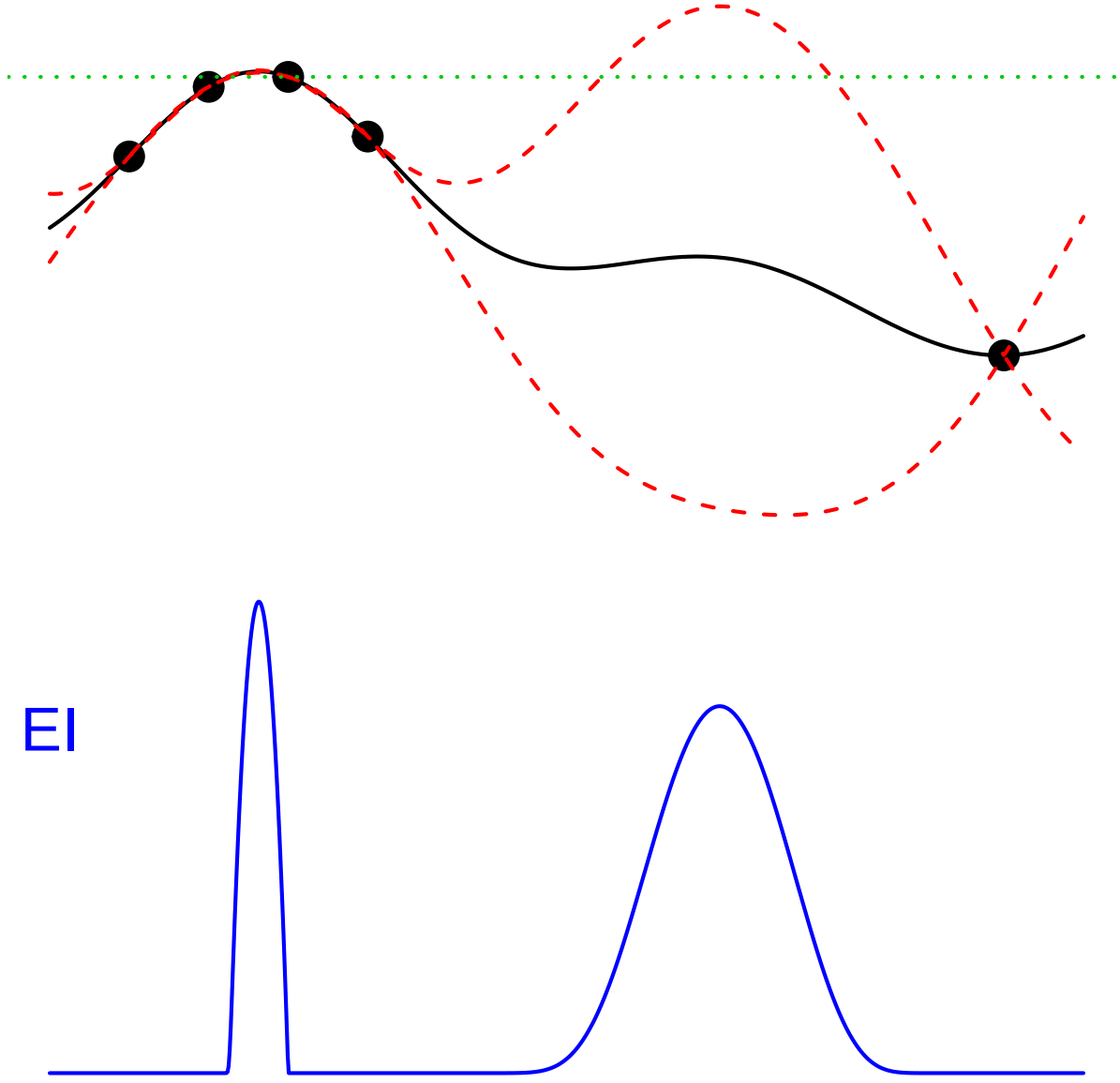
$$\mathrm{EI}(x) = (\mu(x) - y_{\max})\mathrm{CDF}(z) + \sigma(x)\mathrm{PDF}(z)$$

using the PDF and CDF of a standard Gaussian distribution.

Calculating EI

```
argmax <- which.max(yn)
ymax <- yn[argmax]
z <- (p$mean - ymax)/sqrt(p$s2)
ei <- (p$mean - ymax)*pnorm(z) + sqrt(p$s2)*dnorm(z)
```

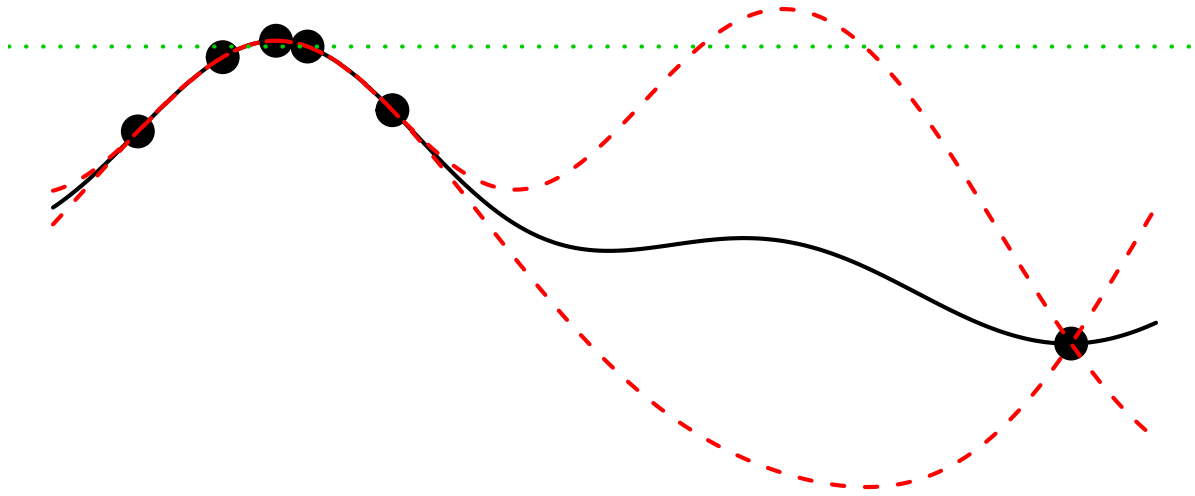
Calculating EI



Picking the next sample x

```
argmaxEI <- which.max(ei)
Xn <- c(Xn, X[argmaxEI])
yn <- c(yn, p$mean[argmaxEI])

updateGP(gp, matrix(X[argmaxEI], ncol=1), p$mean[argmaxEI])
p <- predGP(gp, matrix(X, ncol=1), lite=TRUE)
```



Calculating EI (round 2)

```
argmax <- which.max(yn)
ymax <- yn[argmax]
z <- (p$mean - ymax)/sqrt(p$s2)
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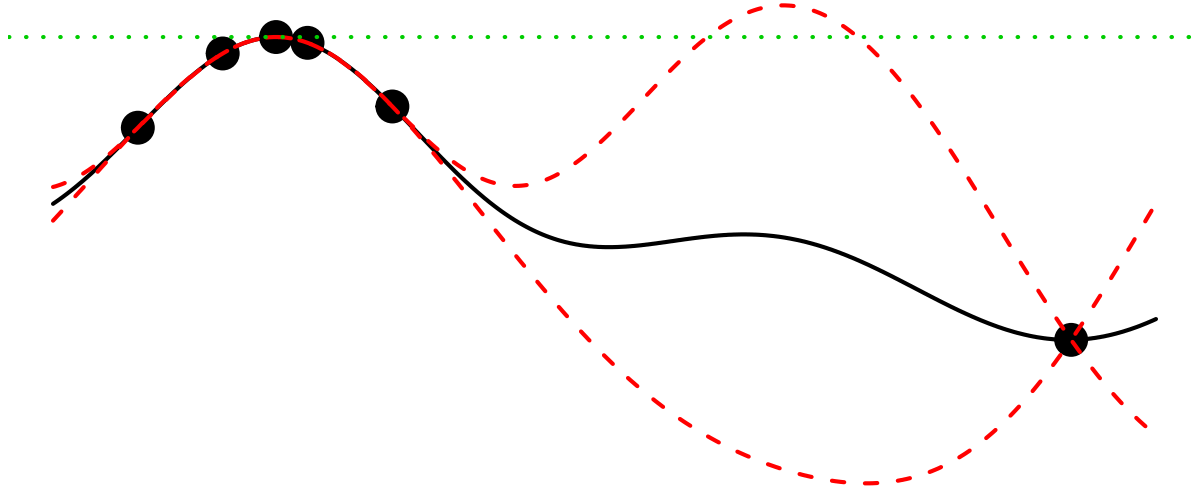
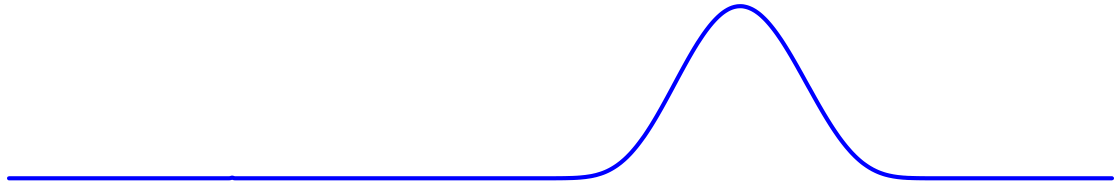


EI

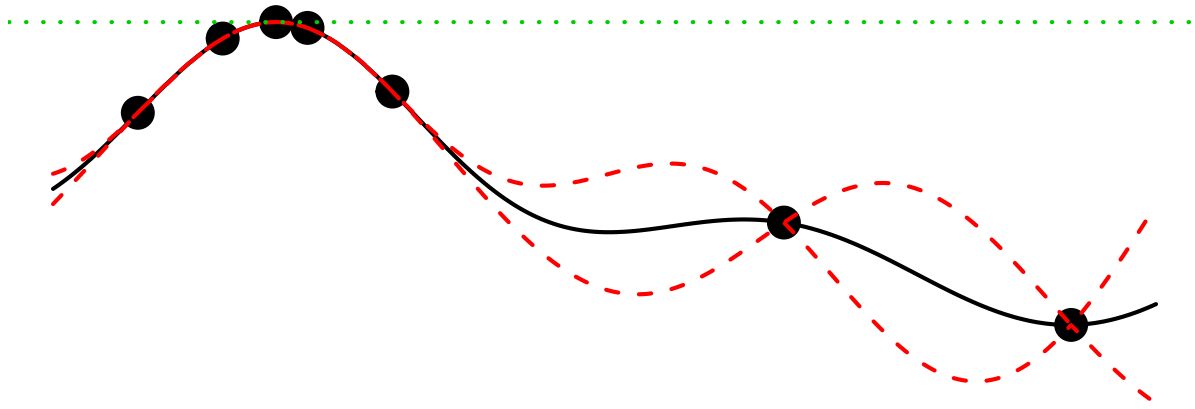


Picking the next sample x (round 2)

```
argmaxEI <- which.max(ei)
Xn <- c(Xn, X[argmaxEI])
yn <- c(yn, p$mean[argmaxEI])

updateGP(gp, matrix(X[argmaxEI], ncol=1), p$mean[argmaxEI])
p <- predGP(gp, matrix(X, ncol=1), lite=TRUE)
```

After the second update



EI

The complete GPR surrogate optimization framework

To maximize the response y of an unknown function f using no more than N function evaluations:

1. Create a space-filling design X_n for $n < N$.
2. Measure the responses $y_n(X_n)$ and train $\mathcal{GP}(X_n, y_n)$.
3. Use a nonlinear optimizer (`optim`) to find the argmax x of a metric (mean, SD, EI).
4. Measure $y(x)$ and update $\mathcal{GP}(X_{n+1}, y_{n+1})$.
5. Go to #3 and repeat until all N runs are used.
6. Search $\mathcal{GP}(X_N, y_N)$ for the global maximum $y^*(x^*)$.

Does sequential design always work?

- Sequential design methods are **last sample optimal**.
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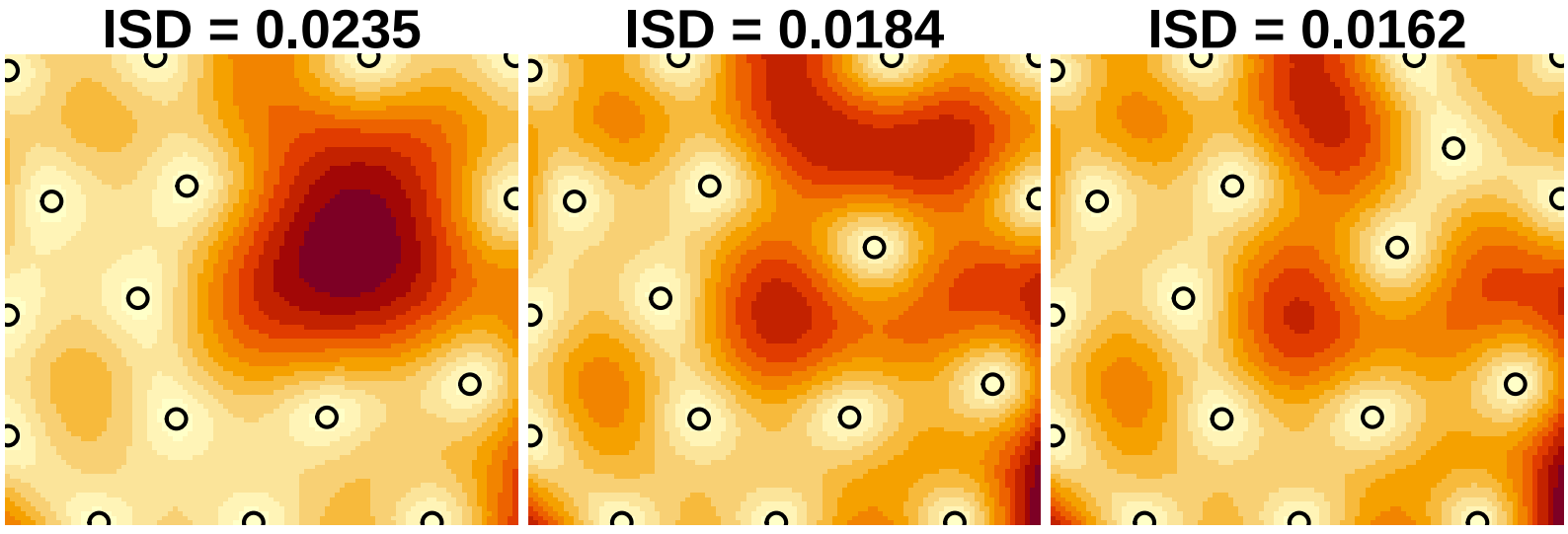
- Sequential design methods are **last sample optimal**.
- After $N-1$ runs, sequential design finds the optimal location for the last run.
- However, sequential design is *greedy*. If $N-2$ of N runs are finished, two rounds of sequential design may not be optimal.

Limited lookahead in active learning



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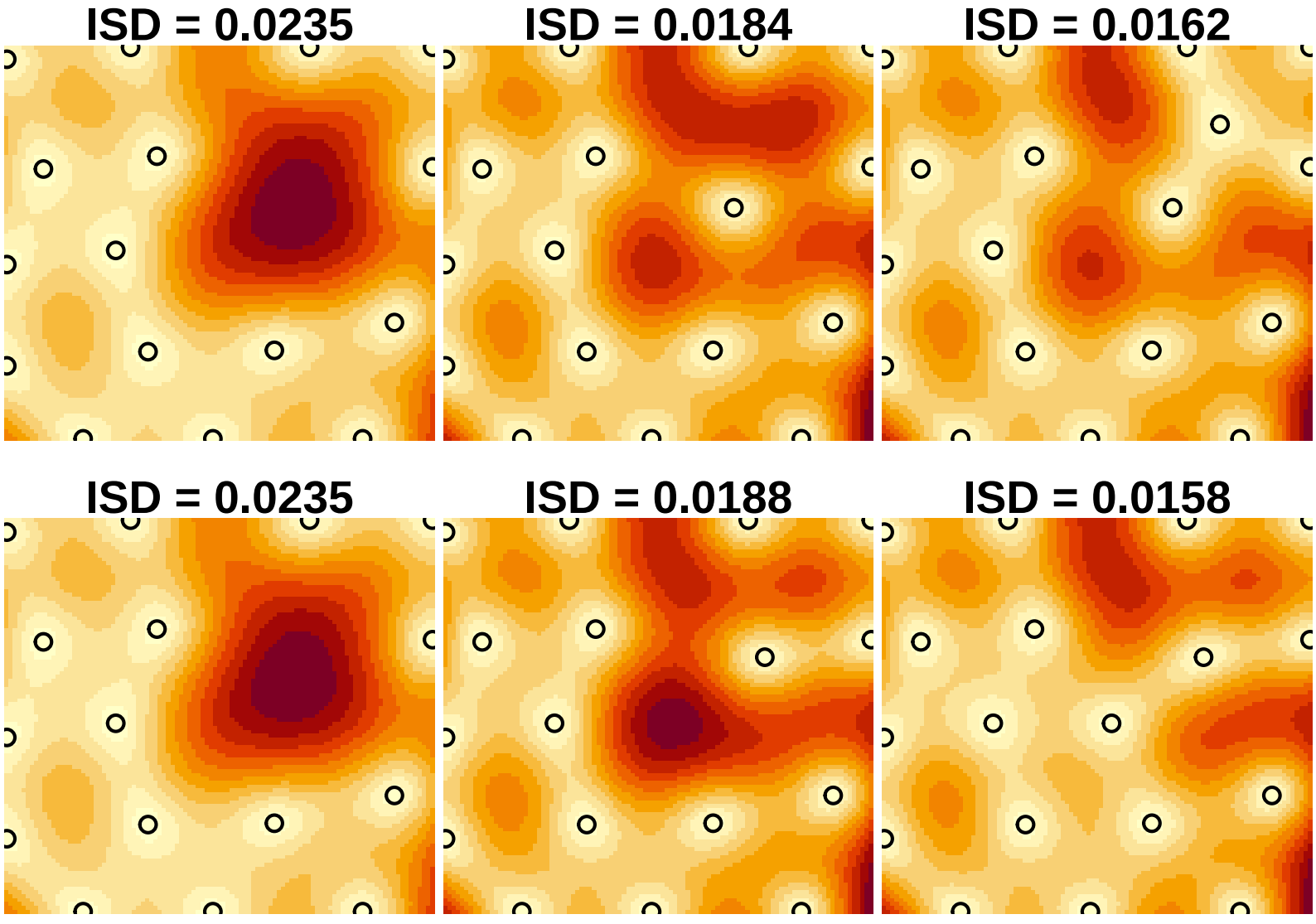

What's wrong with being greedy?

Imagine we have two runs left. There are two strategies:

1. Select both points with our current information $\mathcal{GP}(X_{N-2}, y_{N-2})$. This ignores the new information available in $\mathcal{GP}(X_{N-1}, y_{N-1})$.
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The "best" solution is often a compromise between two extremes. Given a budget of N runs and an initial design X_n, we could

1. Place the remaining $N - n$ runs at once using $\mathcal{GP}(X_n, y_n)$.
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For example, Let $N = 36$ and $n = 16$, so we have 20 runs to go. We could

1. Place runs in 5 batches of 4 points, **or**
2. Place 4 batches of 4 points, followed by 4 one-at-a-time updates.

Summary

- Surrogate optimization with Gaussian processes finds **global** optima for unknown, expensive functions.
- Balancing *exploration* and *exploitation* is critical for finding the best response.
- Sequential design works well but suffers from limited lookahead.