Optimization as Estimation with Gaussian Processes in Bandit Settings

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Black-box function optimization in the bandit setting

maximize $f(x)$

$f(x)$ is expensive to evaluate.

Sequential queries.

At round $t$,

Choose $x_t$; Observe $y_t = f(x_t) + \epsilon$, where $\epsilon \sim N(0,\sigma^2)$;

Goal: Minimize cumulative regret $R_T = \sum_{t=1}^{T} (\max_{x \in X} f(x) - f(x_t))$.
Black-box function optimization in the bandit setting

\[
\begin{align*}
\text{maximize} & \quad f(x) \\
\text{subject to} & \quad x \in \mathcal{X}
\end{align*}
\]

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\end{align*}
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\[ f(x) = f(x_t) + \epsilon, \quad \epsilon \sim N(0, \sigma^2) \]

Goal: Minimize cumulative regret

\[ R_T = \sum_{t=1}^{T} \left( \max_{x \in X} f(x) - f(x_t) \right) \]
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\end{array}
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Gaussian process optimization

Assume \( f \sim GP(\mu, k) \).
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At round $t$,
- Predict $\mu_{t-1}(x)$ and $\sigma_{t-1}^2(x)$
Assume \( f \sim GP(\mu, k) \).

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- Predict \( \mu_{t-1}(x) \) and \( \sigma^2_{t-1}(x) \)
- Pick an input \( x_t \)

**Examples:**
- \( \text{PI}\) (Kushner, 1964)
- \( \text{EI}\) (Mo˘ckus, 1974)
- \( \text{UCB}\) (Srinivas et al., 2010)
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Examples:
- \( \text{PI}(x) = \Pr[f(x) > \theta_t] \) (Kushner, 1964)
- \( \text{EI}(x) = \mathbb{E}[f(x) - \theta_t + \mathbb{E}[f(x)]] \) (Mo˘ckus, 1974)
- \( \text{UCB}(x) = \mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x) \) (Srinivas et al., 2010)
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Examples:
- PI($x$) = $P_r[f(x) > \theta_t]$ (Kushner, 1964)
- EI($x$) = $E[(f(x) - \theta_t)^+]$ (Mockus, 1974)
- UCB($x$) = $\mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x)$ (Srinivas et al., 2010)
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Existing acquisition functions

Upper Confidence Bound (GP-UCB) (Srinivas et al., 2010)

\[ x_t = \arg \max_{x \in \tilde{x}} \mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x) \]

Can set \( \lambda_t \) that guarantees high-probability sub-linear regret in theory.
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Can set \( \lambda_t \) that guarantees high-probability sub-linear regret in theory.

\[ \begin{array}{c|c|c|c|c}
\lambda & 0 & 10 & 20 & 30 \\
\hline
\text{R} & 0.2 & 0.4 & 0.6 & 0.8 & 1.0 & 1.2 & 1.4 & 1.6 \\
\hline
\lambda = 1 & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} \\
\lambda = 2 & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} \\
\lambda = 3 & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} \\
\lambda = 4 & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} \\
\lambda \text{ UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} & \text{UCB} \\
\end{array} \]

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Optimization as Estimation

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Upper Confidence Bound (GP-UCB) (Srinivas et al., 2010)

\[ x_t = \arg \max_{x \in \mathcal{X}} \mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x) \]

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A new method: query the most likely arg max

Given the observations, what is the most likely arg max of the function?
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Notice that, for any $x \in \mathcal{X}$, $f(x)$ has a Gaussian distribution.
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Notice that, for any $x \in \mathcal{X}$, $f(x)$ has a Gaussian distribution.
Optimization as estimation

EST: estimate the arg max of the function $f$. 
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1. What is the function maximum?
Optimization as estimation

EST: estimate the arg max of the function $f$.

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2. How likely is $f(x)$ the maximum?
Step 1: Estimate the function maximum

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   Consider discrete $\mathcal{X}$ and negligible noise,

   $$\hat{m} = \mathbb{E}[\max_{x \in \mathcal{X}} f(x)] = \max_{\tau \in [1, t-1]} y_\tau + \int_{\infty}^\infty \Pr[\max_{x \in \mathcal{X}} f(x) > w] dw \max_{\tau \in [1, t-1]} y_\tau$$

   Approximate the joint Gaussian with independent Gaussians
   $$g(w) = 1 - \Pr[f(x) \leq w, \forall x \in \mathcal{X}] \approx 1 - \prod_{x \in \mathcal{X}} \Phi(w - \mu(x) / \sigma(x))$$

   Integrate numerically (ESTn) or approximately (ESTa)
Step 1: Estimate the function maximum

What is the function maximum?
Consider discrete $\mathcal{X}$ and negligible noise,

$$\hat{m} = \mathbb{E}[\max_{x \in \mathcal{X}} f(x)] = \max_{\tau \in [1, t-1]} y_\tau + \int_0^\infty \Pr[\max_{x \in \mathcal{X}} f(x) > w] \, dw$$

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Step 1: Estimate the function maximum

1. What is the function maximum?
Consider discrete $\mathcal{X}$ and negligible noise,

$$\hat{m} = \mathbb{E}[\max_{x \in \mathcal{X}} f(x)] = \max_{\tau \in [1, t-1]} y_{\tau} + \int_{\max_{x \in \mathcal{X}} f(x) > w} \Pr[\max_{x \in \mathcal{X}} f(x) > w] \, dw$$

- Approximate the joint Gaussian with independent Gaussians

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Step 2: calculate the probability that $x$ is the arg max

2 How likely is $f(x)$ the maximum?
Step 2: calculate the probability that $\mathbf{x}$ is the arg max

2. How likely is $f(\mathbf{x})$ the maximum?

$$\Pr[f(\mathbf{x}) \text{ is the maximum} | \hat{m}] \approx Q\left( \frac{\hat{m} - \mu(\mathbf{x})}{\sigma(\mathbf{x})} \right) \prod_{\mathbf{x}' \neq \mathbf{x}} \Phi\left( \frac{\hat{m} - \mu(\mathbf{x}')}{\sigma(\mathbf{x}')} \right)$$
Step 2: calculate the probability that $\mathbf{x}$ is the arg max

How likely is $f(\mathbf{x})$ the maximum?

$$
\Pr[f(\mathbf{x}) \text{ is the maximum} | \hat{m}] \approx \frac{\Pr[f(\mathbf{x}) \geq \hat{m}]}{Q\left(\frac{\hat{m} - \mu(\mathbf{x})}{\sigma(\mathbf{x})}\right)} \prod_{\mathbf{x'} \neq \mathbf{x}} \Phi\left(\frac{\hat{m} - \mu(\mathbf{x'})}{\sigma(\mathbf{x'})}\right)
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How likely is $f(\mathbf{x})$ the maximum?

$$\Pr[f(\mathbf{x}) \text{ is the maximum} | \hat{m}] \approx \frac{\Pr[f(\mathbf{x}) \geq \hat{m}]}{Q\left(\frac{\hat{m} - \mu(\mathbf{x})}{\sigma(\mathbf{x})}\right)} \prod_{\mathbf{x}' \neq \mathbf{x}} \Phi\left(\frac{\hat{m} - \mu(\mathbf{x}')}{{\sigma(\mathbf{x}')}}\right) \Pr[\forall \mathbf{x}' \neq \mathbf{x}, f(\mathbf{x}') < \hat{m}]$$
Step 2: calculate the probability that \( \mathbf{x} \) is the arg max

How likely is \( f(\mathbf{x}) \) the maximum?

\[
\Pr[f(\mathbf{x}) \text{ is the maximum} | \hat{m}] \approx Q\left( \frac{\hat{m} - \mu(\mathbf{x})}{\sigma(\mathbf{x})} \right) \prod_{\mathbf{x}' \neq \mathbf{x}} \Phi\left( \frac{\hat{m} - \mu(\mathbf{x}')}{\sigma(\mathbf{x}')} \right)
\]

\[
\arg \max_{\mathbf{x} \in \mathcal{X}} \Pr[f(\mathbf{x}) \text{ is the maximum} | \hat{m}] = \arg \min_{\mathbf{x} \in \mathcal{X}} \frac{\hat{m} - \mu(\mathbf{x})}{\sigma(\mathbf{x})}
\]
EST

\[ \Pr[x = \arg\max f(x) | \hat{m}] \]
Connections to GP-UCB and PI

**EST**

\[ \Pr[\mathbf{x} = \text{arg max } f(\mathbf{x}) | \hat{m}] \]

\[ \theta = \hat{m} \]

**PI**

\[ \text{PI}(\mathbf{x}) = \Pr[f(\mathbf{x}) > \theta] \]
Connections to GP-UCB and PI

\[ \text{GP-UCB} \]
\[ UCB(x) = \mu(x) + \lambda \sigma(x) \]

\[ \lambda = \min_{x \in \mathcal{X}} \frac{\hat{m} - \mu(x)}{\sigma(x)} \]

\[ \text{EST} \]
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Connections to GP-UCB and PI

**GP-UCB**

$$\text{UCB}(x) = \mu(x) + \lambda \sigma(x)$$

$$\lambda = \min_{x \in X} \frac{\hat{m} - \mu(x)}{\sigma(x)}$$

$$\theta = \max_{x \in X} \mu(x) + \lambda \sigma(x)$$

**EST**

$$\Pr[x = \arg\max f(x) | \hat{m}]$$

$$\theta = \hat{m}$$

**PI**

$$\text{PI}(x) = \Pr[f(x) > \theta]$$
At round $t$, pick the input that is most likely to reach a target value.

$$\hat{m}_t = \begin{cases} 
\max_{x \in \mathcal{X}} \mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x) & \text{GP-UCB} \\
\theta_t & \text{PI} \\
\mathbb{E}[\max_{x \in \mathcal{X}} f(x)] & \text{EST} 
\end{cases}$$

$$x_t \leftarrow \arg \min_{x \in \mathcal{X}} \frac{\hat{m}_t - \mu_{t-1}(x)}{\sigma_{t-1}(x)}$$
Regret bounds

**Theorem (Regret bounds for EST)**

Assume \( \hat{m}_t \geq \max_{x \in \mathcal{X}} f(x), \forall t \in [1, T] \). Then,

\[
\mathbb{E}[R_T] \leq \nu_* \sqrt{CT\gamma_T}.
\]

With probability at least \( 1 - \delta \),

\[
R_T \leq (\nu_* + \zeta_T) \sqrt{CT\gamma_T},
\]

\( C = \frac{2}{\log(1+\sigma^{-2})}, \nu_t \triangleq \min_{x \in \mathcal{X}} \frac{\hat{m}_t - \mu_{t-1}(x)}{\sigma_{t-1}(x)}, t^* = \arg \max_t \nu_t \).

\( k(x, x') \leq 1, \gamma_T = \max_{A \subseteq \mathcal{X}, |A| \leq T} l(y_A, f_A), \zeta_T = (2 \log(\frac{T}{2\delta}))^{\frac{1}{2}}. \)
Theorem (Regret bounds for EST)

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Slepian’s Comparison Lemma (Slepian, 1962; Massart, 2007)

Let $\mathbf{u}, \mathbf{v} \in \mathbb{R}^n$ be two multivariate Gaussian random vectors with the same mean and variance, such that

$$E[\mathbf{v}_i \mathbf{v}_j] \leq E[\mathbf{u}_i \mathbf{u}_j], \forall i, j.$$

Then,

$$E[\sup_{i \in [1,n]} \mathbf{v}_i] \geq E[\sup_{i \in [1,n]} \mathbf{u}_i].$$
Slepian’s Comparison Lemma (Slepian, 1962; Massart, 2007)

Let \( u, v \in \mathbb{R}^n \) be two multivariate Gaussian random vectors with the same mean and variance, such that

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E[v_i v_j] \leq E[u_i u_j], \quad \forall i, j.
\]

Then,

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E[\sup_{i \in [1,n]} v_i] \geq E[\sup_{i \in [1,n]} u_i].
\]

Ignoring positive covariance gives higher expected maximum.
Experiments

More results at Session 2 Poster 47
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Optimization as Estimation
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Robotics

Vision

More results at Session 2 Poster 47
A new BO strategy from the viewpoint of estimating arg max.

Adaptively tuning $\lambda$ and $\theta$ in GP-UCB and PI.

Sub-linear regret bounds and good empirical results.

Source code: https://github.com/zi-w/GP-EST
• A new BO strategy from the viewpoint of estimating arg max.
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Summary: Optimization as Estimation

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