Optimization as Estimation with Gaussian Processes in Bandit Settings

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May 9, 2016
Black-box function optimization in the bandit setting

\[
\text{maximize } \quad f(x)
\]

\[
\text{subject to } \quad x \in \mathcal{X}
\]

Function $f$ is expensive to evaluate.

Sequential queries.

At round $t$,

Choose $x_t$;

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

Goal: Minimize cumulative regret $R_T = \sum_{t=1}^{T} (\max_{x \in \mathcal{X}} f(x) - f(x_t))$. 

Zi Wang (MIT CSAIL)

Optimization as Estimation

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Black-box function optimization in the bandit setting

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\end{align*}
\]

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\[
\begin{align*}
\text{INPUT } x \\
\text{FUNCTION } f: \\
\text{NOISY OUTPUT } y
\end{align*}
\]
Black-box function optimization in the bandit setting

\[ \max_{x \in X} f(x) \]

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At round \( t \),

\[ f(x) \]

\[ x \]
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Gaussian process optimization

Assume $f \sim GP(\mu, k)$. 

Prior distribution
Gaussian process optimization

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At round $t$,
- Predict $\mu_{t-1}(x)$ and $\sigma^2_{t-1}(x)$

Prior distribution

Posterior distribution

Examples:
- $\text{PI}(x) = \text{Pr}[f(x) > \theta]$
  (Kushner, 1964)
- $\text{EI}(x) = E[(f(x) - \theta)^+]$
  (Mo˘ckus, 1974)
- $\text{UCB}(x) = \mu_{t-1}(x) + \lambda_t \sigma_{t-1}(x)$
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Existing acquisition functions

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

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

Can set \( \lambda_t \) that guarantees high-probability sub-linear regret in theory.
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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.
A new method: query the most likely arg max

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Notice that, for any $x \in \mathcal{X}$, $f(x)$ has a Gaussian distribution.
EST: estimate the arg max of the function $f$. 
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Step 1: Estimate the function maximum

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

$$\hat{m} = \mathbb{E}_{x \in \mathcal{X}}[\max f(x)] = \max_{\tau \in [1, t-1]} y_{\tau} + \int_{\max_{\tau \in [1, t-1]} y_{\tau}}^{\infty} \Pr_{x \in \mathcal{X}}[\max f(x) > w] \, dw$$
Step 1: Estimate the function maximum

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

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

   - Approximate the joint Gaussian with independent Gaussians

   $$g(w) = 1 - \Pr[f(x) \leq w, \forall x \in \mathcal{X}] \approx 1 - \prod_{x \in \mathcal{X}} \Phi\left(\frac{w - \mu(x)}{\sigma(x)}\right)$$
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Consider discrete $\mathcal{X}$ and negligible noise,

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

- Integrate numerically (ESTn) or approximately (ESTa)
Step 2: calculate the probability that \( x \) is the arg max

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

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

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

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

$$\Pr[f(x) \text{ is the maximum} \mid \hat{m}] \approx \Pr[f(x) \geq \hat{m}]$$

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

- How likely is $f(x)$ the maximum?

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

\[
\Pr[\forall x' \neq x, f(x') < \hat{m}]
\]

arg max $x \in X$ $\Pr[f(x) \text{ is the maximum} | \hat{m}] = \arg \min x \in X \frac{\hat{m} - \mu(x)}{\sigma(x)}$
Connections to GP-UCB and PI

\[ \text{EST} \]

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

EST

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

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

PI

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

GP-UCB

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

$$\lambda = \min_x \frac{\hat{m} - \mu(x)}{\sigma(x)}$$

EST

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

PI

$$\text{PI}(x) = \Pr[f(x) > \theta]$$
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**

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

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

**PI**

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

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

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

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

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

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

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

where

- \( \nu_t = \min_{x \in \mathcal{X}} \frac{\hat{m}_t - \mu_{t-1}(x)}{\sigma_{t-1}(x)} \), \( t^* = \arg \max_t \nu_t \).
- \( C = \frac{2}{\log(1 + \sigma^{-2})} \), \( \nu_t \triangleq \min_{x \in \mathcal{X}} \frac{\hat{m}_t - \mu_{t-1}(x)}{\sigma_{t-1}(x)} \), \( t^* = \arg \max_t \nu_t \).
- \( k(x, x') \leq 1 \), \( \gamma_T = \max_{A \subseteq \mathcal{X}, |A| \leq T} I(y_A, f_A) \), \( \zeta_T = (2 \log(\frac{T}{2\delta}))^{\frac{1}{2}} \).
Regret bounds

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

\[k(x, x') \leq 1, \quad \gamma_T = \max_{A \subseteq \mathcal{X}, |A| \leq T} l(y_A, f_A), \quad \zeta_T = (2 \log(\frac{T}{2\delta}))^{\frac{1}{2}}.\]
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

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

Then,

\[
\mathbb{E}[\sup_{i \in [1,n]} \mathbf{v}_i] \geq \mathbb{E}[\sup_{i \in [1,n]} \mathbf{u}_i].
\]
Estimating an upper bound on the function maximum

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

Ignoring positive covariance gives higher expected maximum.
Experiments

accuracy on val set

Caltech101
SUN397

More results at Session 2 Poster 47
Zi Wang (MIT CSAIL)

Optimization as Estimation
May 9, 2016
Experiments

More results at Session 2 Poster 47
Summary: Optimization as Estimation

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
Summary: Optimization as Estimation

- A new BO strategy from the viewpoint of estimating arg max.
- Adaptively tuning $\lambda$ and $\theta$ in GP-UCB and PI.
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