A Hierarchical Expected Improvement method for effective Bayesian optimization

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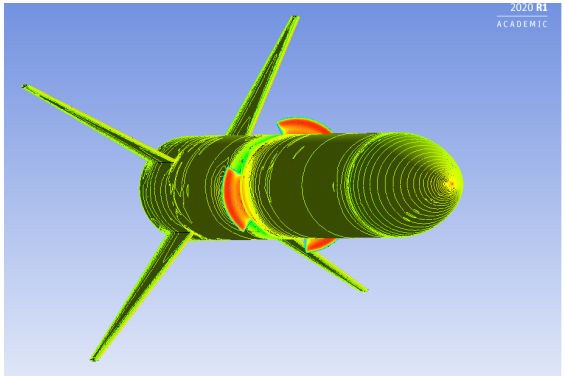
Joint work with **Zhehui Chen** (Google) and **Simon Mak** (Duke University)

[1]The paper appeared in JASA 2024.

Outline

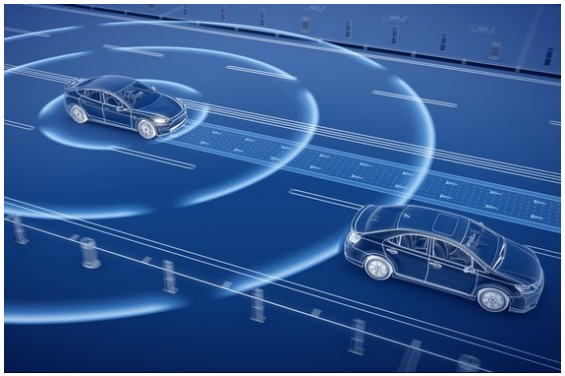
- Why **Bayesian optimization**?
- **Kriging** and **Expected Improvement (EI)**
- **Hierarchical Kriging** and **Hierarchical EI (HEI)**
- **Hyperprior specification** for HEI
- Global **convergence rates**
- Two **applications**: process optimization for **semiconductor manufacturing**, hyperparameter tuning for **deep learning**

Motivation

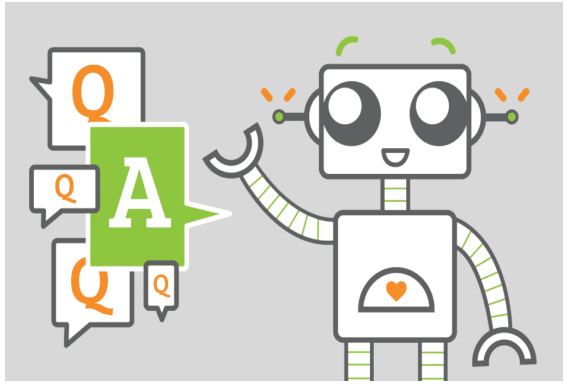


Engineering design

Portfolio management



Autonomous vehicles



Q&A bot

Want to find the **best** setting(s) under a **black-box** objective f'n

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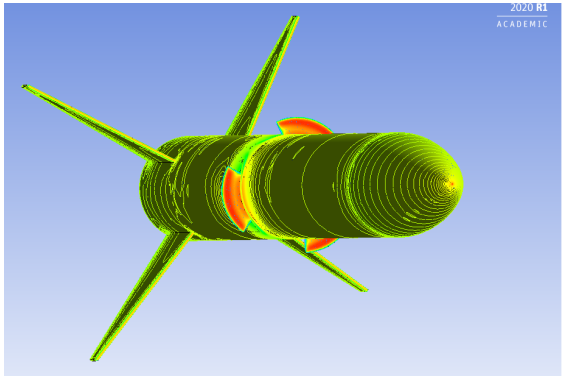

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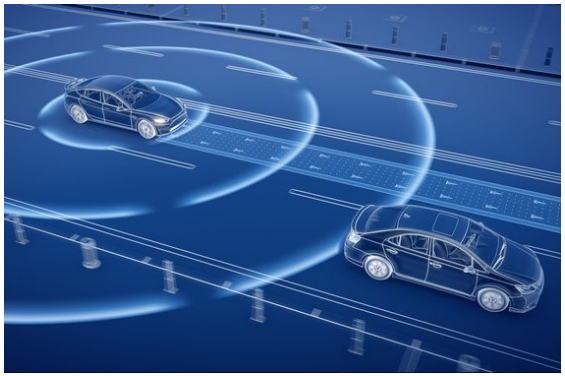

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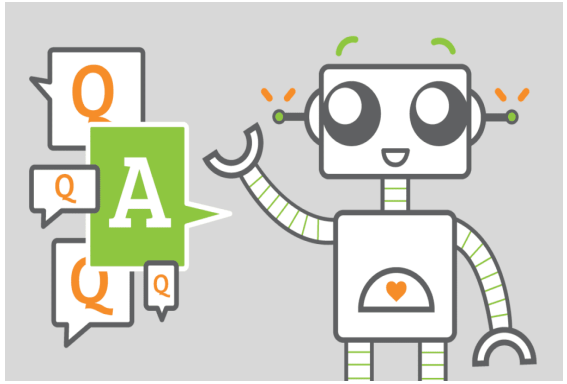

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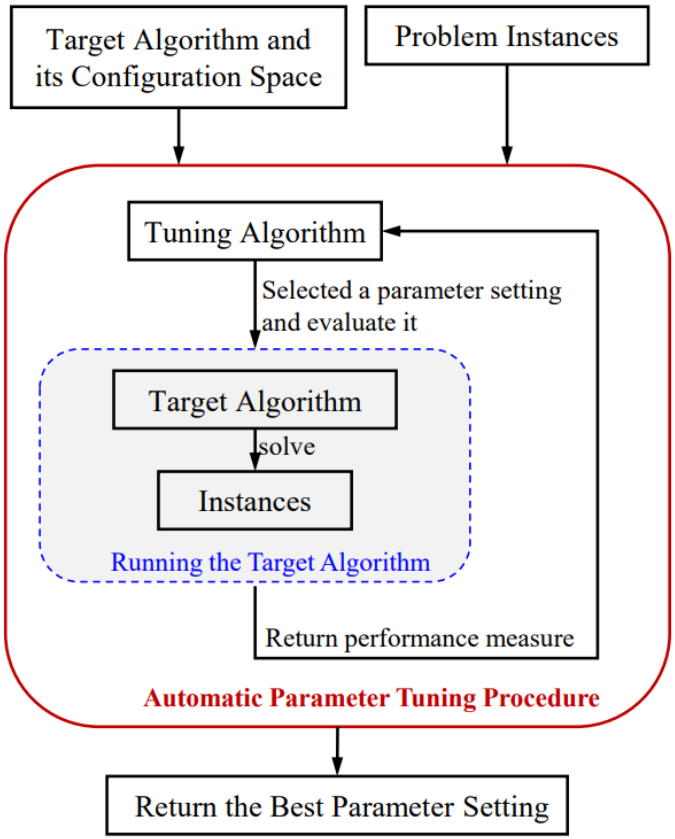
Application in AI

Black-box optimization can be used to tune **hyper-parameters** automatically.



Examples of hyper-parameters in neural networks

- learning rate: $\log U(0.001, 10)$;
- n.layers: 1 to 3;
- batch size: 20 or 100;
- n.hidden units: $\log U(128, 4096)$;
- ...

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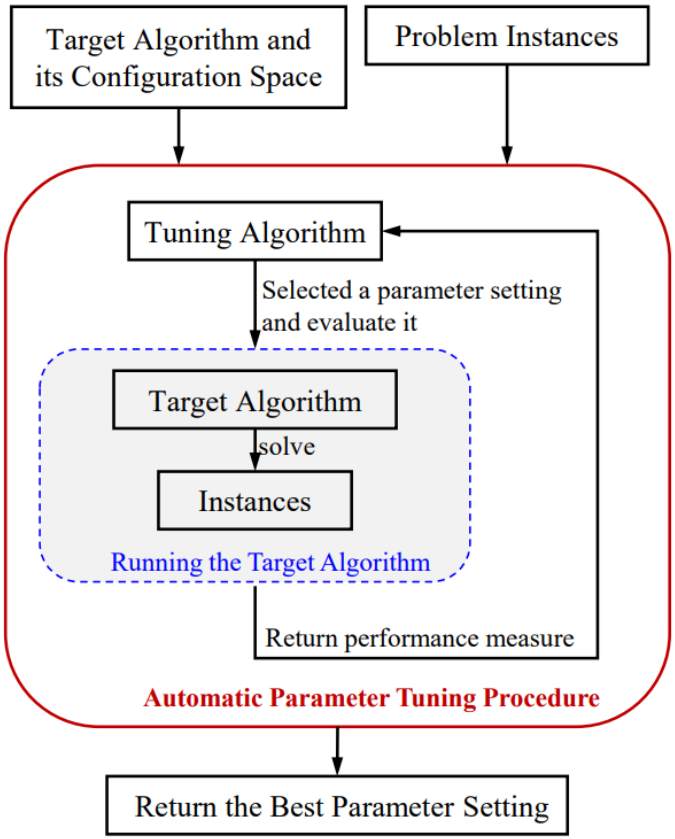

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$$\boldsymbol{x}^* \in \arg\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x})$$

- Ω: **feasible** domain for parameters $\boldsymbol{x}$
- f: an unknown **black-box objective** function
  - Functional form **unknown** prior to **data**
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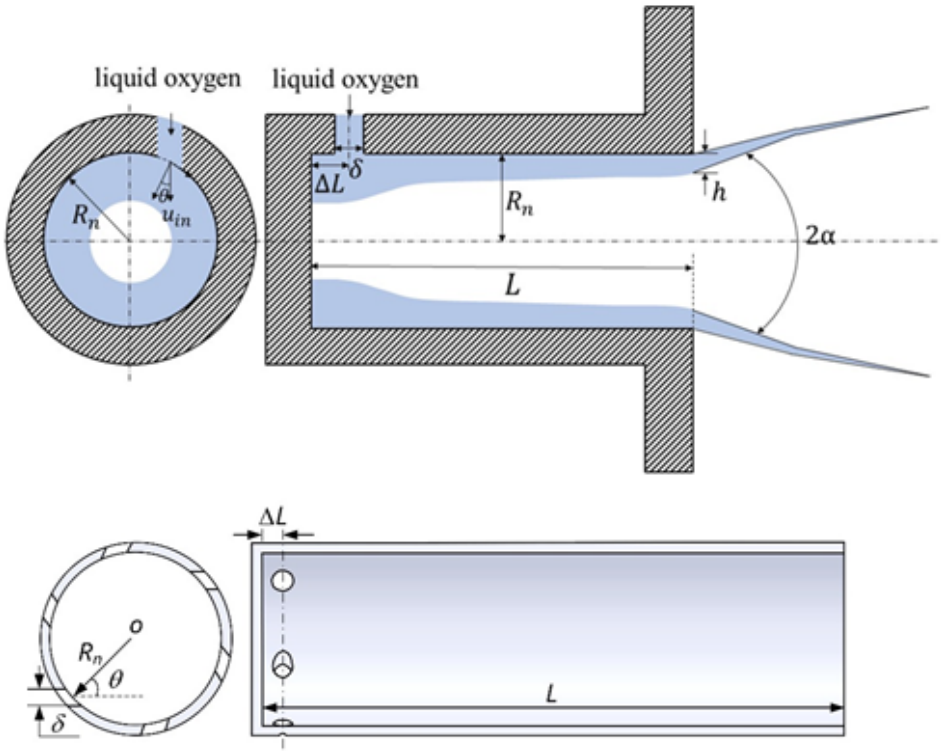
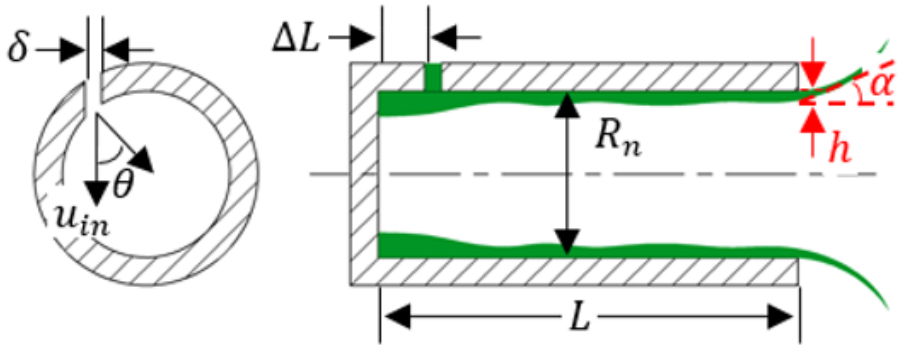
Rocket design

Collaboration project with GT Aerospace (Air Force / SpaceX)

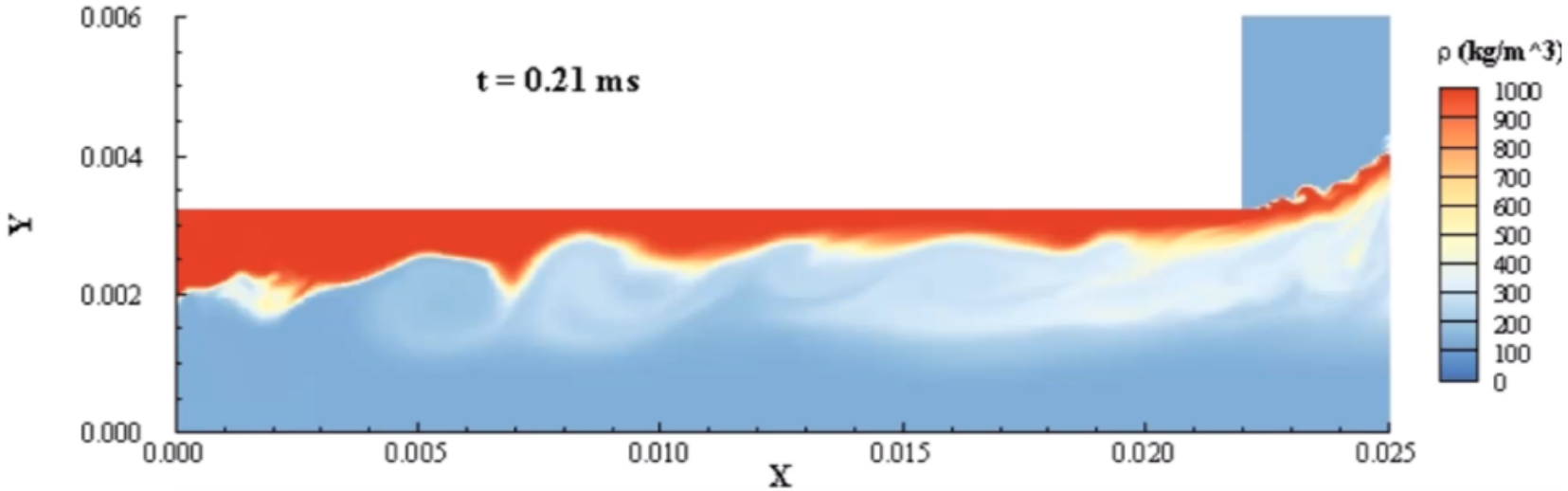


Rocket design

Optimizing **rocket injector** designs over a geometric **design space** (Mak et al. 2018; Yeh et al. 2018; Chang et al. 2019)



L	20-100 mm
R_n	2-5 mm
θ	45°-75°
δ	0.5-2 mm
ΔL	1-4 mm



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Simulations are very **expensive**: **14 days** per **injector design** (each evaluation of f), **parallelized** over millions of cores

- **Exploring** the 5D domain Ω by simulations **alone** will take 1000's of simulations $\Rightarrow$ **years** of **computation**

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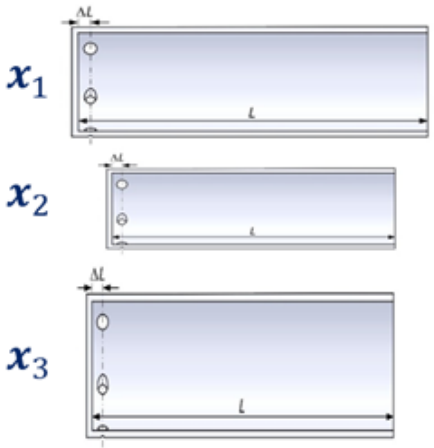
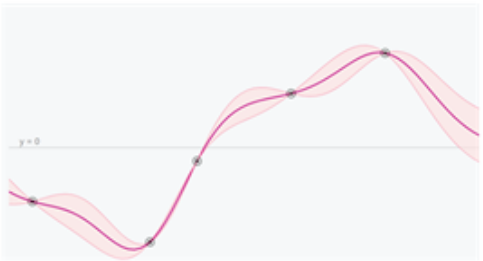


Run a few experiments at different injector geometries



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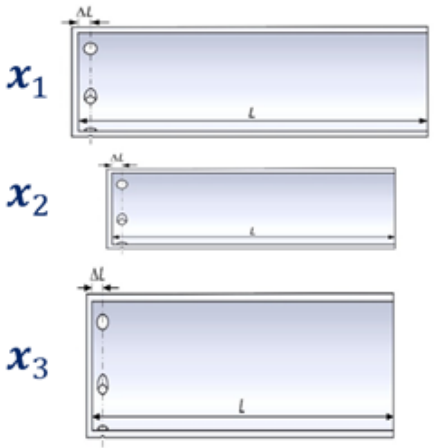

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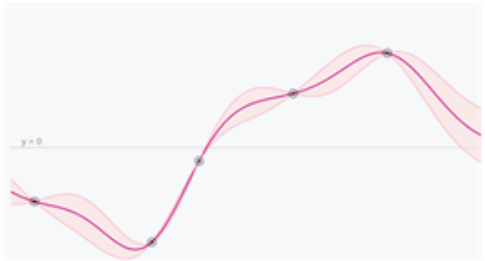

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- **Bayesian** (probabilistic) model on **objective** f'n f:
  - Provide **predictor** of f: $\widehat{f} = \mathbb{E}\{f|\text{data}\}$
  - Quantify **uncertainty** on f: $\text{Var}\{f|\text{data}\}$
- **Acquisition function** for choosing **next** point x_{new}
  - **Exploitation**: want x's with low **predictions** $\widehat{f}$
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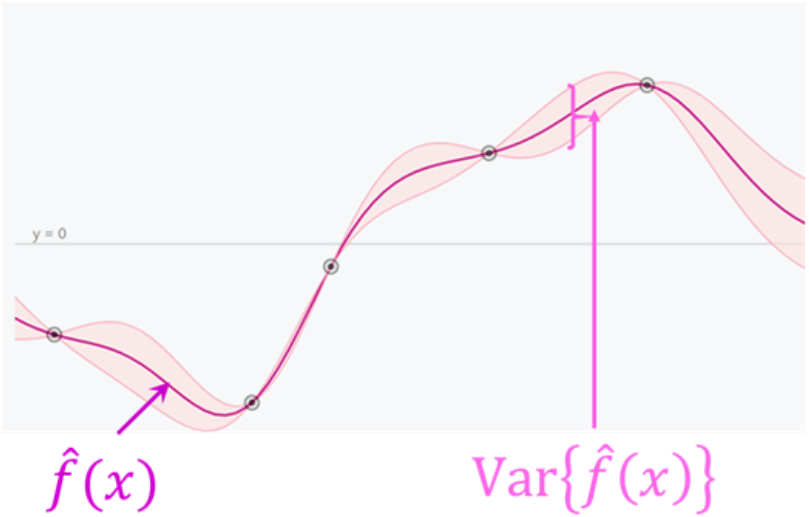

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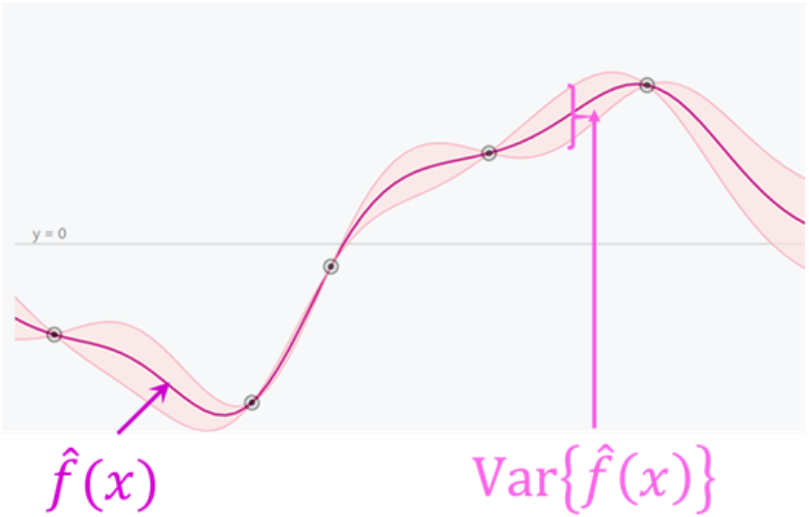

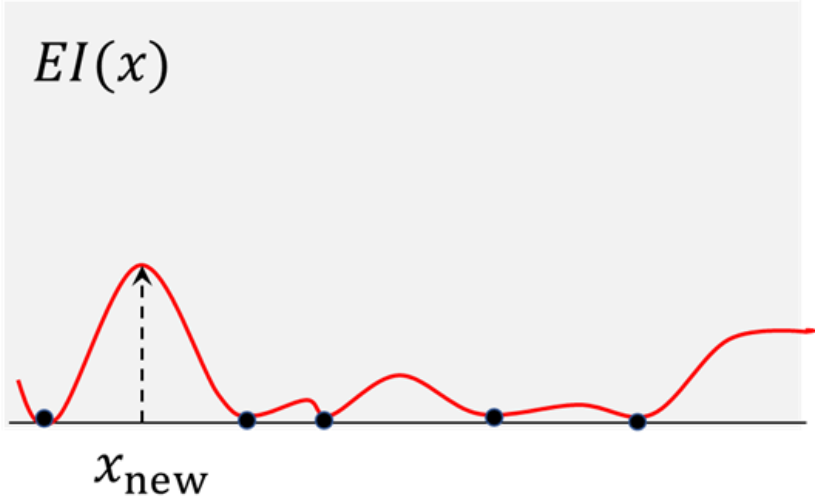

Bayesian optimization

A **widely-used** setting in **Bayesian optimization**:

- **Bayesian** model on f: **Gaussian process** (kriging)
  - **Nonparametric** form $\Rightarrow$ **powerful approximation**
  - **Probabilistic** model $\Rightarrow$ **uncertainty quantification** (UQ)
  - **Closed-form** prediction & UQ $\Rightarrow$ **efficient modeling**
- **Acquisition function**: **Expected Improvement** (Jones et al. 1997)
  - **Closed-form** expression for $\mathrm{EI}(x)$ $\Rightarrow$ **efficient queries**
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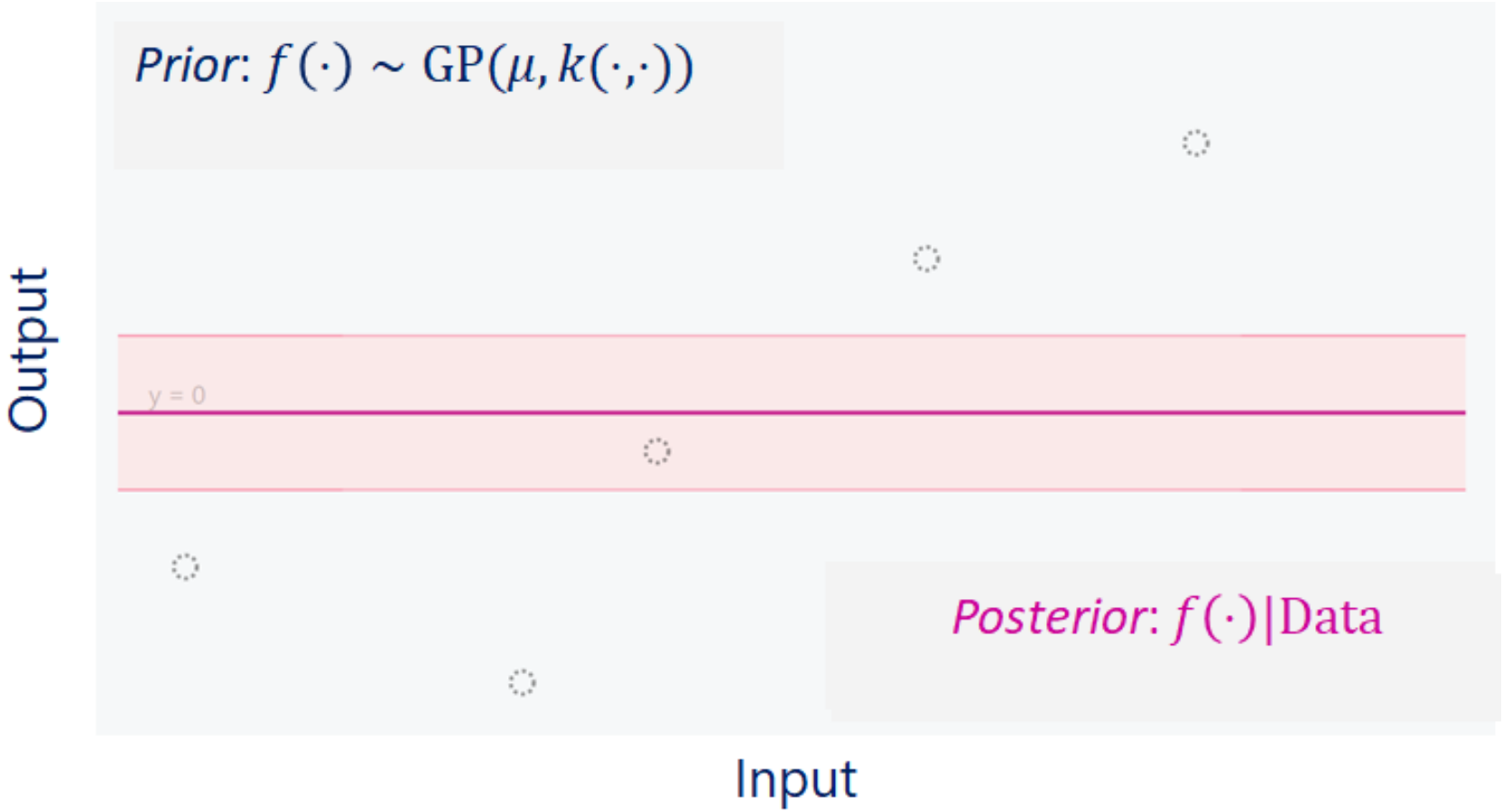

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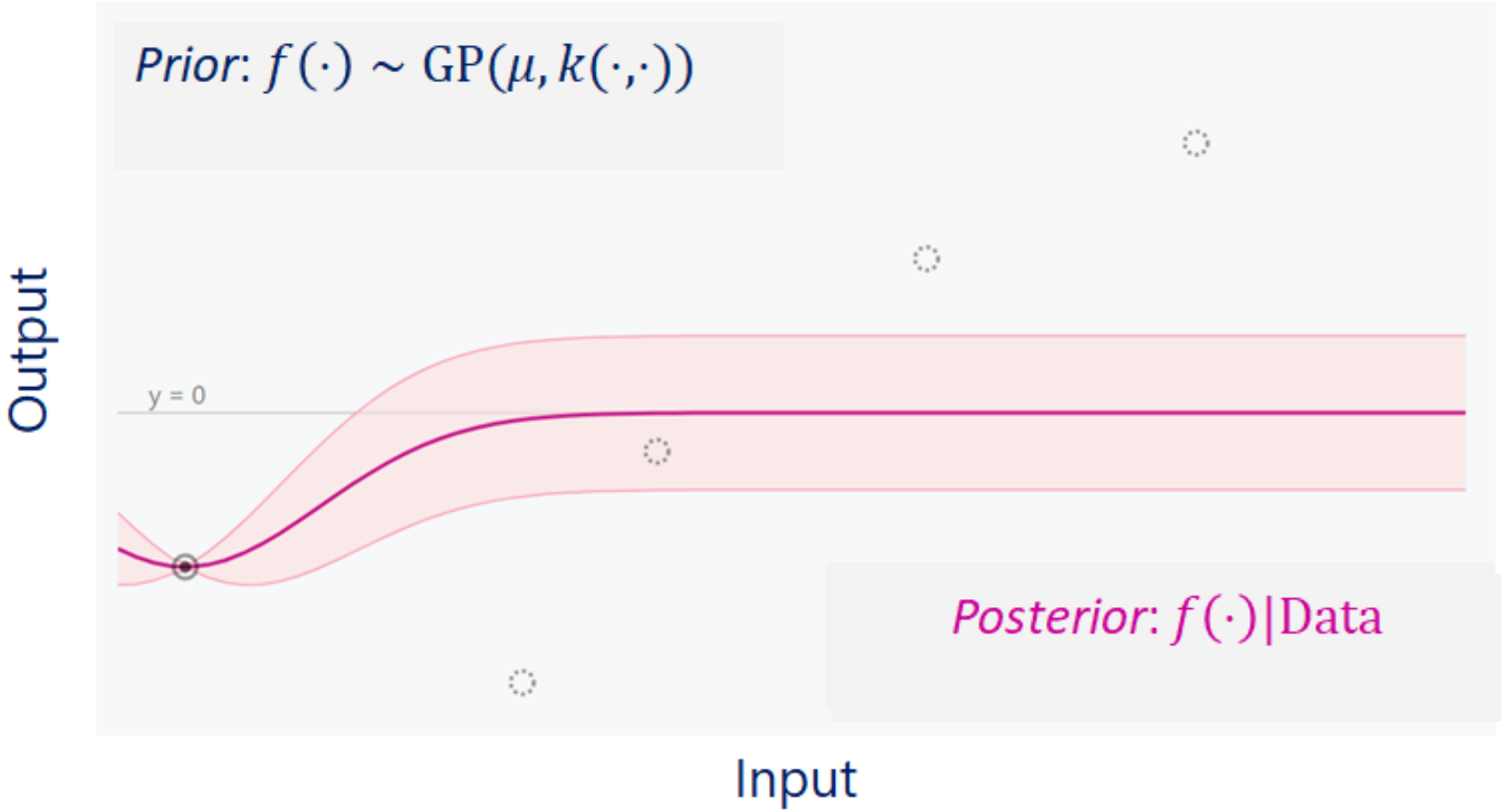

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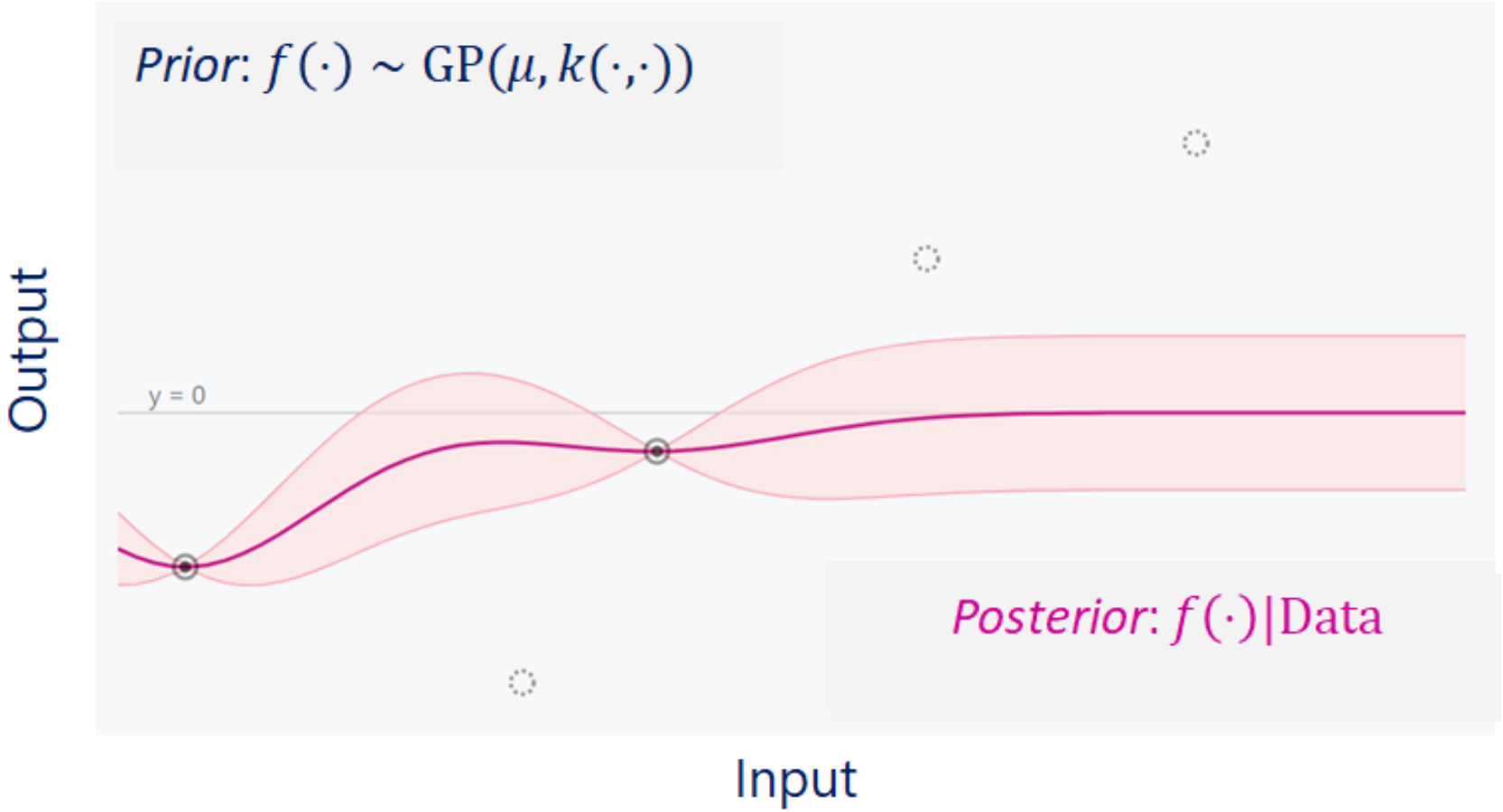

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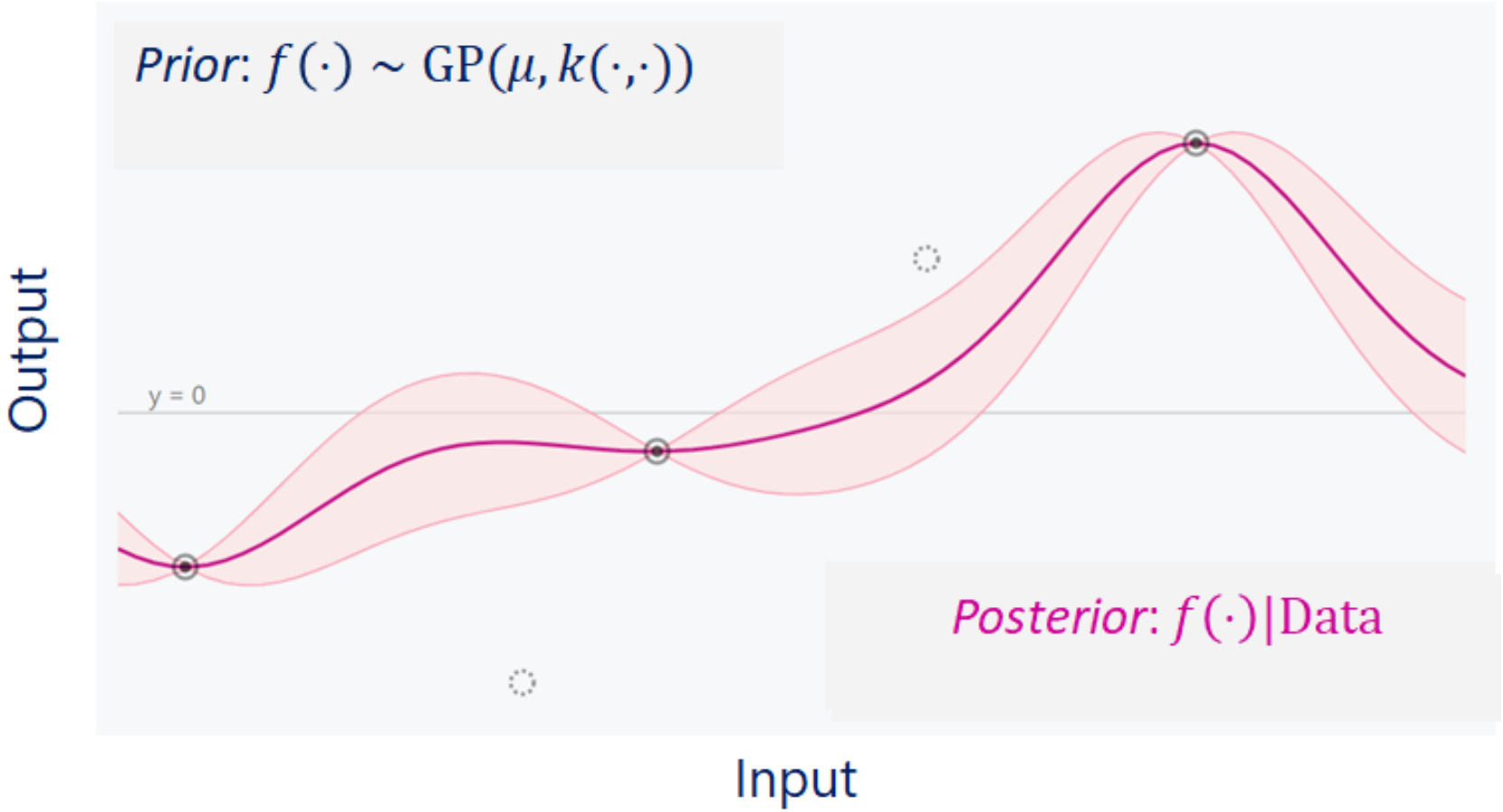

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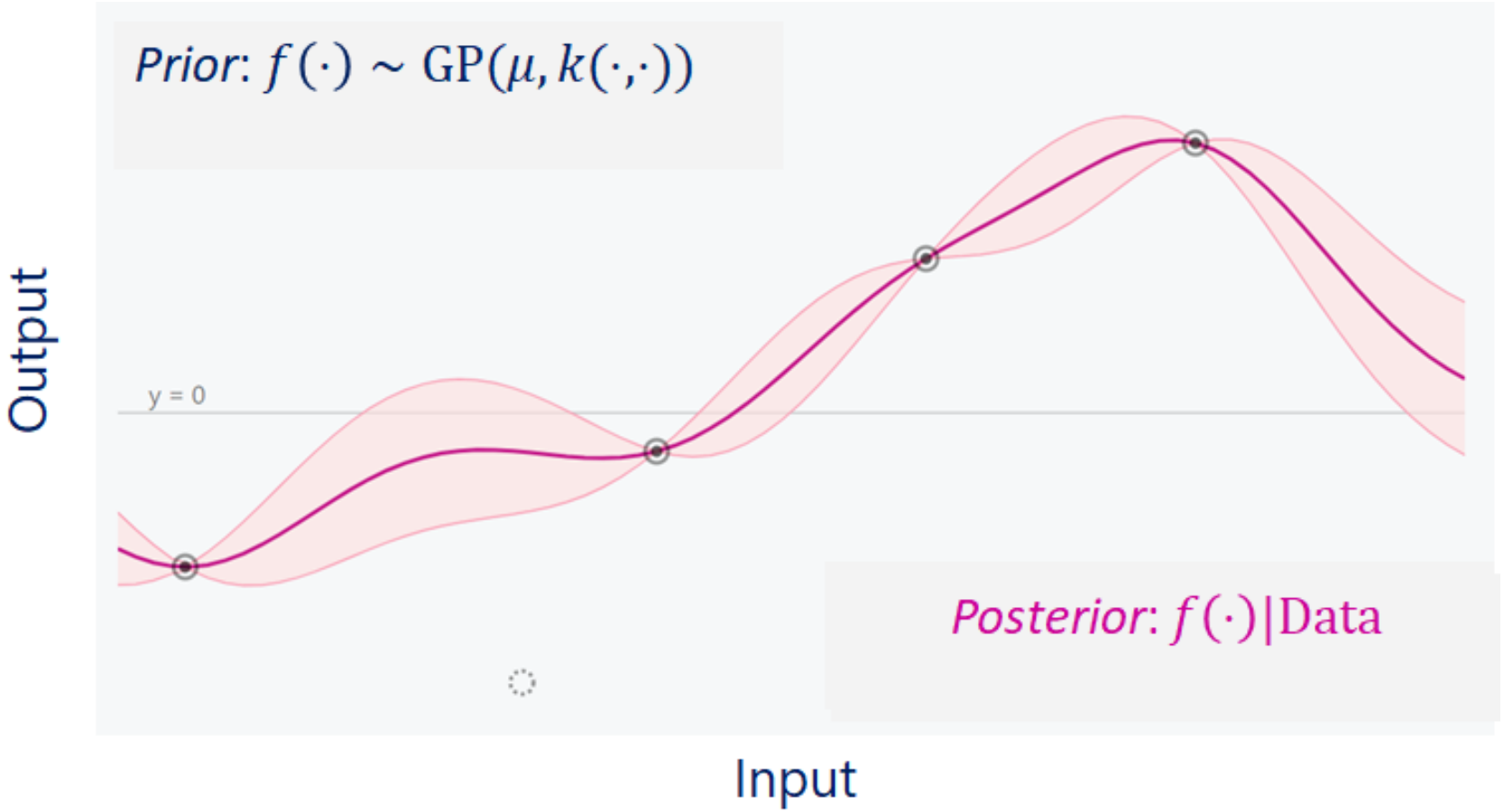

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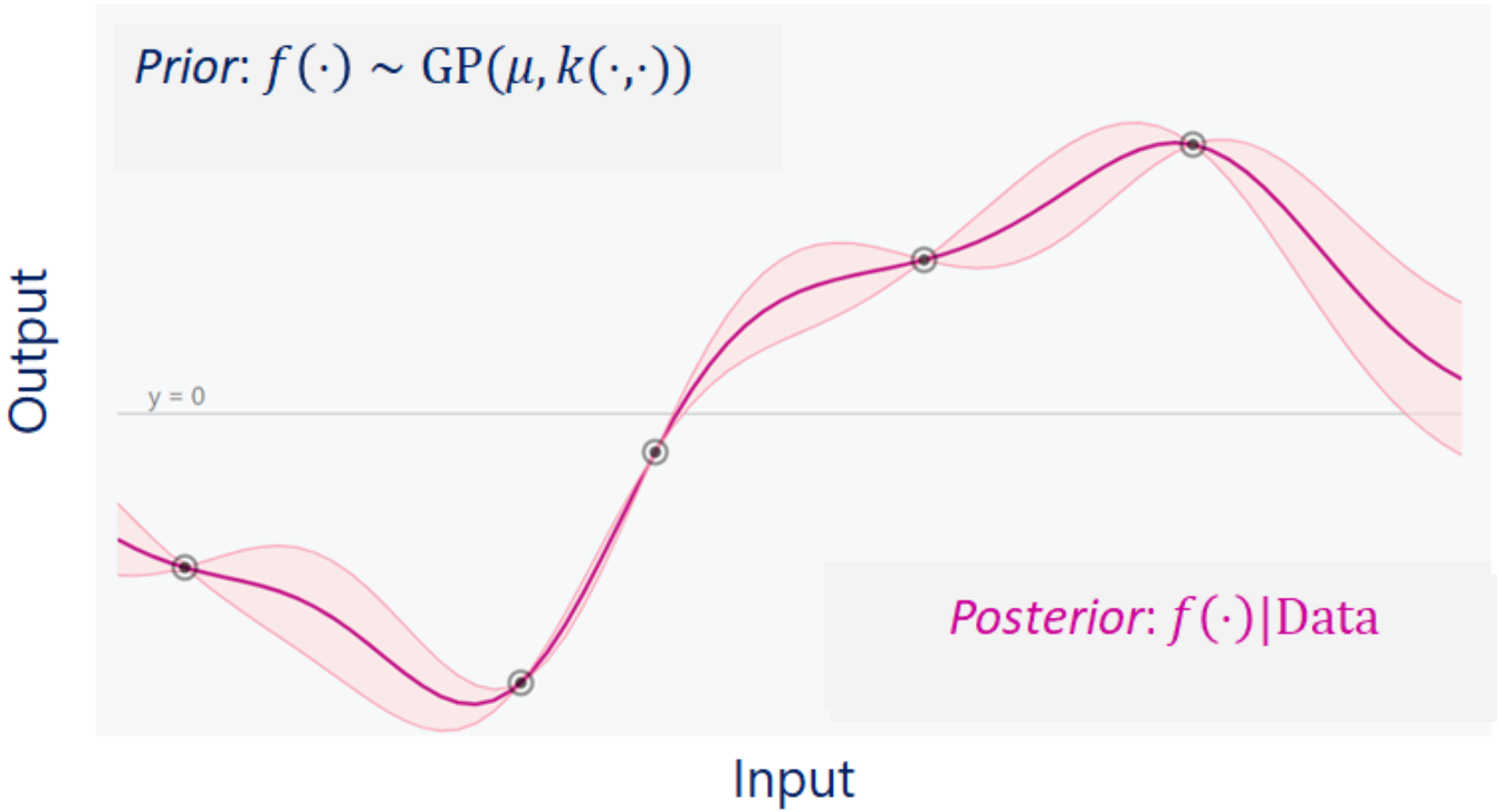


Gaussian process (kriging) model

Universal kriging model (see, e.g., Santner et al. 2013):

$$f(\cdot) \sim GP\{\mu(\cdot), \sigma^2 r(\cdot,\cdot)\}, \quad \boldsymbol{x} \in \mathbb{R}^d.$$

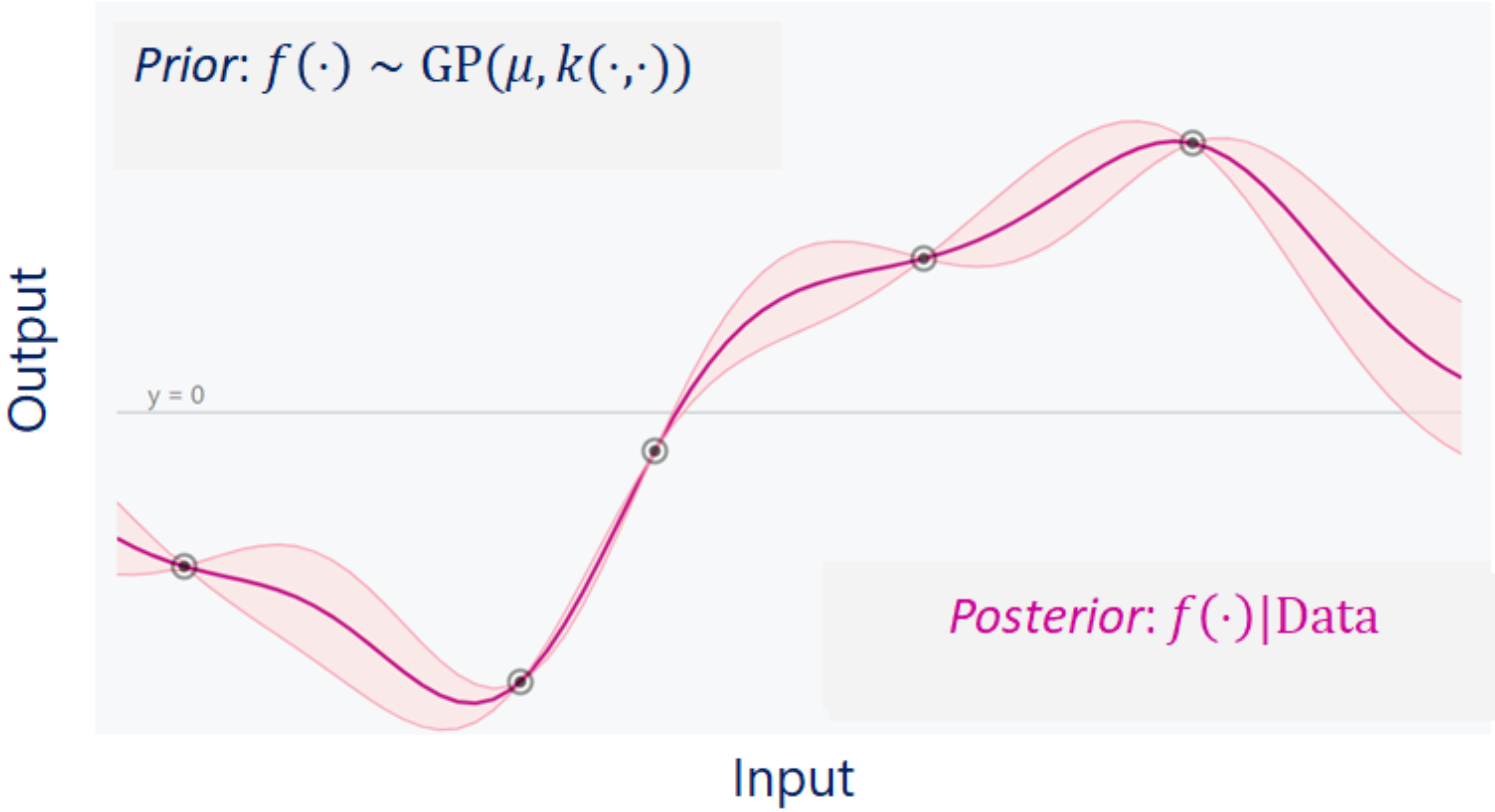
- **Mean** function: $\mu(\boldsymbol{x}) = \boldsymbol{p}^\top(\boldsymbol{x})\boldsymbol{\beta}$
- **Basis** functions: $\boldsymbol{p}(\boldsymbol{x}) = [p_1(\boldsymbol{x}), \cdots, p_q(\boldsymbol{x})]^\top$
- Process **variance**: $\sigma^2 = \mathrm{Var}\{f(\boldsymbol{x})\}$
- **Correlation** function: $r(\boldsymbol{x}, \boldsymbol{x}') = r(\boldsymbol{x} - \boldsymbol{x}')$

When **no** basis functions are used (i.e., $p(\boldsymbol{x}) = 1$), UK reduces to **ordinary kriging** (OK)

Gaussian process (kriging) model

Given **data** $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, the posterior of $f(\boldsymbol{x})$ is **Gaussian**:

$$\left[f(\boldsymbol{x})\middle|\mathcal{D}\right] \sim \mathcal{N}\left(\widehat{f}_n(\boldsymbol{x}), \sigma^2 s^2(\boldsymbol{x})\right)$$



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- Posterior **mean**: $\widehat{f}_n(\boldsymbol{x}) = \boldsymbol{p}^\top(\boldsymbol{x})\widehat{\boldsymbol{\beta}} + \boldsymbol{r}^\top(\boldsymbol{x})\boldsymbol{R}^{-1}(\boldsymbol{y} - \boldsymbol{P}\widehat{\boldsymbol{\beta}})$
  - $\widehat{\boldsymbol{\beta}} = (\boldsymbol{P}^\top \boldsymbol{R}^{-1}\boldsymbol{P})^{-1}\boldsymbol{P}^\top \boldsymbol{R}^{-1}\boldsymbol{y}$
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  - $s^2(\boldsymbol{x}) = r(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{r}^\top(\boldsymbol{x})\boldsymbol{R}^{-1}\boldsymbol{r}(\boldsymbol{x}) + \boldsymbol{p}^\top(\boldsymbol{x})\boldsymbol{G}^{-1}\boldsymbol{p}(\boldsymbol{x})$, where $\boldsymbol{G} = \boldsymbol{P}^\top \boldsymbol{R}^{-1}\boldsymbol{P}$

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  - $\boldsymbol{y} = [y_1, \cdots, y_n]^\top$, $\boldsymbol{P} = [\boldsymbol{p}(\boldsymbol{x}_1), \cdots, \boldsymbol{p}(\boldsymbol{x}_n)]^\top$
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Gaussian process (kriging) model

Given **data** $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$, the posterior of $f(\boldsymbol{x})$ is **Gaussian**:

$$\left[f(\boldsymbol{x})\middle|\mathcal{D}\right] \sim \mathcal{N}\left(\widehat{f}_n(\boldsymbol{x}), \sigma^2 s^2(\boldsymbol{x})\right)$$

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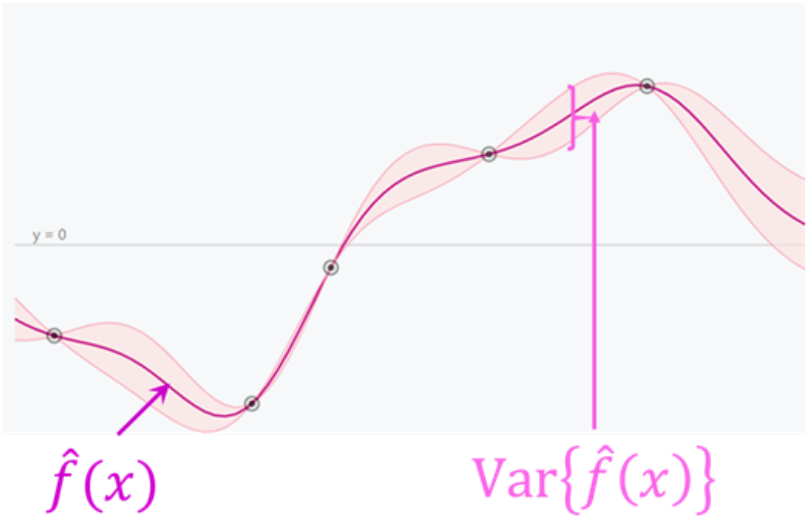
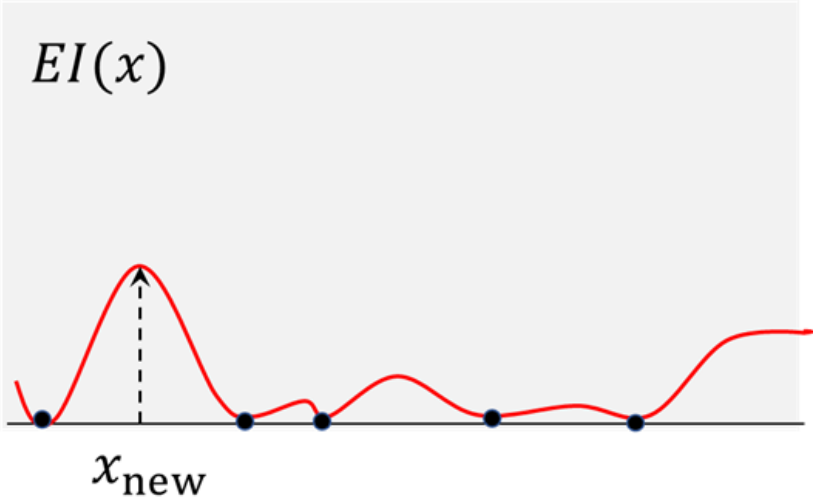
How to incorporate this **probabilistic** predictor within the **acquisition function**?





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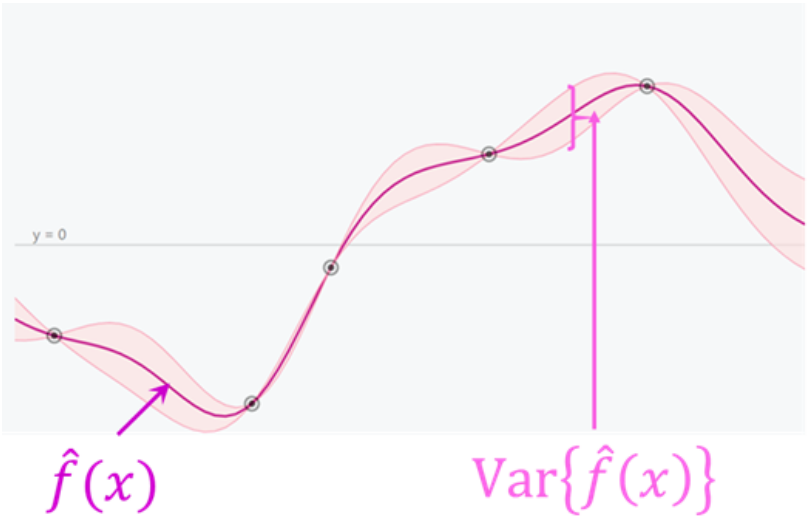

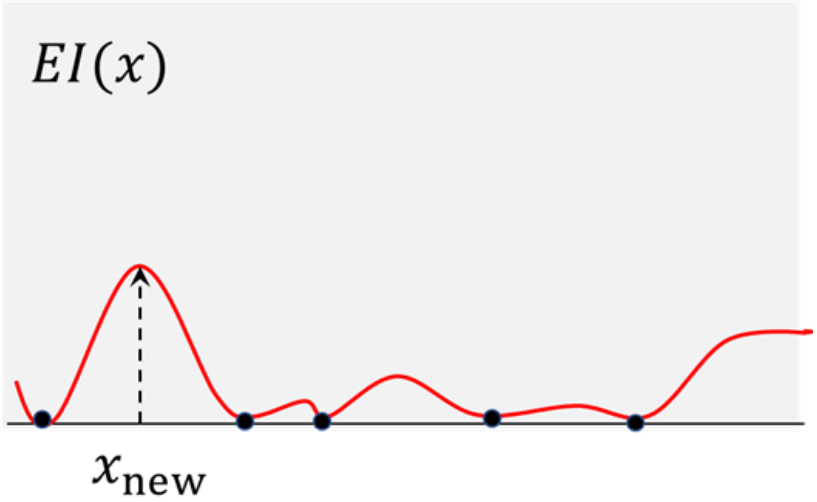

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Expected improvement (Jones et al. 1997)

$$\arg\max_{\boldsymbol{x}\in\Omega} \mathsf{EI}(\boldsymbol{x}) := \mathbb{E}[\max(y^* - f(\boldsymbol{x}), 0)|\mathcal{D}]$$

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In practice, the GP **variance** parameter σ^2 is **unknown** and needs to be **estimated**:

- **Estimate** σ^2 via MLE

$$\widehat{\sigma}^2 = \frac{1}{n}(\boldsymbol{y} - \boldsymbol{P}^\top \widehat{\boldsymbol{\beta}})^\top \boldsymbol{R}^{-1}(\boldsymbol{y} - \boldsymbol{P}^\top \widehat{\boldsymbol{\beta}})$$

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Sounds reasonable... what can go wrong?

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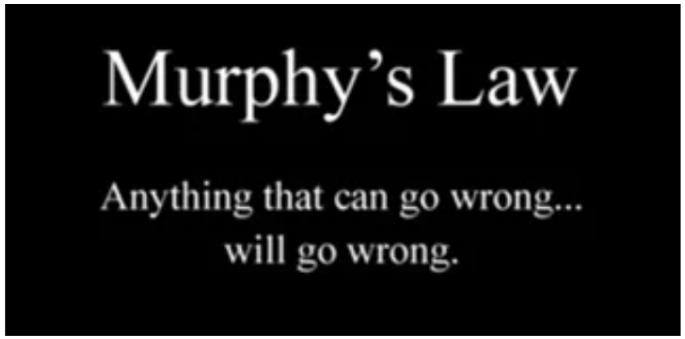

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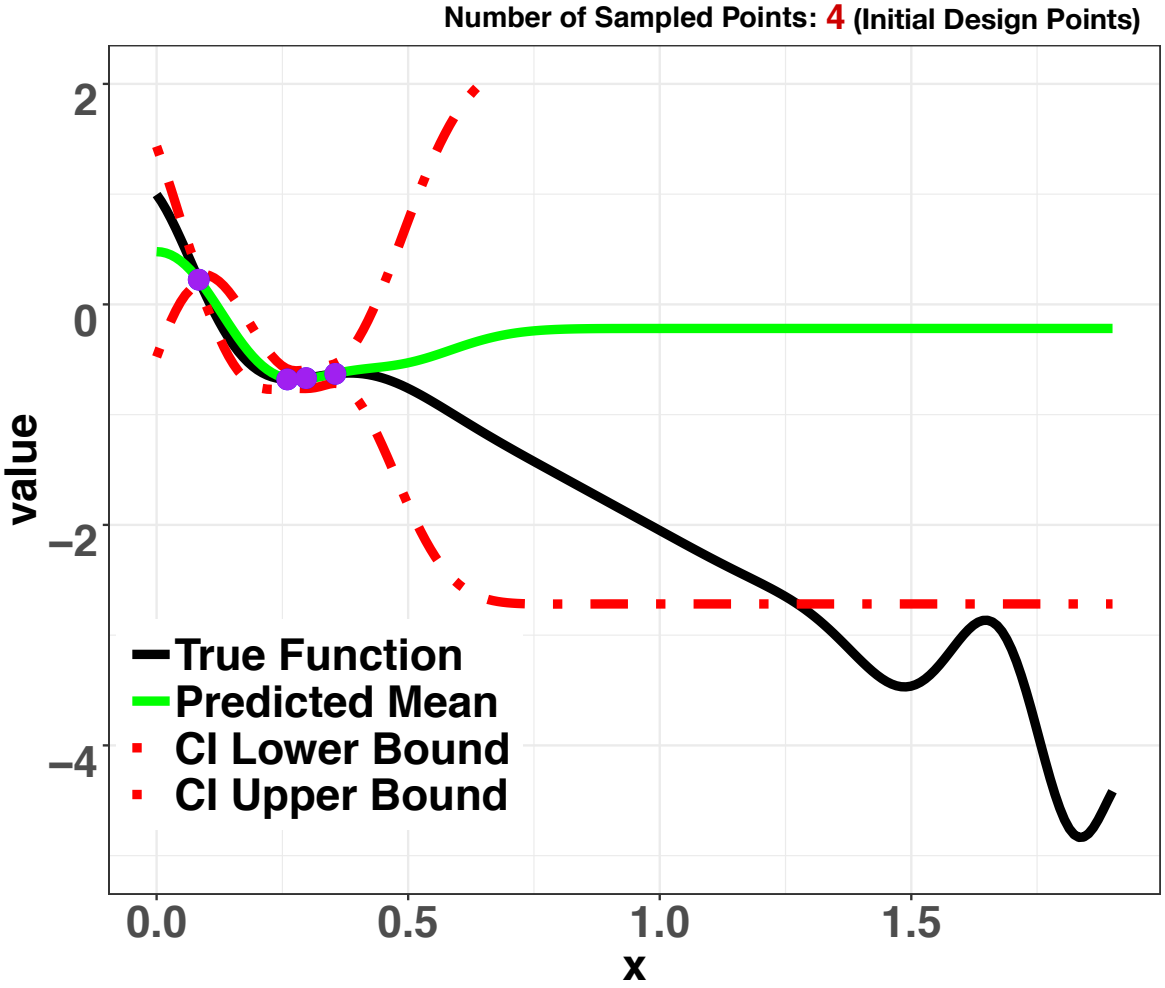
Let's try this **plug-in EI** approach:



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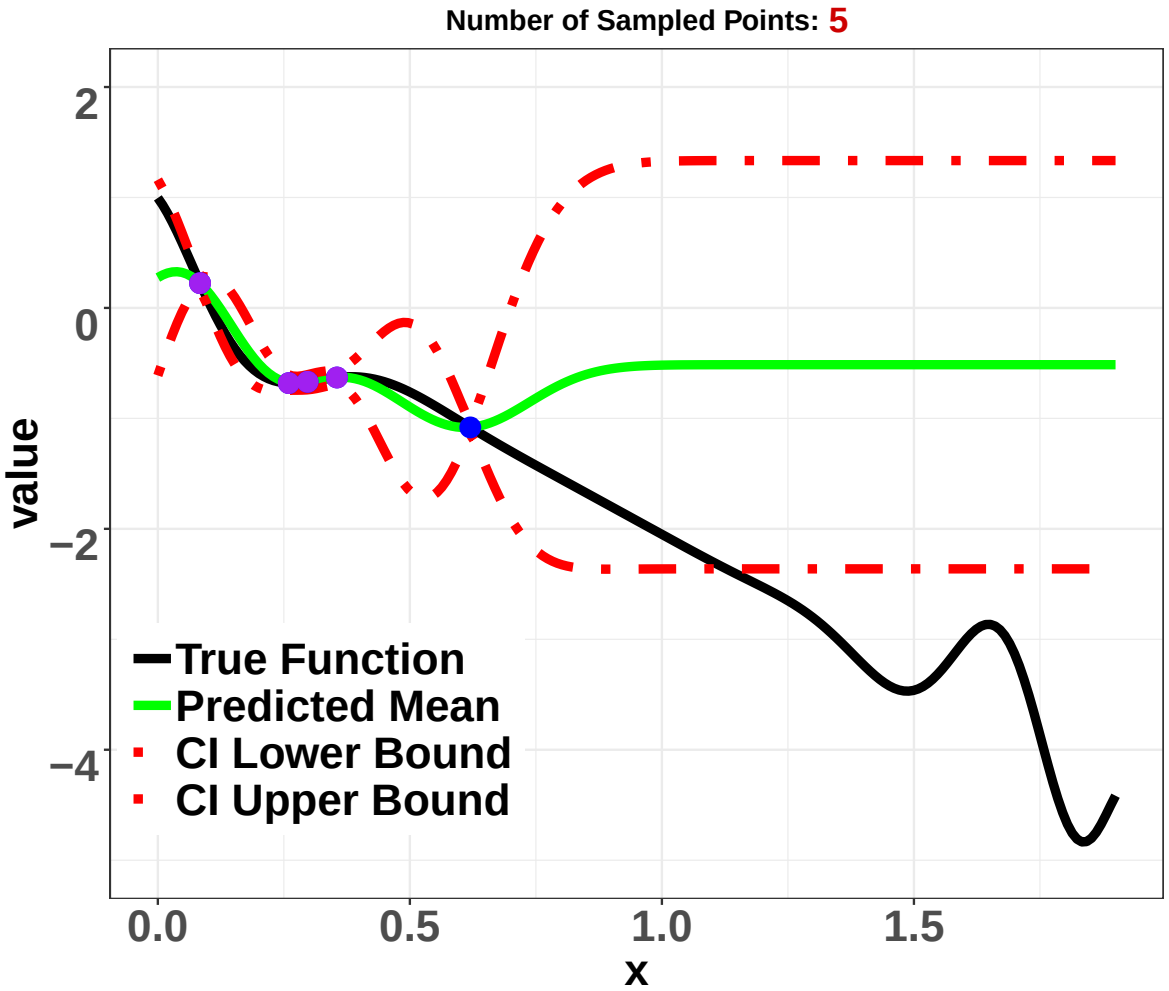

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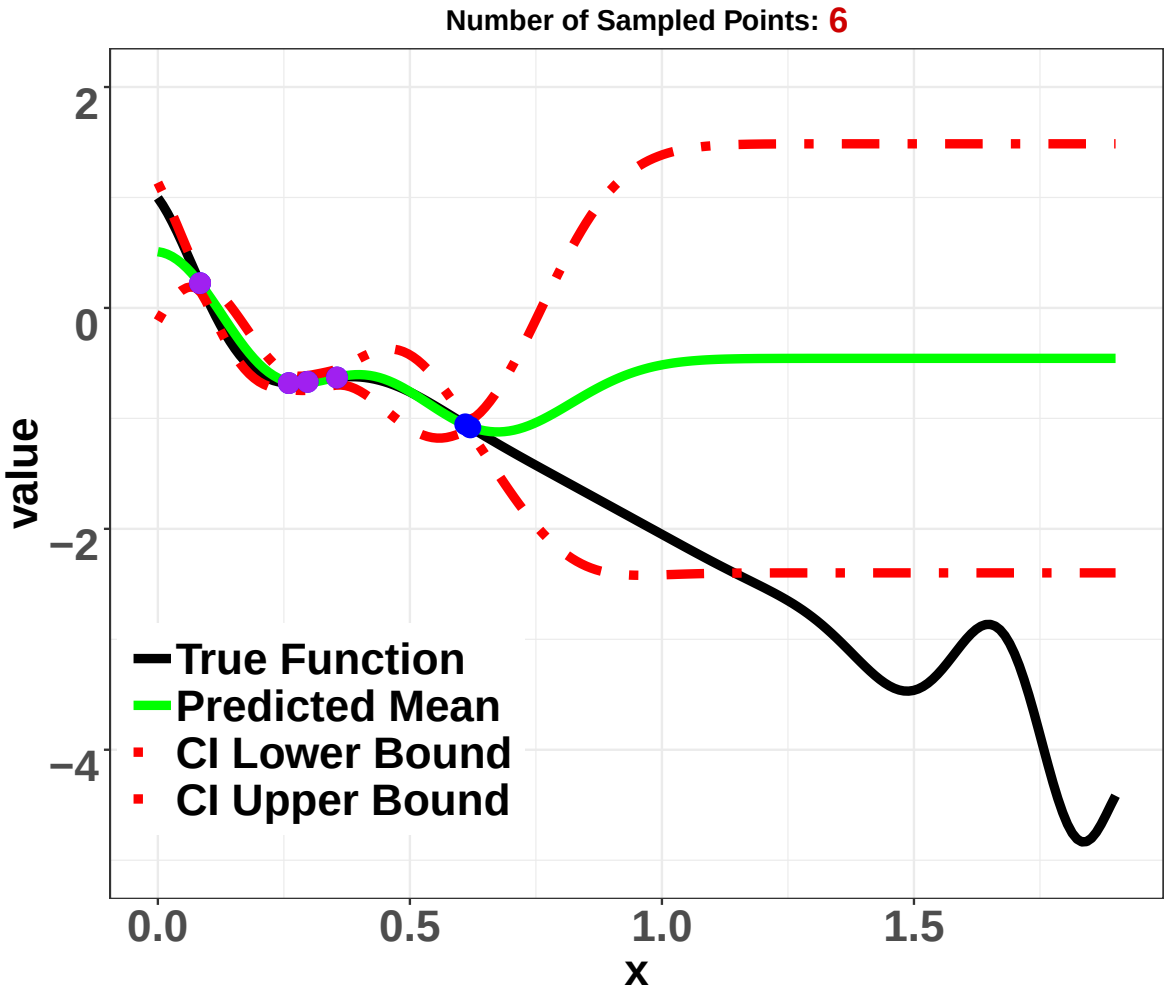

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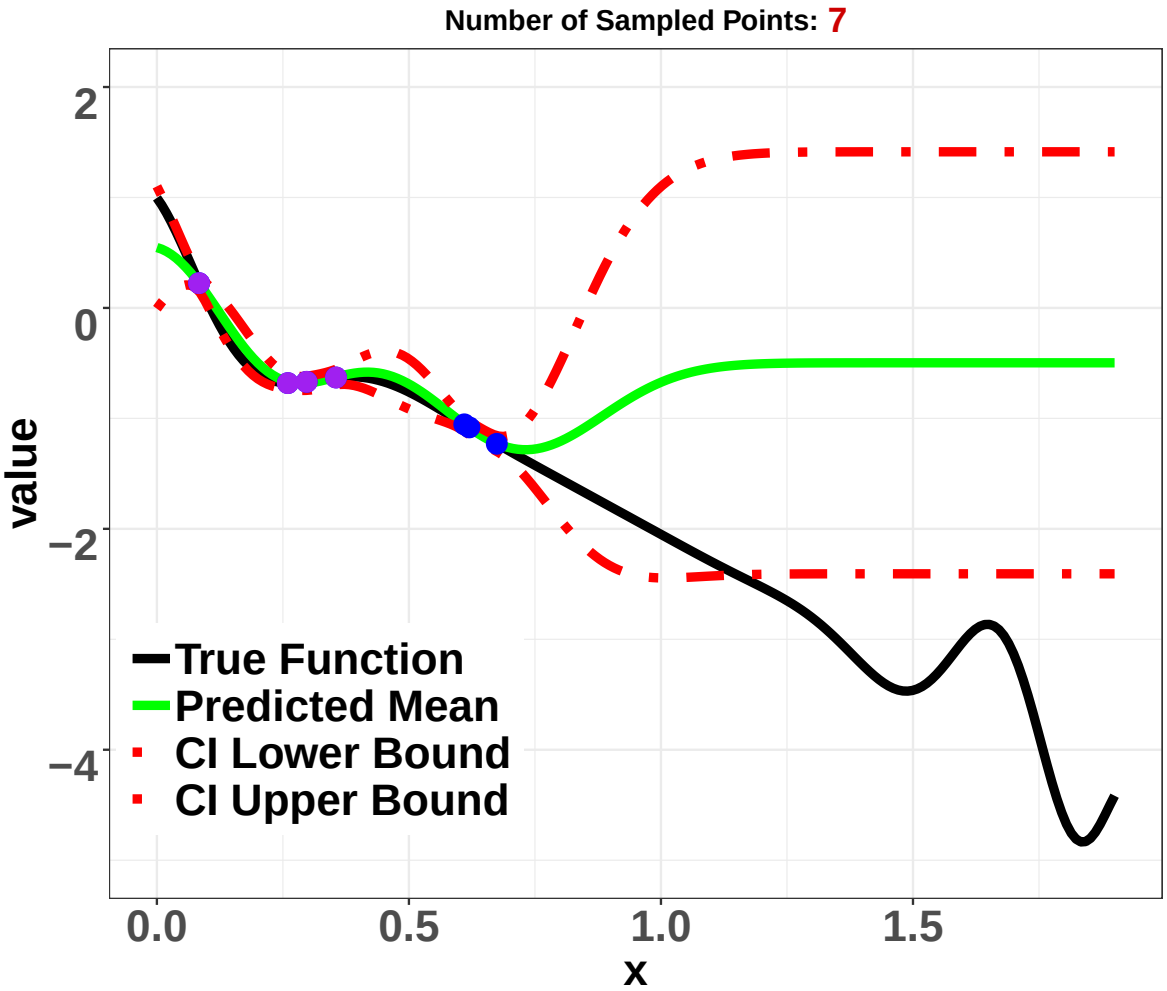

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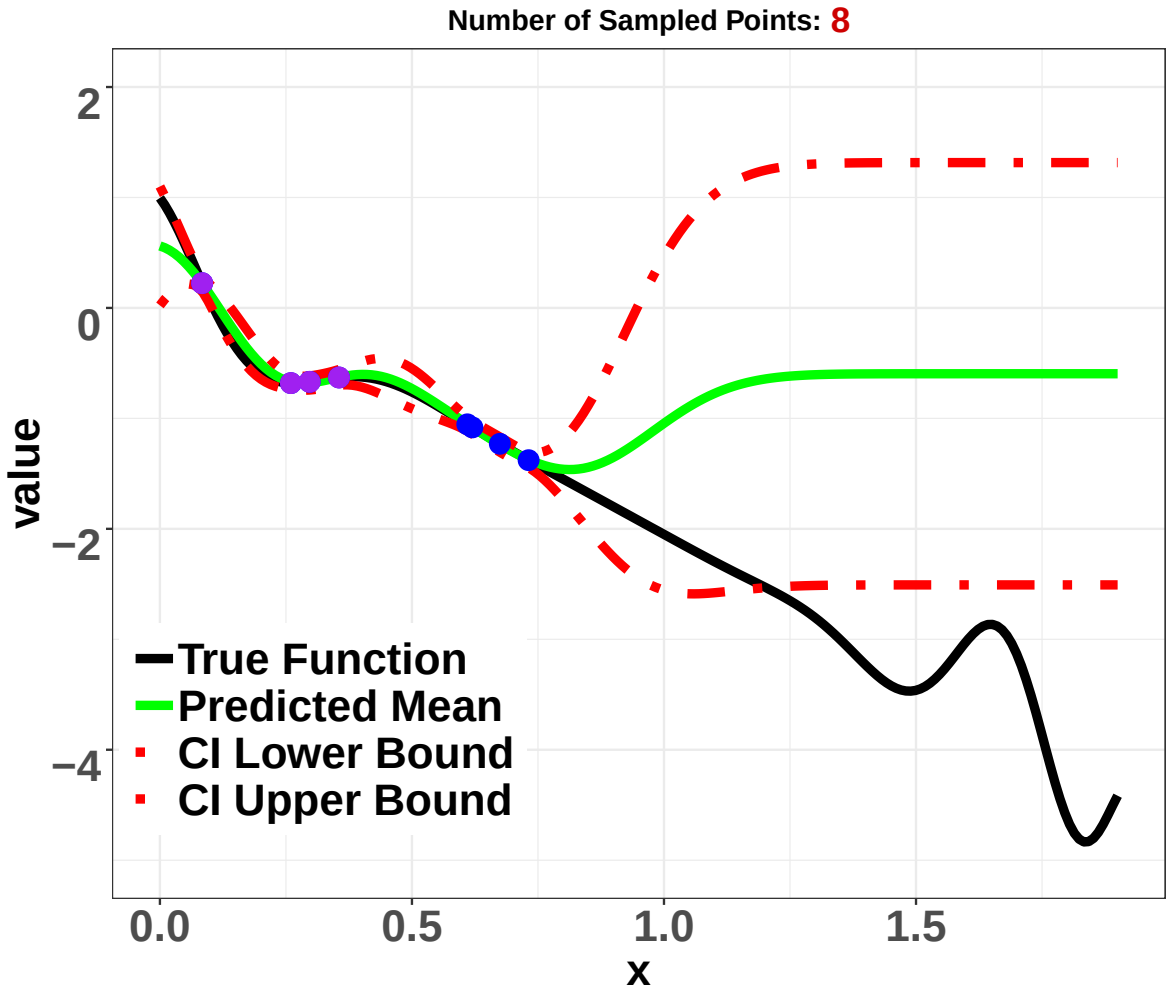

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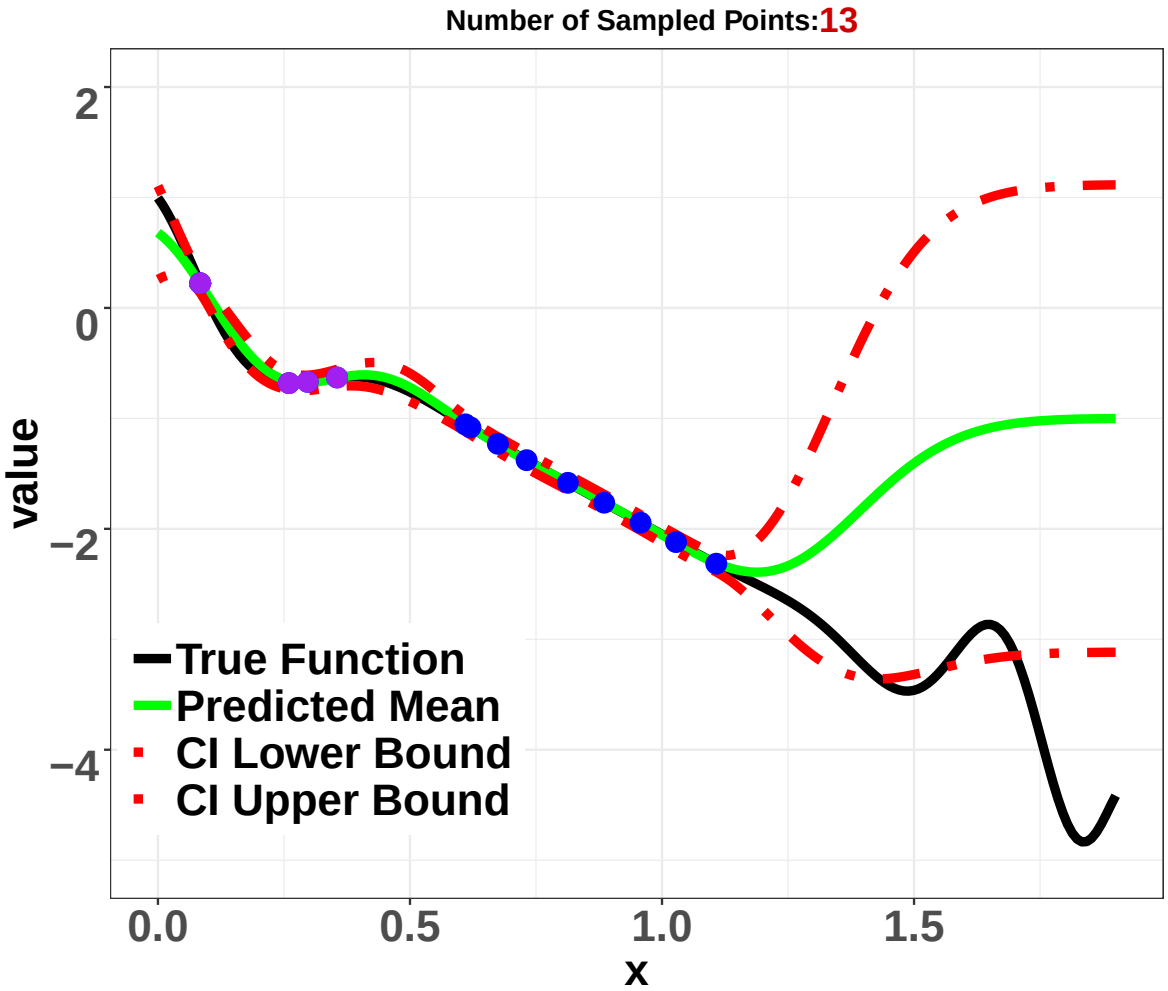

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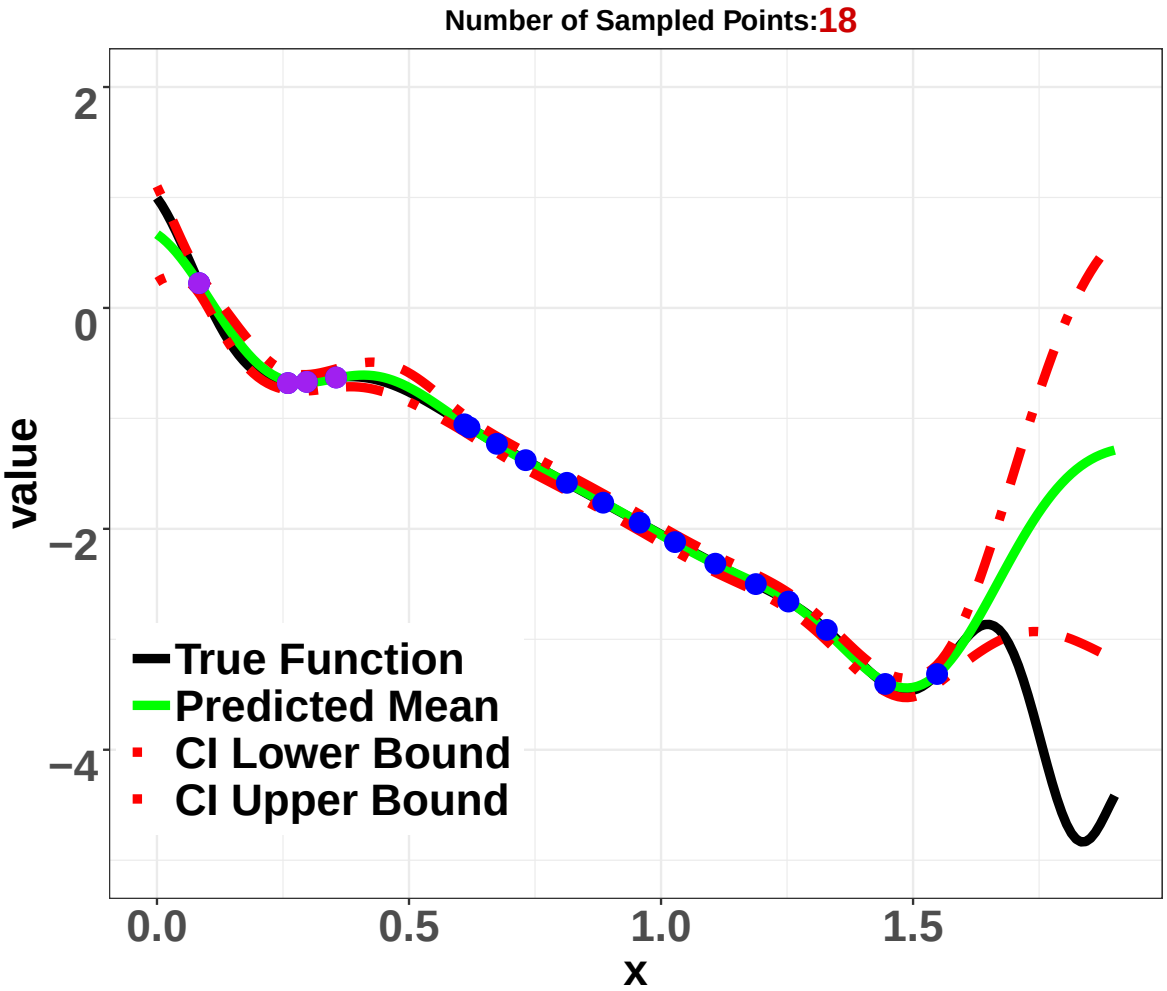

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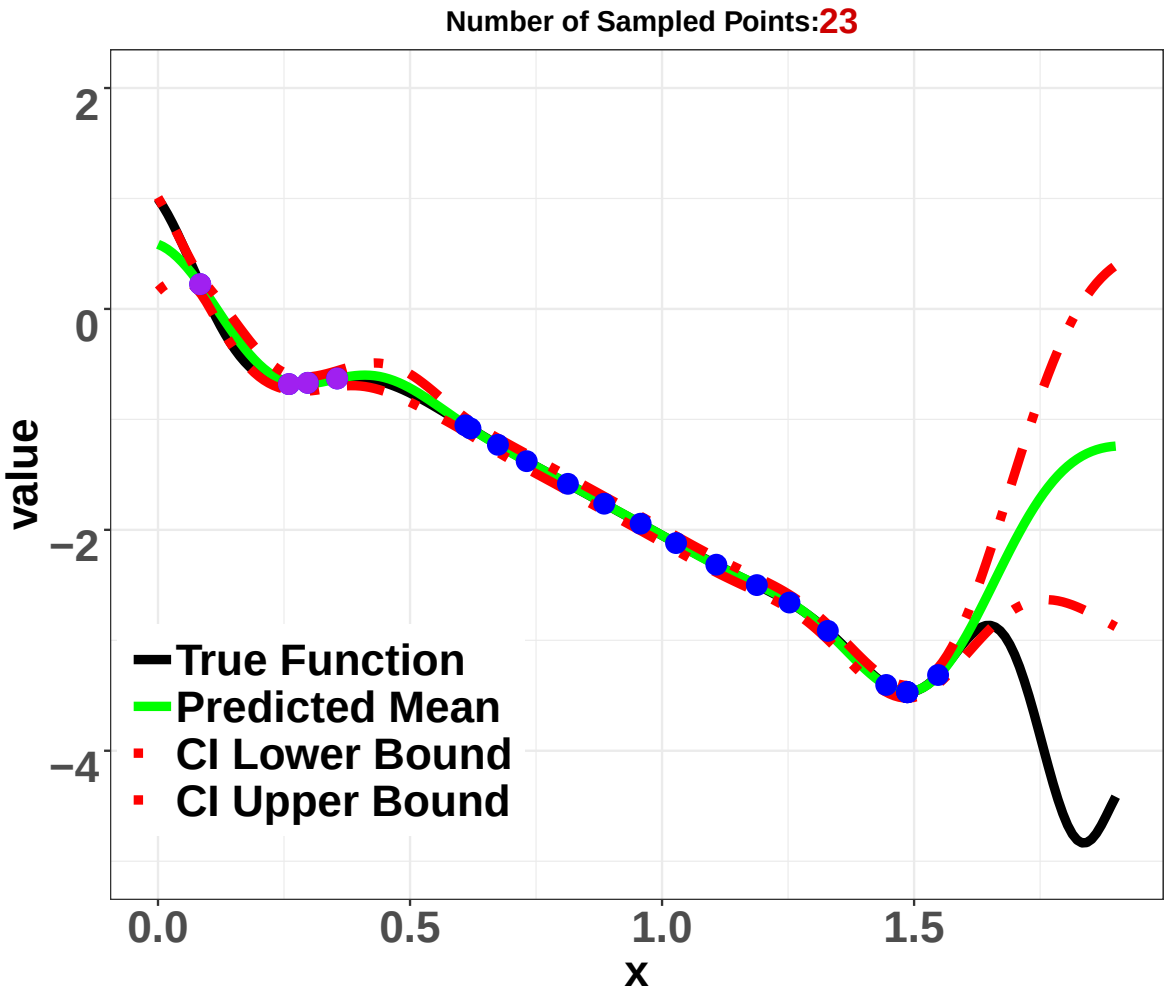

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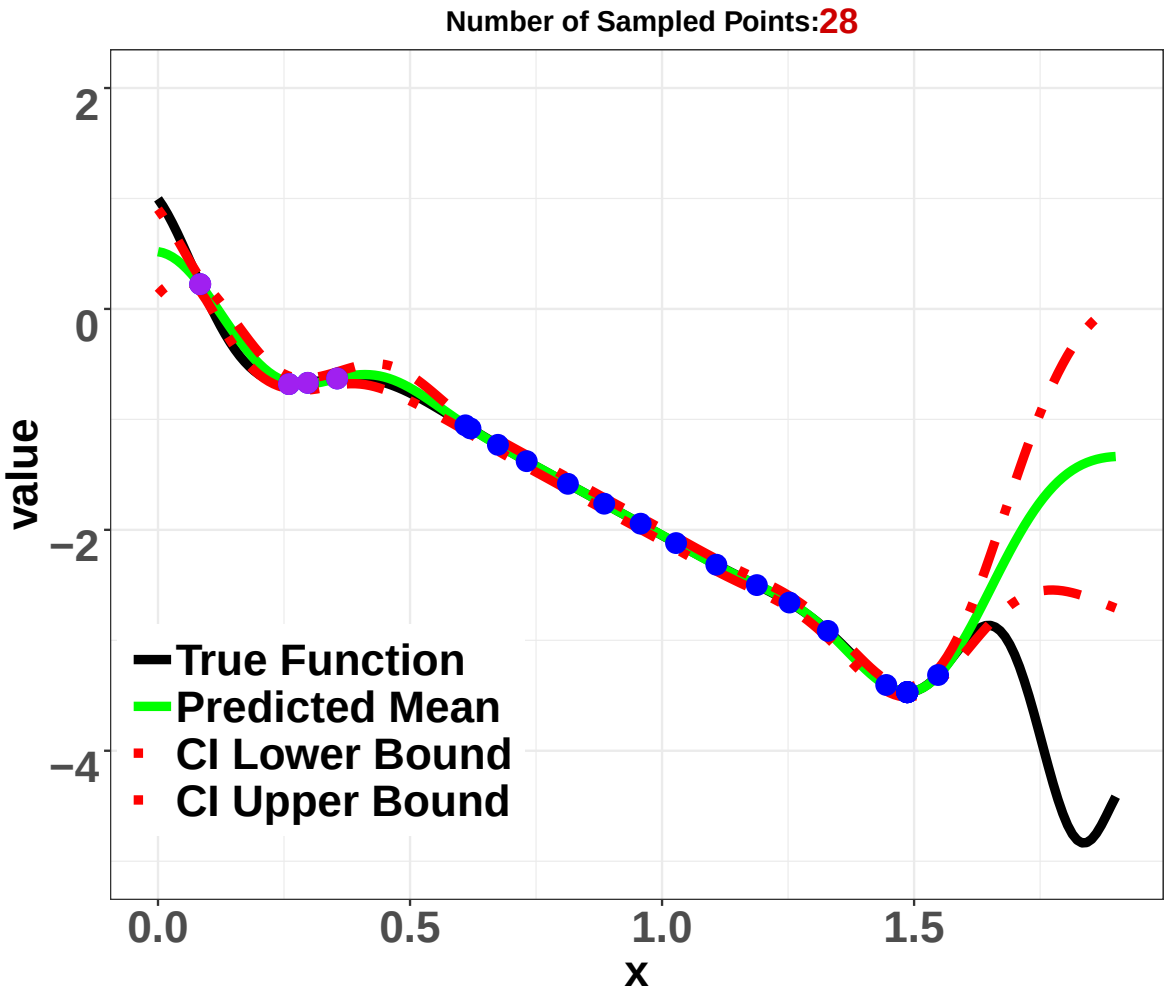

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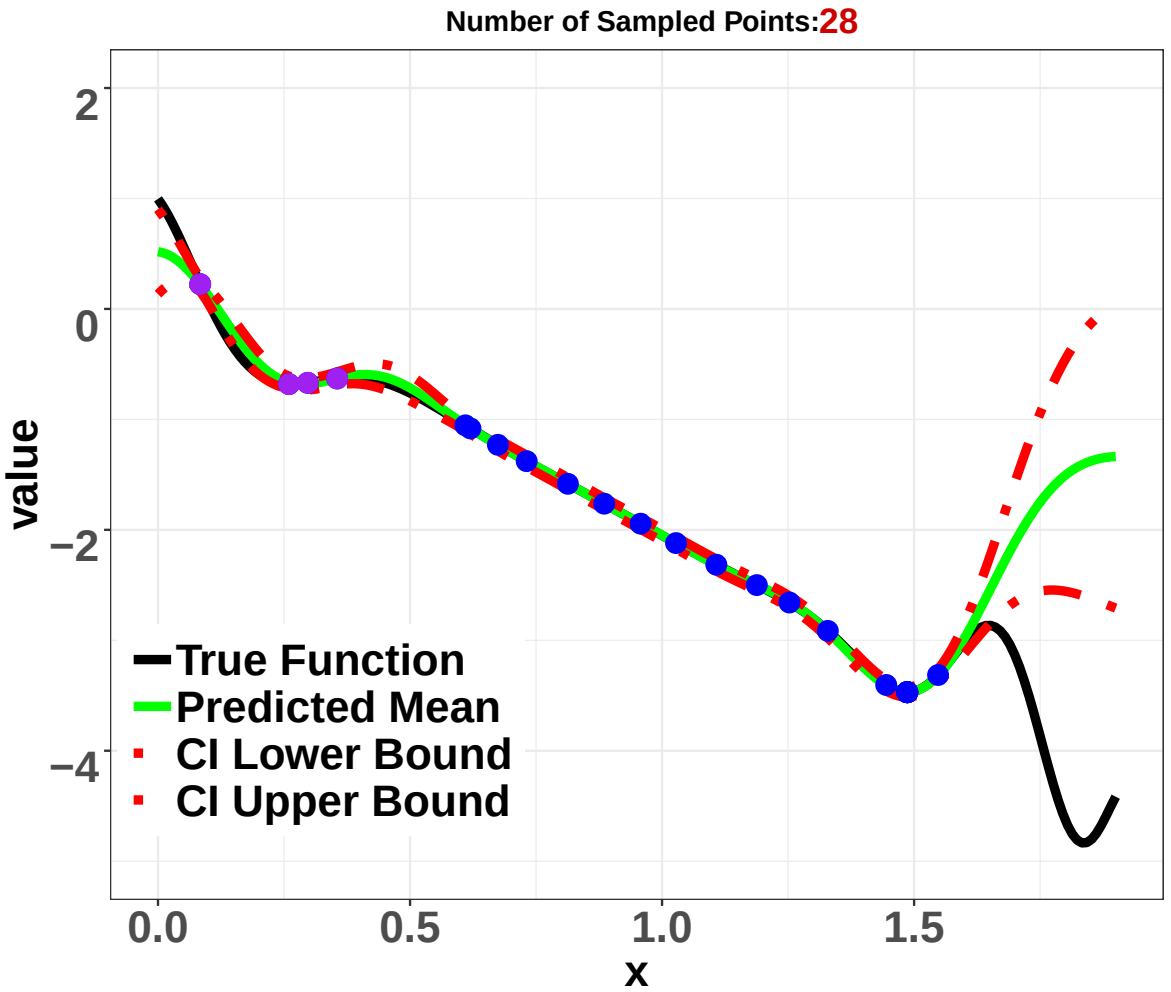

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- Bull (2011): EI can **fail** to find the global optima!

Theorem (Bull, 2011)

Given any $\epsilon > 0$ and any random initial design F, there exist some $\delta > 0$ and some f in a certain space,

$$\mathbb{P}_F(\min_n f(\boldsymbol{x}_n) - \min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) > \delta) \geq 1 - \epsilon,$$

where $(\boldsymbol{x}_n)_{n=1}^{\infty}$ is a solution sequence maximizing EI with plug-in MLEs $(\widehat{\beta}, \widehat{\sigma}^2)$.

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These methods encourage **more exploration**, but in *ad hoc* ways! Can we provide a **principled** solution to **over-exploitation** via a **hierarchical Bayesian** view on EI?

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$$\textbf{UK}: \quad f(\cdot) = \mu(\cdot) + Z(\cdot), \qquad Z(\cdot) \sim GP\{0, \sigma^2 r(\cdot,\cdot)\}$$

$$\textbf{Mean}: \quad \mu(\boldsymbol{x}) = \boldsymbol{p}^\top(\boldsymbol{x})\boldsymbol{\beta}, \qquad \textbf{Prior:} \quad [\boldsymbol{\beta}] \propto \mathbf{1}$$

$$\textbf{Covariance}: \quad \sigma^2 r(\cdot,\cdot), \qquad \textbf{Prior:} \quad [\sigma^2] \sim \text{Inv-Gamma}(a, b)$$

Still a **closed-form posterior** distribution (Santner et al., 2018):

$$\left[f(\boldsymbol{x})\middle|\mathcal{D}\right] \sim T(2\widetilde{a}, \widehat{f}_n(\boldsymbol{x}), \widetilde{\sigma}^2 s^2(\boldsymbol{x})).$$

- $T(2\widetilde{a}, \cdot, \cdot)$: **Student** t-distribution with d.f. $2\widetilde{a}$
- $\widetilde{a} = a + (n-q)/2$, $\widetilde{b} = b + n\widehat{\sigma}^2/2$, $\widetilde{\sigma}^2 = \widetilde{b}/\widetilde{a}$

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Hierarchical Expected Improvement

Do we get a **closed-form** expression for **expected improvement** under this **hierarchical** GP model?

$$\begin{aligned}\mathrm{HEI}(\boldsymbol{x}) &= \mathbb{E}[\max(y^* - f(\boldsymbol{x}), 0)|\mathcal{D}] \\ &= I(\boldsymbol{x})\Phi_{2\widetilde{a}}\left(\frac{I(\boldsymbol{x})}{\widetilde{\sigma}\, s_n(\boldsymbol{x})}\right) + \kappa\widetilde{\sigma}\, s_n(\boldsymbol{x})\phi_{2\widetilde{a}-2}\left(\frac{I(\boldsymbol{x})}{\kappa\widetilde{\sigma}\, s_n(\boldsymbol{x})}\right)\end{aligned}$$

- ϕ_ν, Φ_ν: p.d.f. and c.d.f. of a t-**distribution** with d.f. ν

Why is this **important**?

- Function **queries** are obtained via **maximizing** $\mathrm{HEI}(\boldsymbol{x})$

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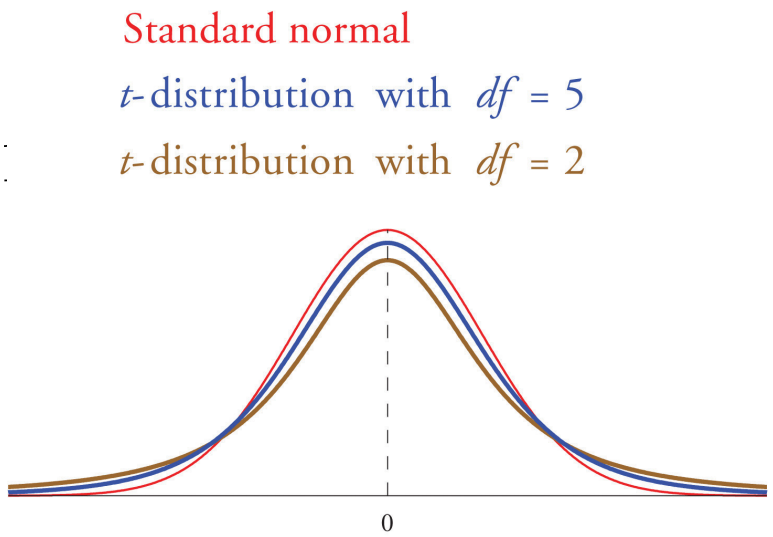

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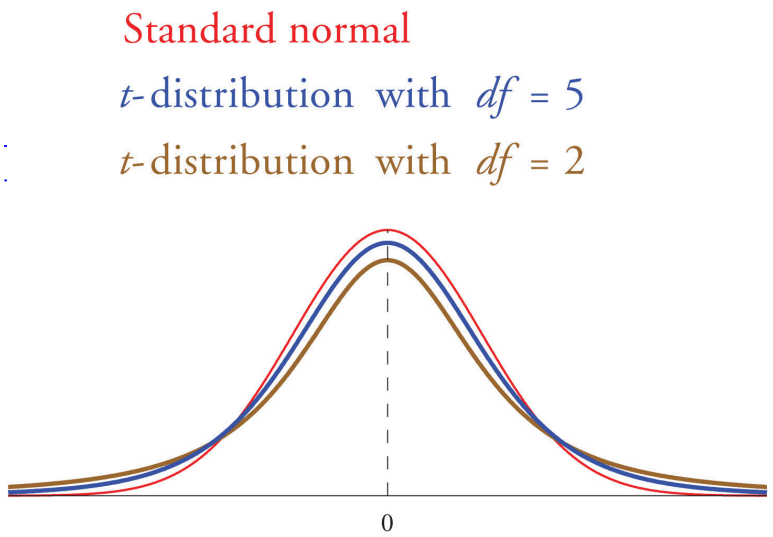

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How to set **hyperparameters** a and b in $[\sigma^2] \sim$ Inv-Gamma(a, b)?

- **HEI-Weak: Weakly informative** (Gelman et al 2004)

  $a = b$ small, *e.g.*, 0.1

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  Estimate hyperprior parameters via marginal likelihood

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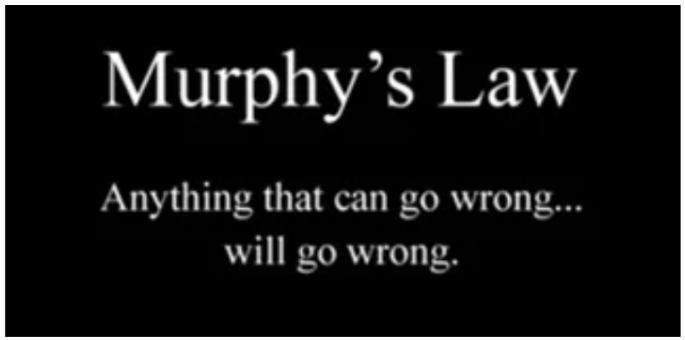

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Assume the following independent hyperpriors:

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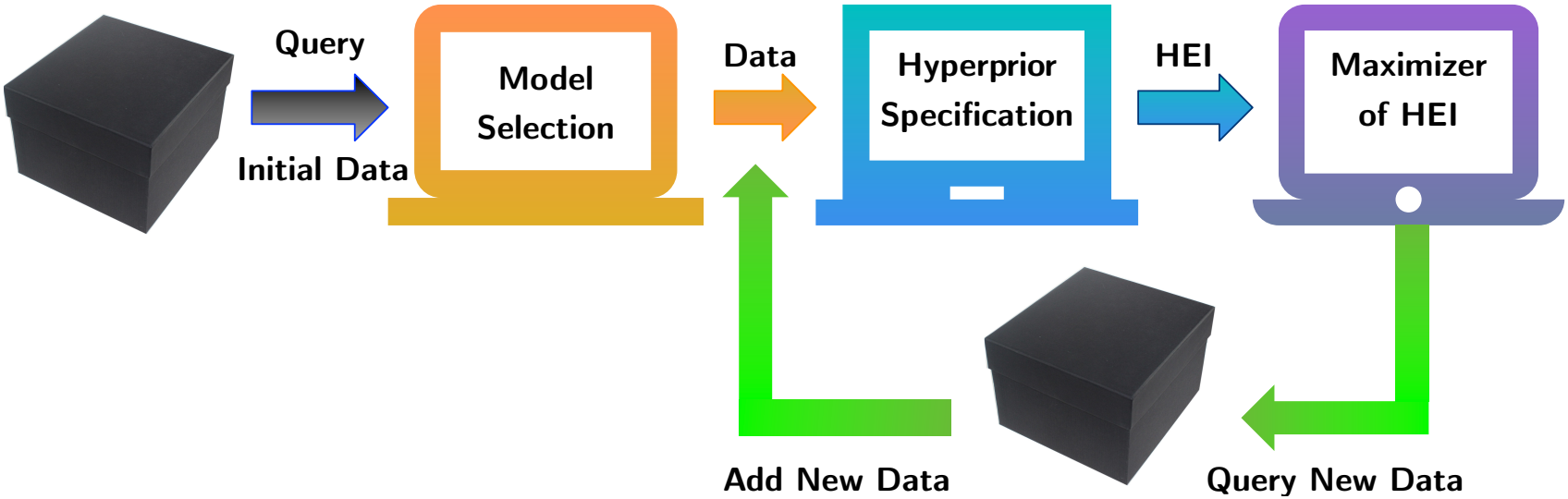

Query
Initial Data
Model Selection
Data
Hyperprior Specification
HEI
Maximizer of HEI
Add New Data
Query New Data

Algorithm

Algorithm 1 Hierarchical Expected Improvement for Bayesian Optimization

Initialization

- Generate n_{ini} space-filling design points $\{\mathbf{x}_1, \cdots, \mathbf{x}_{n_{\text{ini}}}\}$ on Ω.
- Evaluate function points $y_i = f(\mathbf{x}_i)$, yielding the initial dataset $\mathcal{D}_{n_{\text{ini}}} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n_{\text{ini}}}$.

Model selection

- Select model order via BIC using (21).
- Estimate hyperparameters (a, b) via MMAP using (18).

Optimization

for $n \leftarrow n_{\text{ini}}$ *to* $n_{\text{tot}} - 1$ **do**

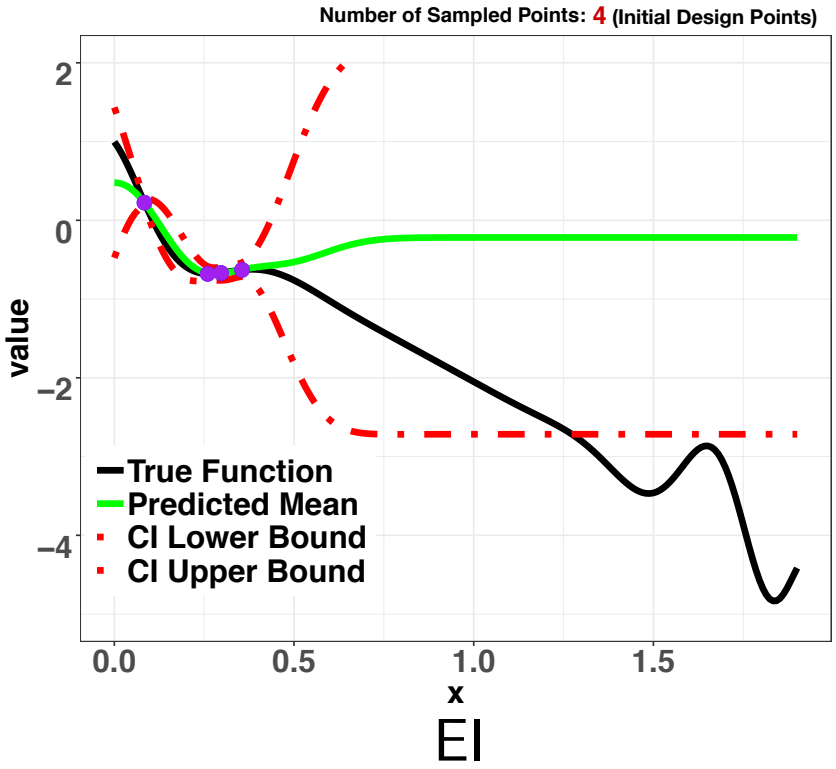
- Given $\mathcal{D}_n$, estimate length-scale parameters $\boldsymbol{\theta}$ via MAP and compute $\text{HEI}_n(\mathbf{x})$.
- Obtain the next evaluation point $\mathbf{x}_{n+1}$ by maximizing $\text{HEI}_n(\mathbf{x})$:

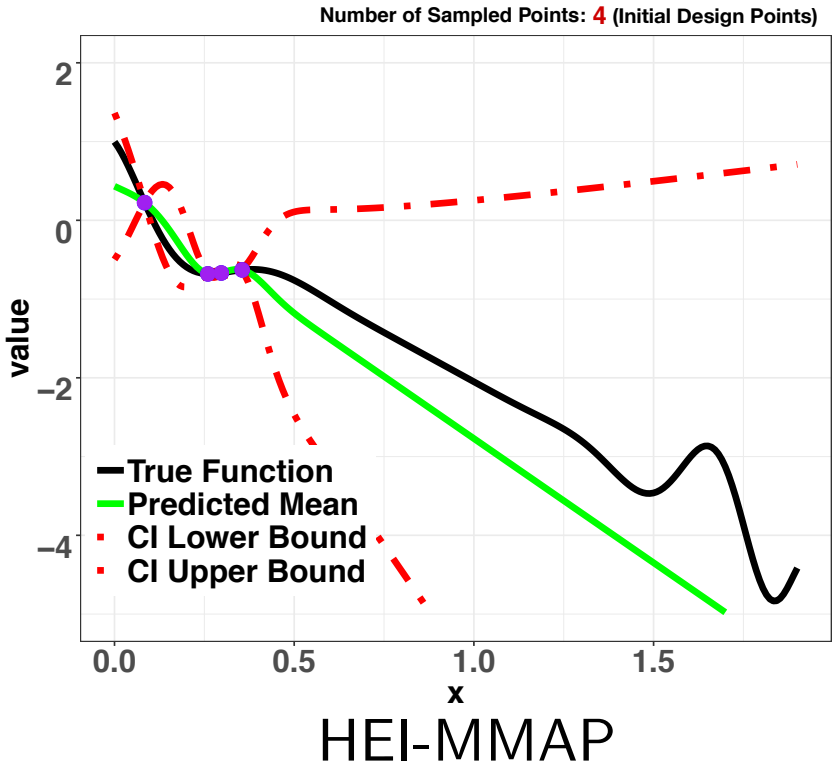
$$\mathbf{x}_{n+1} \leftarrow \underset{\mathbf{x} \in \Omega}{\text{argmax}}\, \text{HEI}_n(\mathbf{x}).$$

- Evaluate $y_{n+1} = f(\mathbf{x}_{n+1})$, and update data $\mathcal{D}_{n+1} = \mathcal{D}_n \cup \{(\mathbf{x}_{n+1}, y_{n+1})\}$.

Return: The best observed solution $\mathbf{x}_{i^*}$, where $i^* = \text{argmin}_{i=1}^{n_{\text{tot}}} f(\mathbf{x}_i)$.

Back to example





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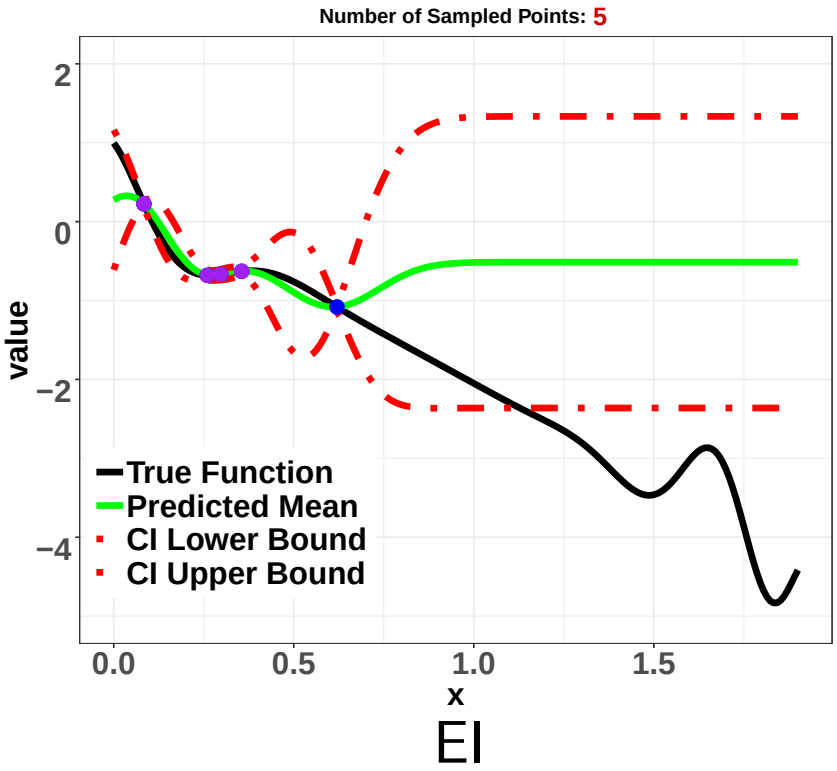

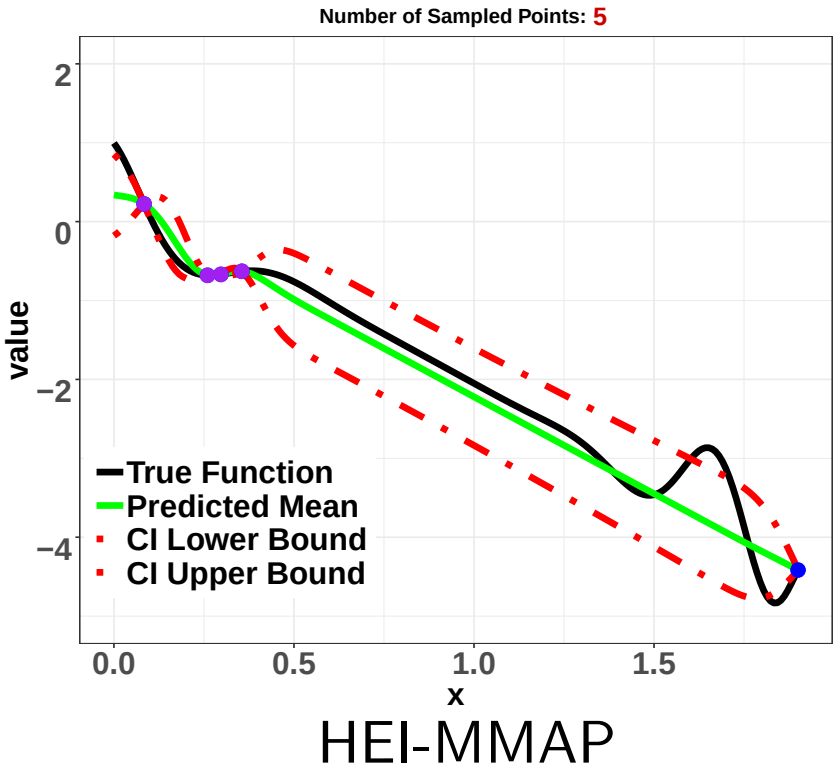

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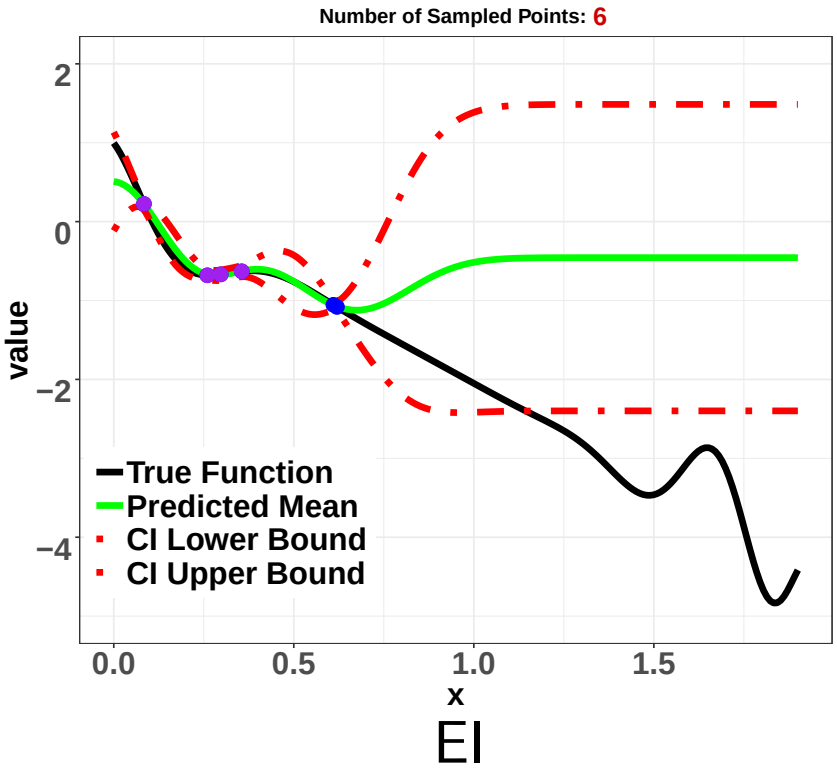

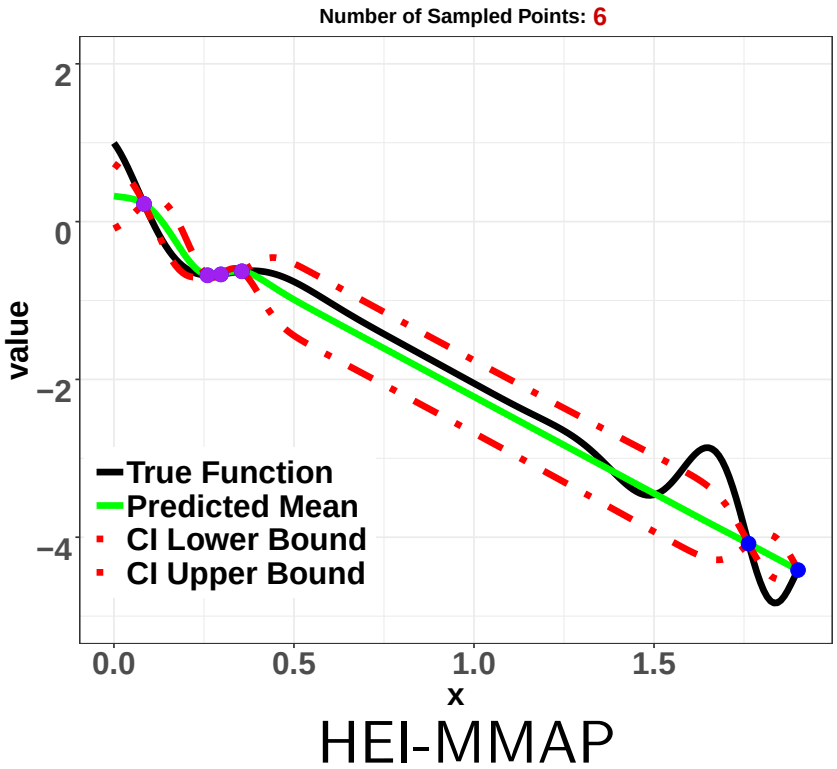

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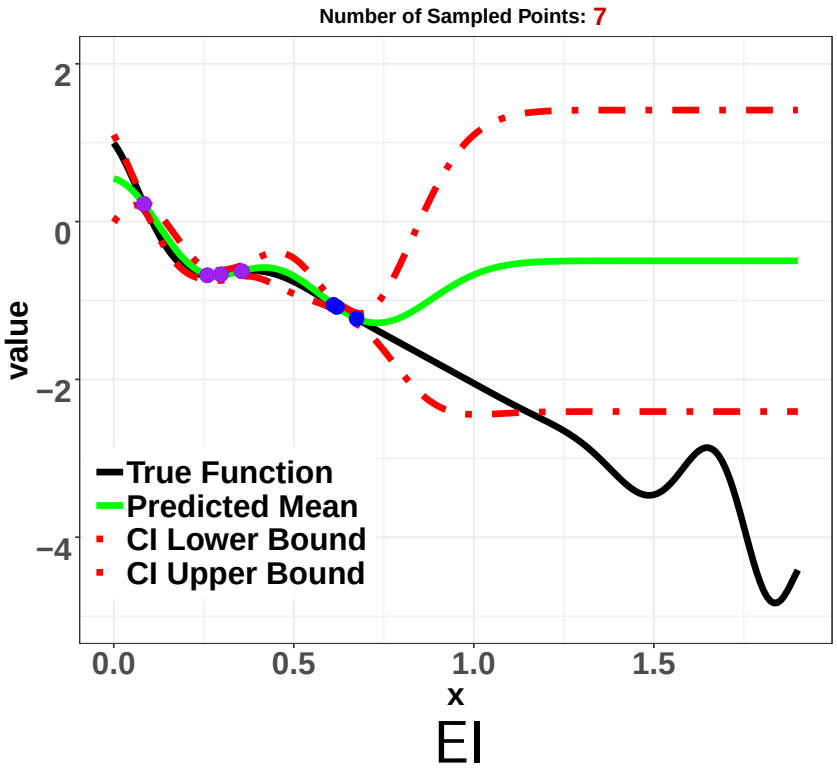

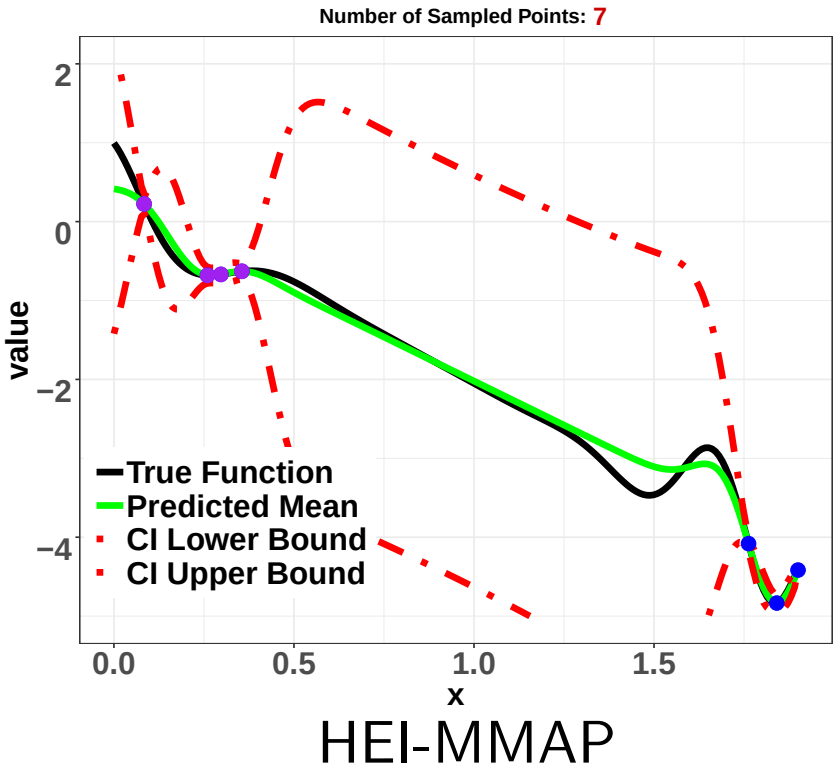

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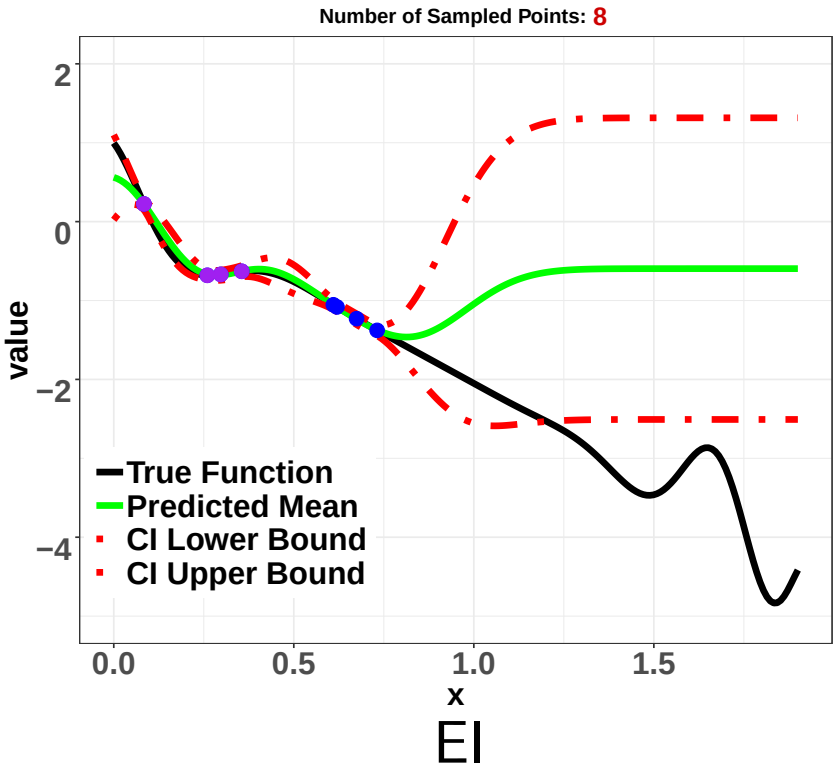

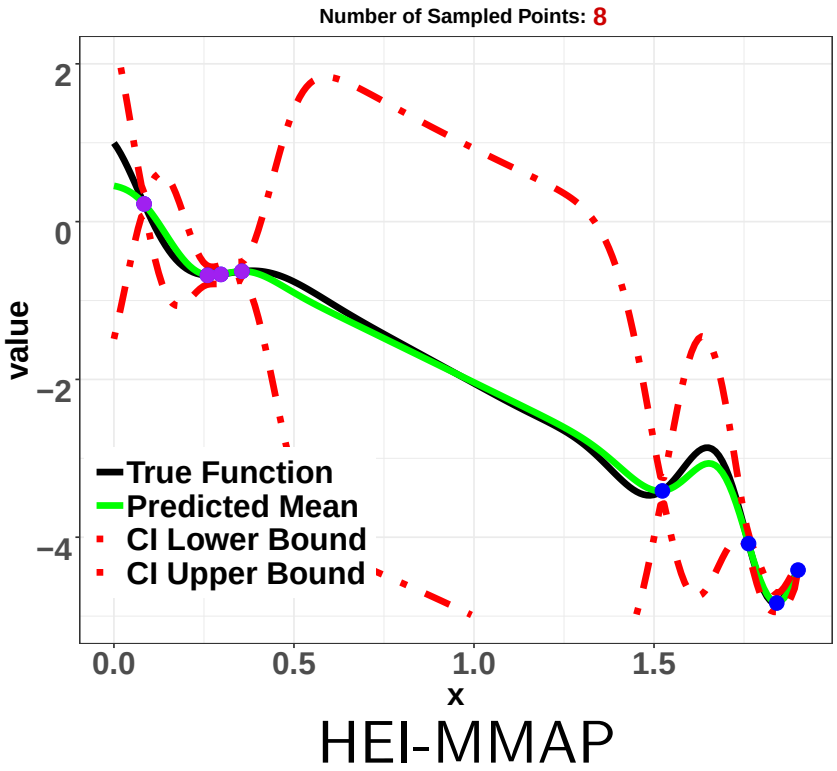

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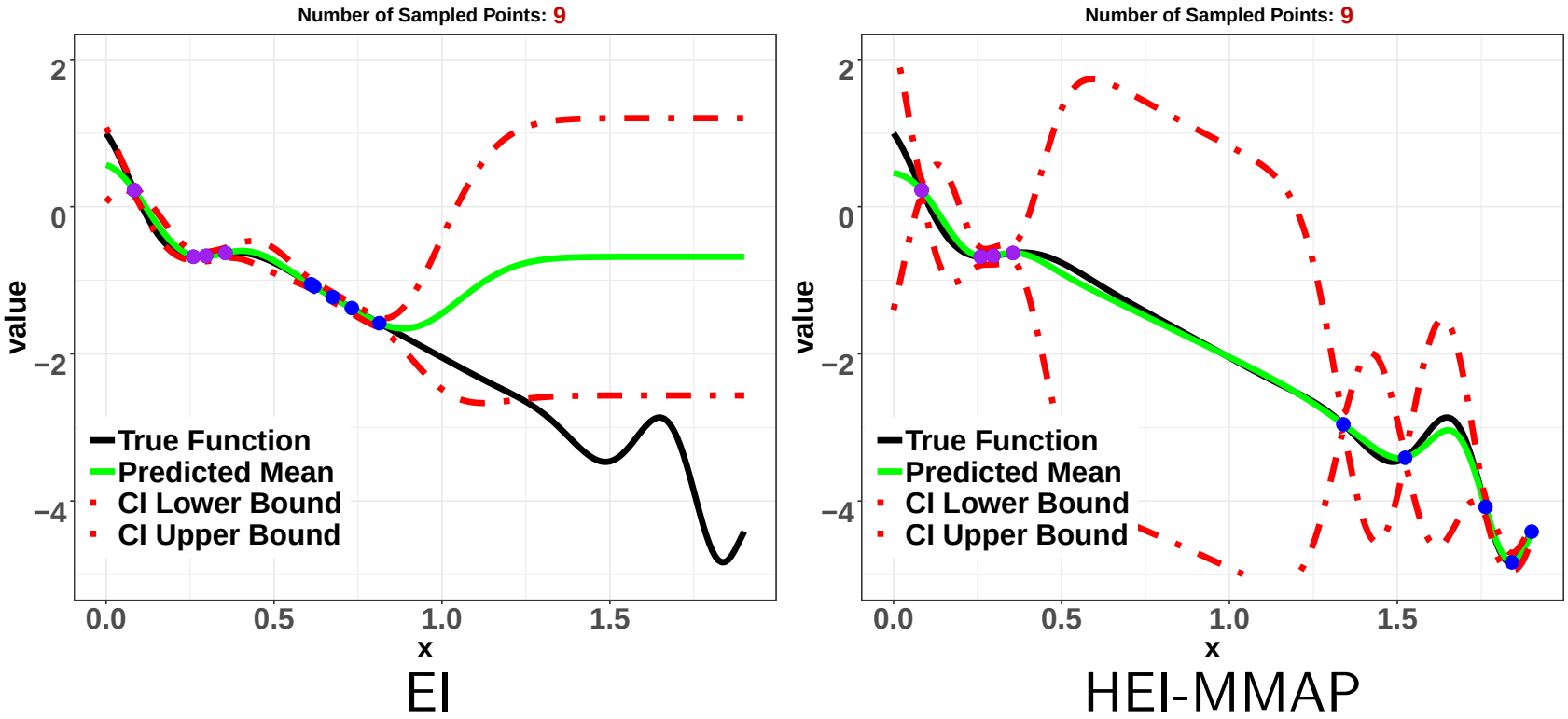

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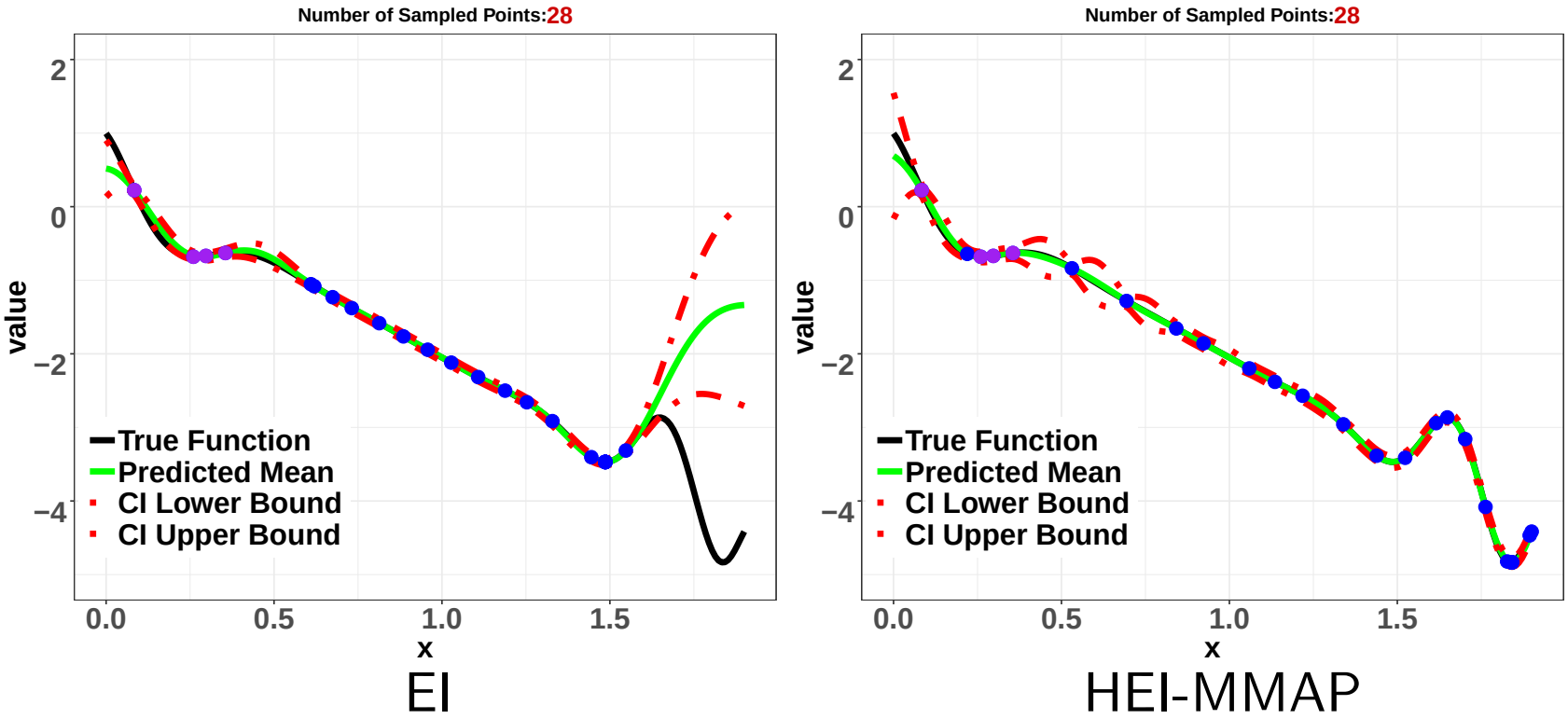

- EI gets **stuck** at **local optimum**, HEI **finds** the **global optimum**

Global convergence

Theorem (Chen, Mak, Wu 2023)

Suppose a is a constant, $b = \Theta(n)$, and correlation $r(\boldsymbol{x})$ satisfies

$$|r(\boldsymbol{x}) - Q_{\lfloor 2\nu \rfloor}(\boldsymbol{x})| = \mathcal{O}\big(\|\boldsymbol{x}\|^{2\nu}(-\log\|\boldsymbol{x}\|)^{2\alpha}\big), \quad \text{as } \|\boldsymbol{x}\| \to 0,$$

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$$\min_n f(\boldsymbol{x}_n) - \min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) = \begin{cases} \mathcal{O}(n^{-\nu/d}(\log n)^{\alpha}), & \nu \le 1 \\ \mathcal{O}(n^{-1/d}), & \nu > 1 \end{cases},$$

where $(\boldsymbol{x}_n)_{n=1}^{\infty}$ is the solution sequence by maximizing HEI.

- Theory requires a **data size dependent** hyperprior on $\sigma^2 \sim IG(a, b)$, namely $b = \Theta(n)$
- **Matérn correlation** (Stein 2012) satisfies the conditions on $r(\boldsymbol{x})$

Minimax rate

γ-**stability** condition (Wynne et al. 2020):

$$s_n(\boldsymbol{x}_{n+1}) \geq \gamma \|s_n(\boldsymbol{x})\|_\infty \quad \text{for all } n = 1, 2, \cdots, \tag{1}$$

- $s_n(\boldsymbol{x})$: **posterior variance** term from GP

With this, we can then show the following optimization rate:

Theorem (Chen, Mak, Wu 2023)

Assume the earlier conditions hold. Then for any $f \in \mathcal{H}_r(\Omega)$:

$$\min_n f(\boldsymbol{x}_n) - \min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}) = O(n^{-\nu/d}),$$

where $(\boldsymbol{x}_n)_{n=1}^\infty$ is the solution sequence maximizing HEI with the γ-stability condition, with $\gamma \in (0, 1)$.

This is precisely the **minimax** rate for $f \in \mathcal{H}_r(\Omega)$ (Bull 2011)!

Minimax rate

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Minimax rate

Algorithm 1 Hierarchical Expected Improvement for Bayesian Optimization

Initialization

- Generate n_{ini} space-filling design points $\{\mathbf{x}_1, \cdots, \mathbf{x}_{n_{\text{ini}}}\}$ on Ω.
- Evaluate function points $y_i = f(\mathbf{x}_i)$, yielding the initial dataset $\mathcal{D}_{n_{\text{ini}}} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n_{\text{ini}}}$.

Model selection

- Select model order via BIC using (21).
- Estimate hyperparameters (a, b) via MMAP using (18).

Optimization

for $n \leftarrow n_{\text{ini}}$ *to* $n_{\text{tot}} - 1$ **do**

- Given $\mathcal{D}_n$, estimate length-scale parameters $\boldsymbol{\theta}$ via MAP and compute $\text{HEI}_n(\mathbf{x})$.
- Obtain the next evaluation point $\mathbf{x}_{n+1}$ by maximizing $\text{HEI}_n(\mathbf{x})$:

Add in stability condition as constraint

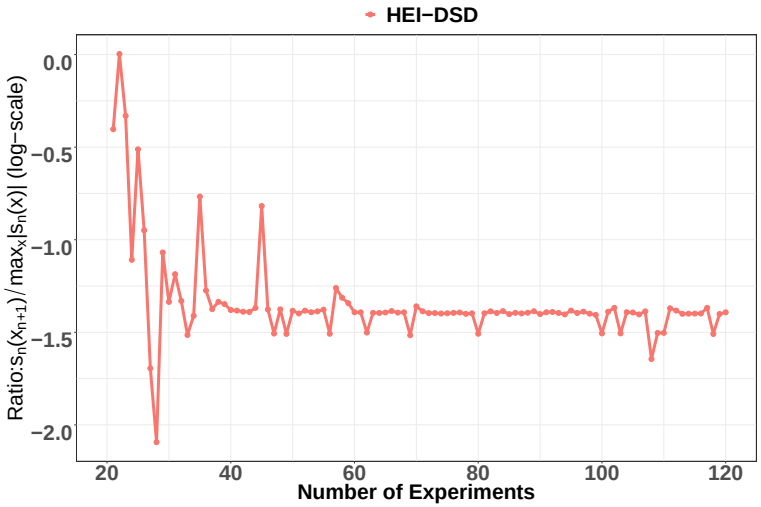
$$\mathbf{x}_{n+1} \leftarrow \underset{\mathbf{x} \in \Omega}{\text{argmax}}\, \text{HEI}_n(\mathbf{x}).$$

- Evaluate $y_{n+1} = f(\mathbf{x}_{n+1})$, and update data $\mathcal{D}_{n+1} = \mathcal{D}_n \cup \{(\mathbf{x}_{n+1}, y_{n+1})\}$.

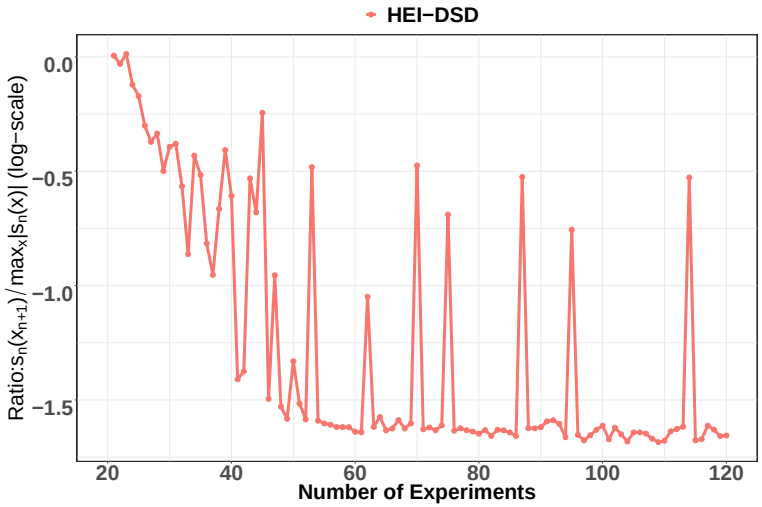
Return: The best observed solution $\mathbf{x}_{i^*}$, where $i^* = \text{argmin}_{i=1}^{n_{\text{tot}}} f(\mathbf{x}_i)$.

Minimax rate

... but in practice, this γ-**stability condition** seems to **hold** without an **explicit** constraint on the HEI



Branin



Camel Three-Hump

Minimax rate

Why is our rate $O(n^{-\nu/d})$ **minimax**?

- Bull (2011): the minimax rate is $O(n^{-\nu/d})$ for $f \in \mathcal{H}_r(\Omega)$
- This rate, however, can be achieved by a **non-adaptive quasi-uniform** strategy, which performs **terribly** in practice!

Rates don't tell the whole story!

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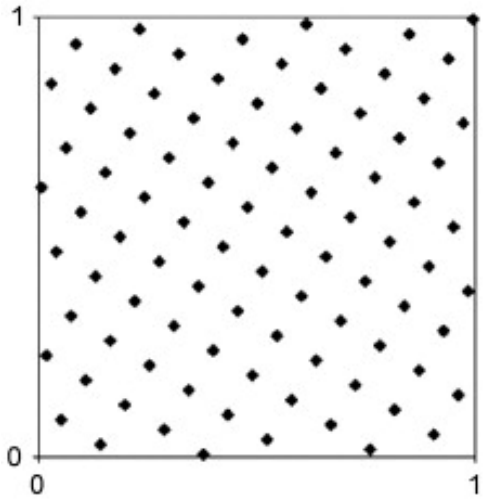

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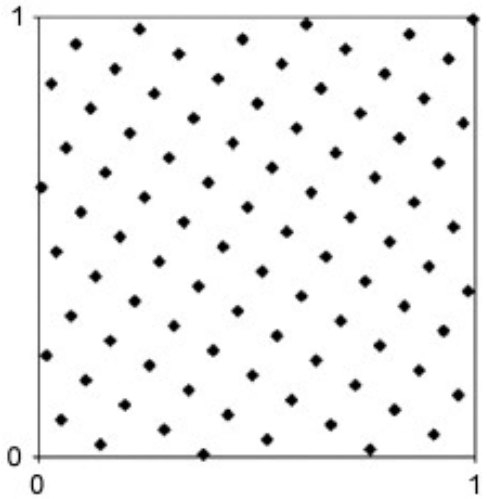


Rates don't tell the whole story!

Test functions

HEI methods:

- HEI-Weak, HEI-MMAP, HEI-DSD

Plug-in EI methods (Jones et al 1997):

- EI-OK, EI-UK

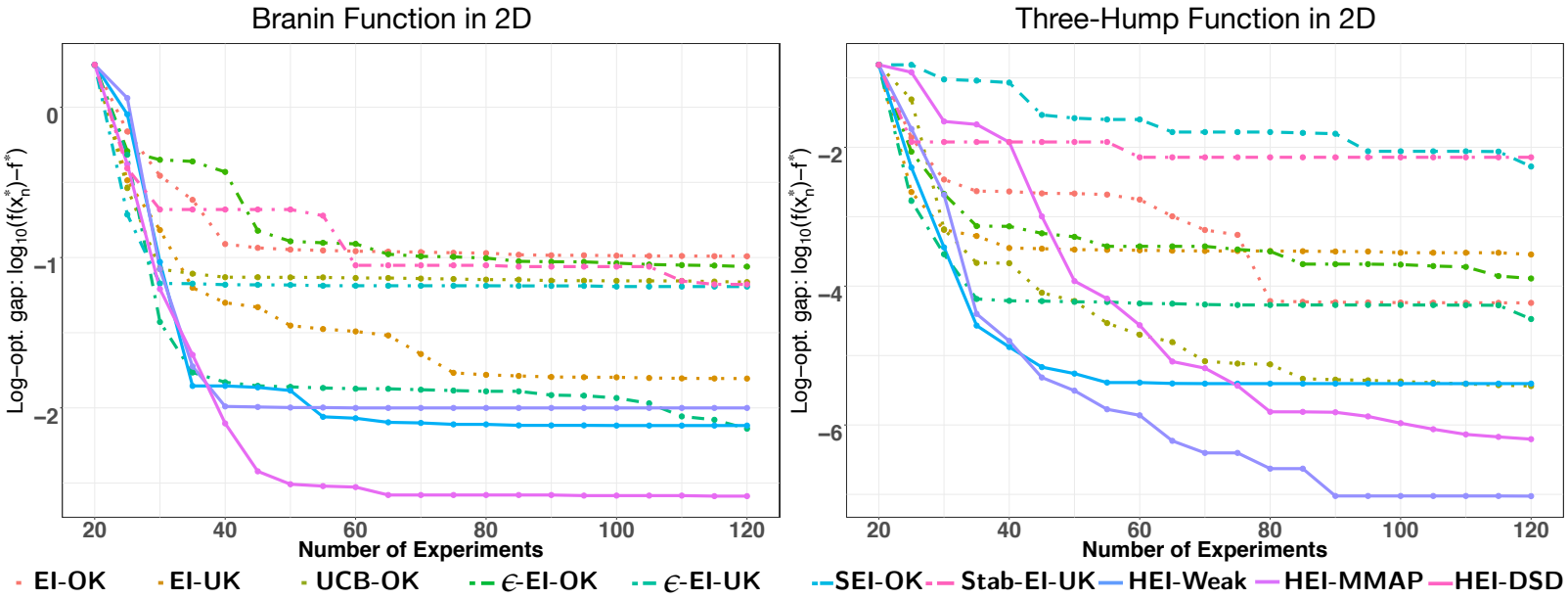
ϵ-**greedy EI** methods (Bull 2011):

- ϵ-EI-OK, ϵ-EI-UK, with $\epsilon = 0.1$ (Sutton & Barto 2018)

UCB-EI methods (Srinivas et al 2010):

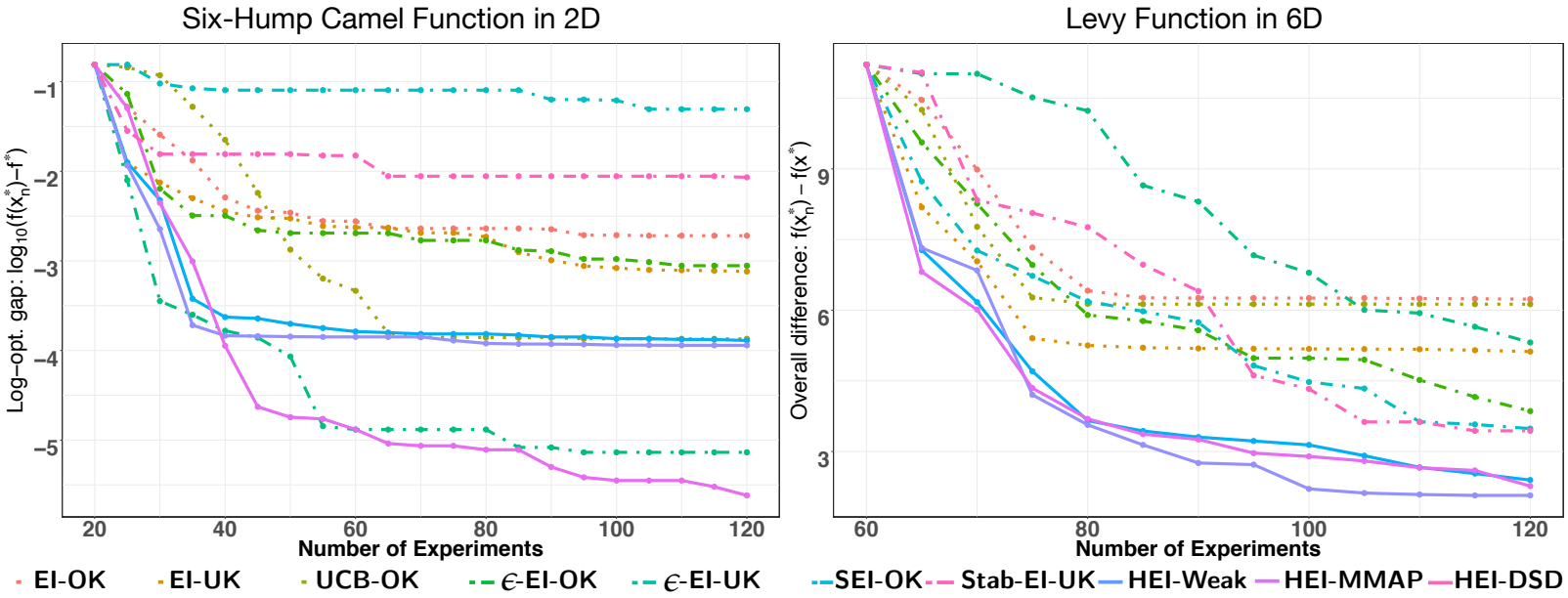
- Exploration parameter $\rho = 2.96$

Test functions



- HEI-MMAP & HEI-DSD perform **best**, EI **stuck** in **local optima**
- ϵ-greedy approaches **not bad**, but not as **effective** as HEI (**ad-hoc** fix to **over-exploitation**)
- HEI provides a **principled** correction via **hierarchical modeling**

Test functions



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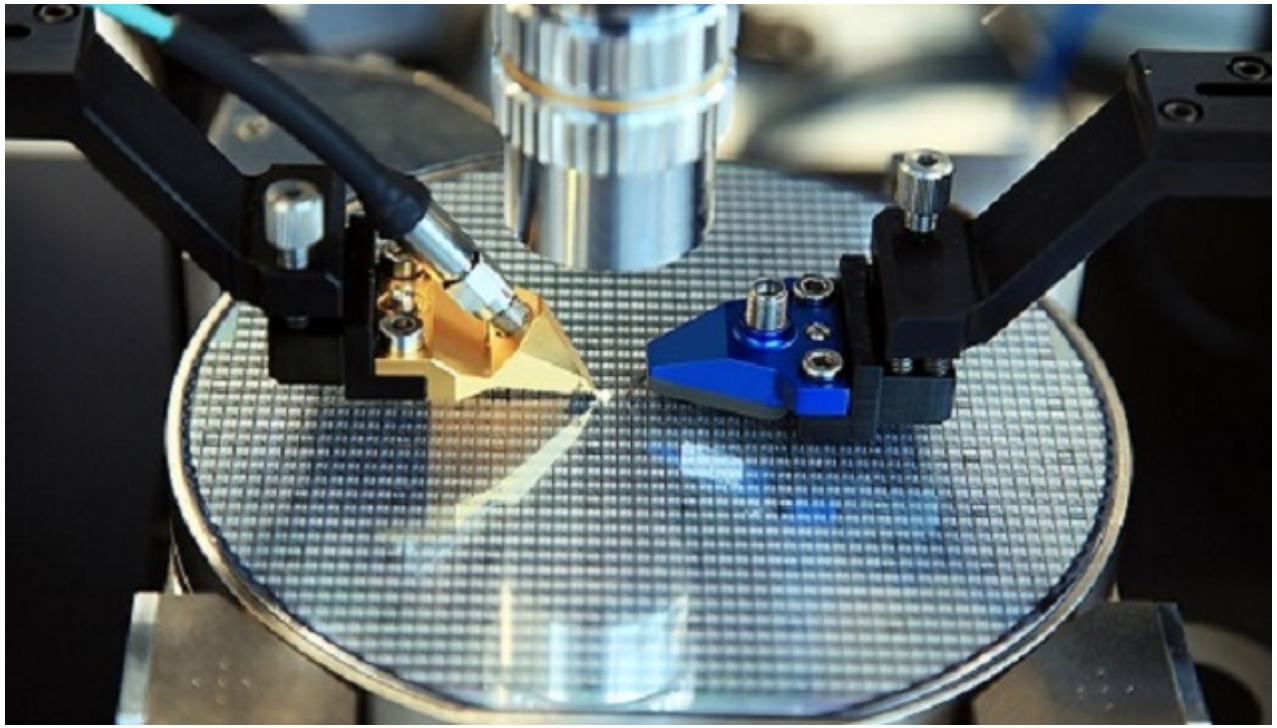
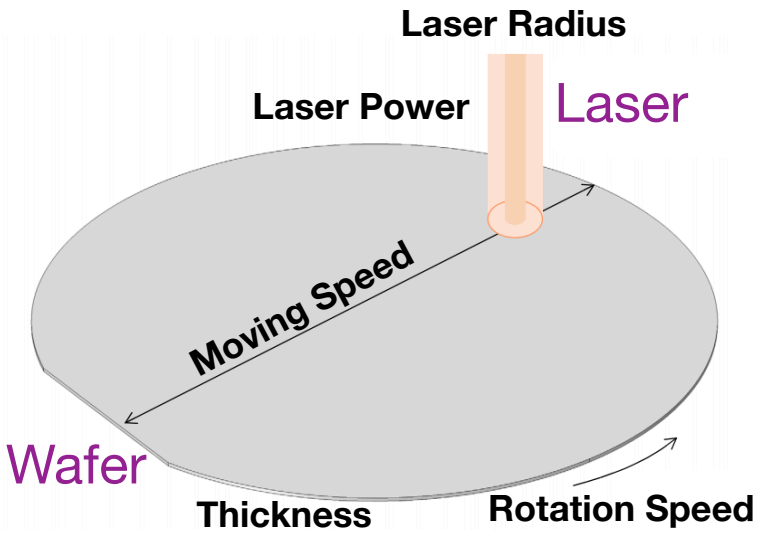
Semiconductor manufacturing optimization



- **Semiconductor manufacturing**: process for manufacturing **integrated circuit chips** used in **electrical devices**
- **Thermal processing** is a crucial stage, allowing for necessary **chemical reactions** and **surface oxidation** (Singh et al 2000)

Semiconductor manufacturing optimization



- $d = 5$ **control variables** for **optimization**
- **Goal**: heat **silicon wafer** to a **target** temperature T $= 600$F **quickly** and **smoothly**

Semiconductor manufacturing optimization

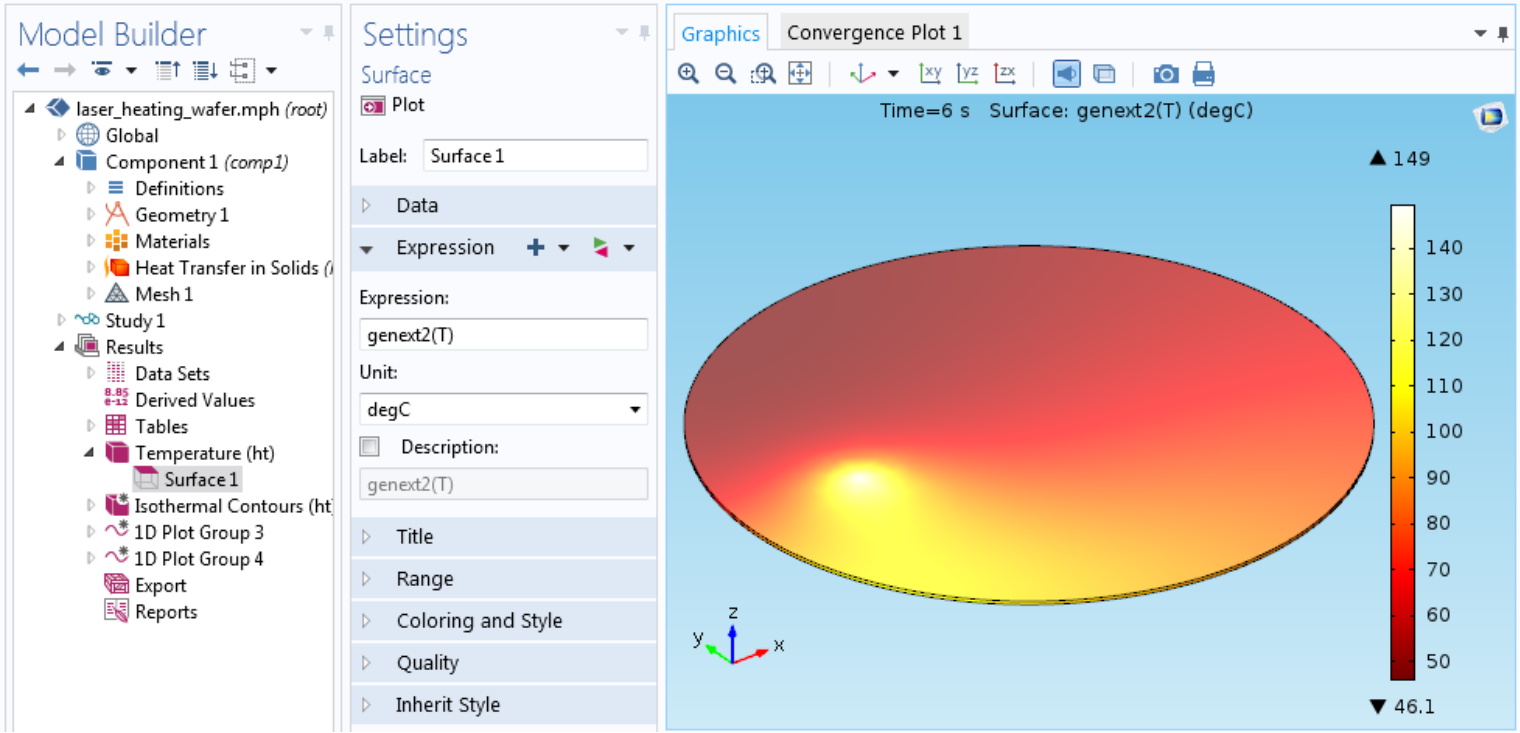
Objective function $f(\boldsymbol{x})$ to minimize:

$$f(\boldsymbol{x}) := \sum_{t=1}^{60} \max_{\mathbf{s}\in\mathcal{S}} \underbrace{\left|\mathcal{T}_t(\mathbf{s};\boldsymbol{x}) - 600\right|}_{\textbf{Gap to Target}}$$

- $\mathbf{s}$: **location** on wafer $\mathcal{S}$
- $\mathcal{T}_t(\mathbf{s};\boldsymbol{x})$: **temperature** at time t and location $\mathbf{s}$

Settings $\boldsymbol{x}$ with **small** $f(\boldsymbol{x})$ ensure that thermal processing is performed **quickly** and **smoothly**

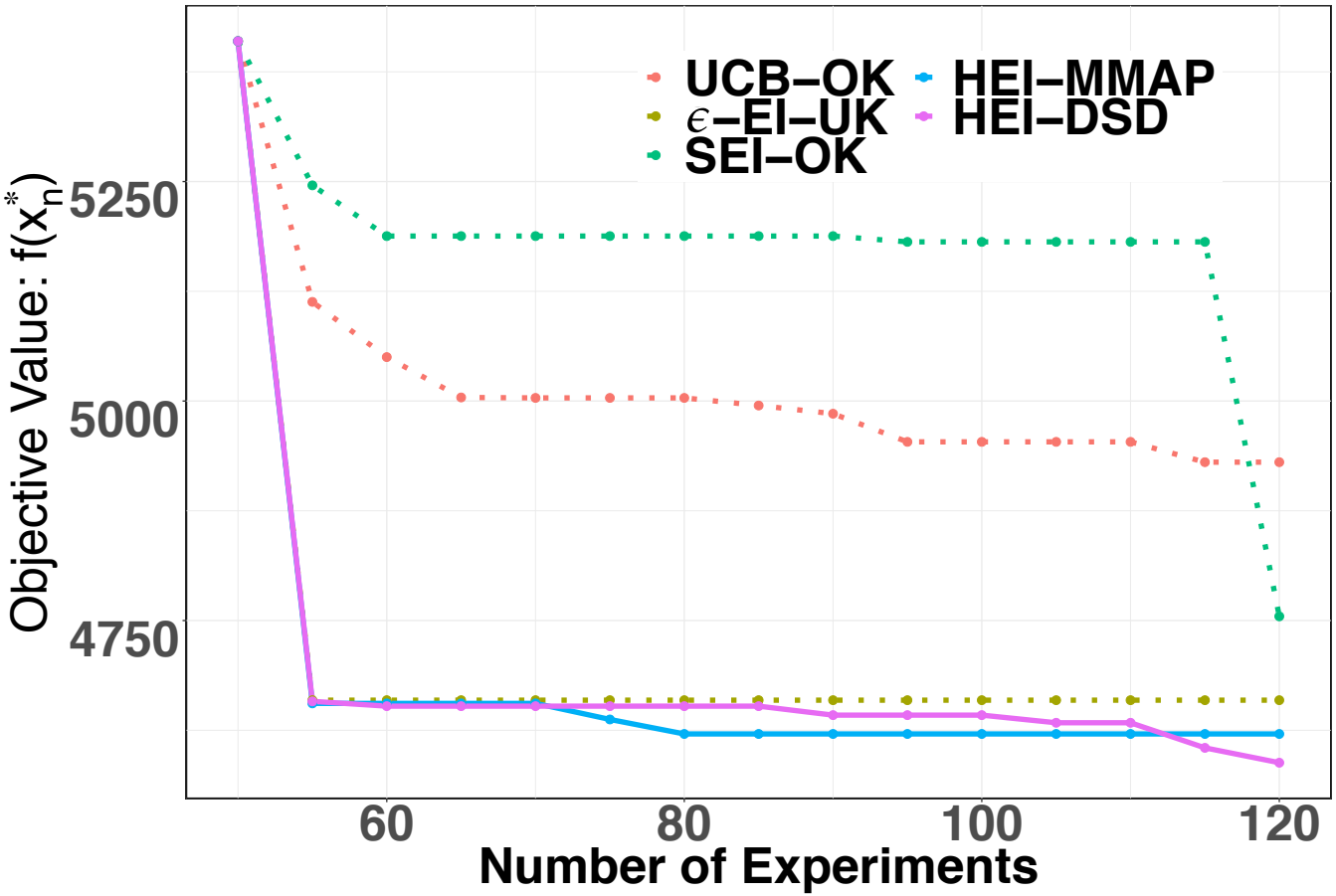
Semiconductor manufacturing optimization



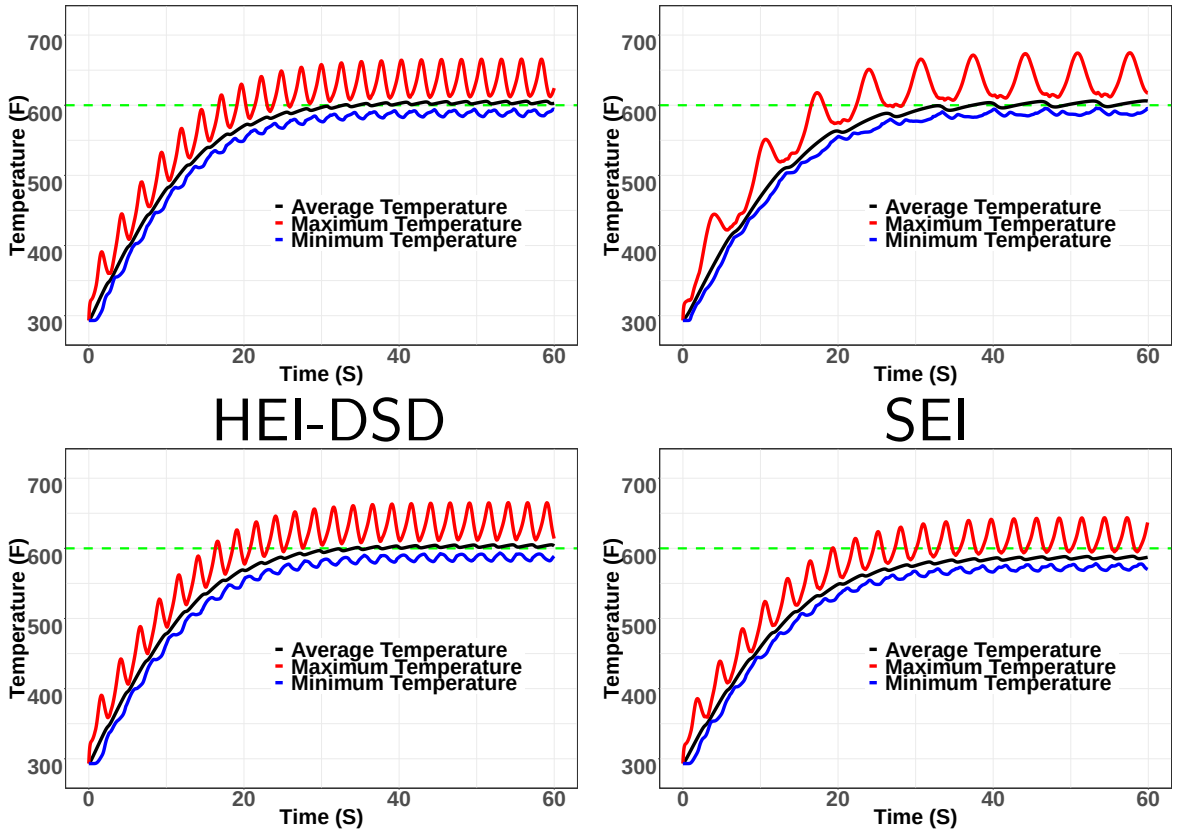
f is **expensive** and **black-box**:

- **Experiments** are **costly** and require **prototyping**
- **Simulations** can be performed on **COMSOL**, but require **30 minutes** for **each** setting

Semiconductor manufacturing optimization

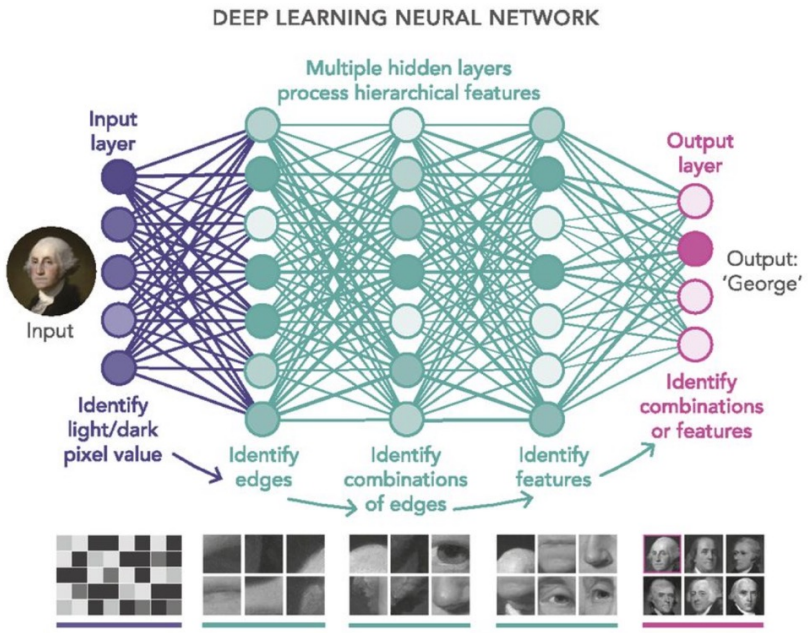


Semiconductor manufacturing optimization



- Visually, HEI-DSD and ϵ-EI-UK give the **best** settings: **average** temperature reaches **target** T **quickly** and **smoothly** (variation over wafer is **small**)

Hyperparameter tuning in deep learning

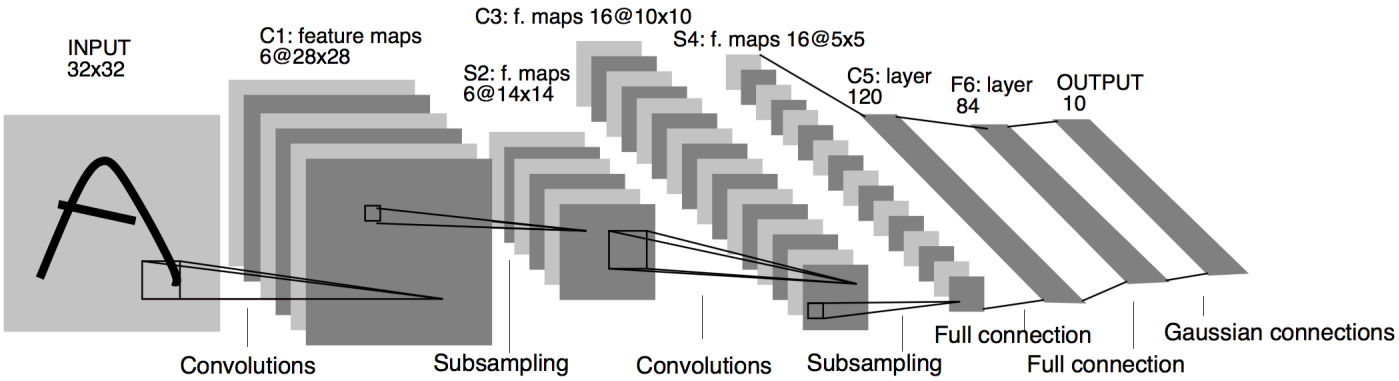


Neural networks (NNs) are widely used in **ML** problems:

- ... but in order to work **well**, many **hyperparameters** need to be carefully **tuned**
- NN training is **expensive** even for a **single** hyperparameter setting (several **hours** for real image databases, such as CIFAR)

Hyperparameter tuning in deep learning

- **Architecture**: LeNet-5 (LeCun et al. 1998)



- **Formulation**: **NN training** solves the following problem

$$\min_{\boldsymbol{w}} \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}} \ell(\mathcal{F}(\boldsymbol{x};\boldsymbol{w}), y)$$

  - ℓ: **loss** function (**softmax** used here)
  - $\mathcal{F}(\cdot;\boldsymbol{w})$: **neural network** with weight matrix $\boldsymbol{w}$
  - $(\boldsymbol{x}, y) \sim \mathcal{D}$: **image** and corresponding **label**

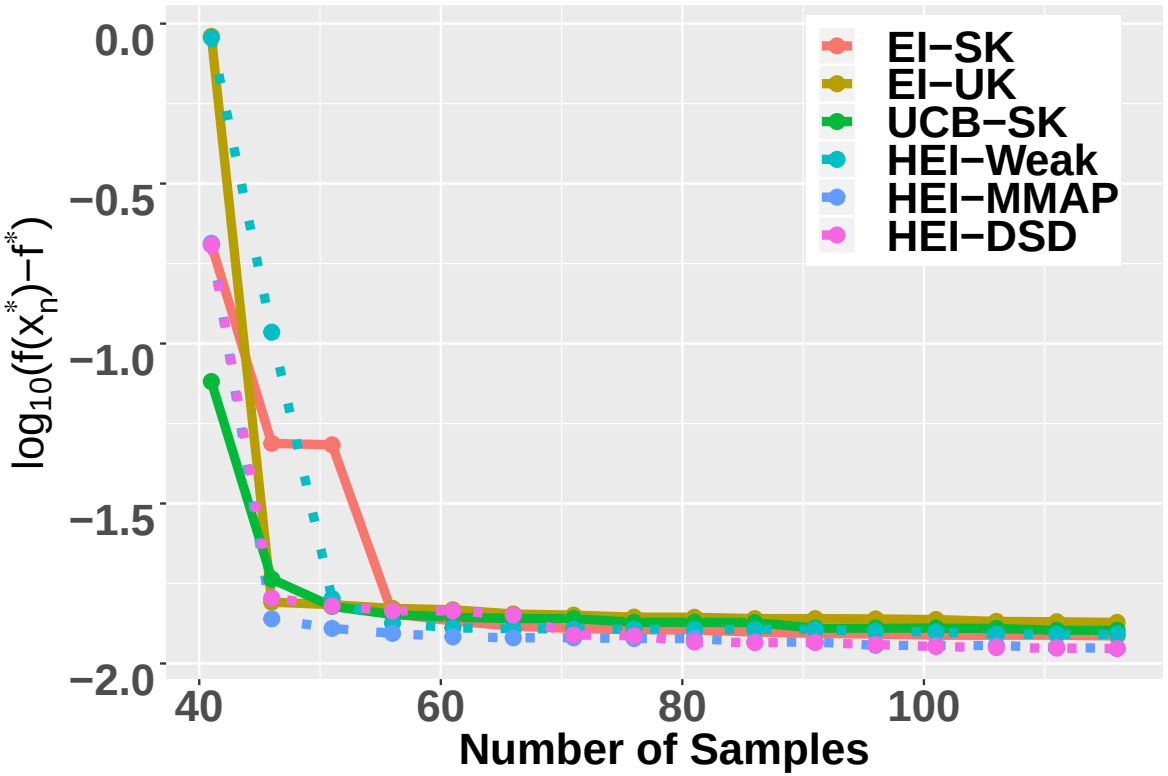
Hyperparameter tuning in deep learning

- **Training Method**:
  Momentum stochastic gradient descent with weight decay:

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - \underbrace{\eta \cdot \nabla_{\boldsymbol{w}} \ell(\mathcal{F}(\boldsymbol{x}_{i_t}, \boldsymbol{w}^{(t)}), y_{i_t})}_{\text{Gradient Descent Term}} + \underbrace{\mu \cdot (\boldsymbol{w}^{(t)} - \boldsymbol{w}^{(t-1)})}_{\text{Momentum Term}} - \underbrace{\lambda \cdot \boldsymbol{w}^{(t)}}_{\text{Weight Decay Term}}$$

- **Hyperparameters**:
  - η: learning rate
  - μ: momentum
  - τ: weight matrix initialization variance
  - λ: weight decay

Hyperparameter tuning in deep learning



- y-**axis**: **log-validation error** of trained NN
- HEI-DSD & HEI-MMAP perform **best**: **lowest** errors
- Existing tuning method (**gradient-based tuning**, Bengio 2000) gives a **higher** **log-error** of -1.854

Conclusions

- **Exploration** is important for **learning** and **optimizing** expensive **black-box** functions
- A **closed-form acquisition function** allows for **efficient optimization**
- A **hierarchical** Bayesian model which considers parameter **uncertainties** can encourage more **exploration** and **correct** the **greediness** (**overexploitation**) of EI

Questions?