Gaussian Processes For Global Optimization

Ludwig Winkler

Methods of Artificial Intelligence and Machine Learning
TU Berlin

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Outline

Problem Setting

- Optimization of a function
- Function is computationally expensive
- Trying to find optimum with few evaluations
- Do so with the help of Gaussian Processes

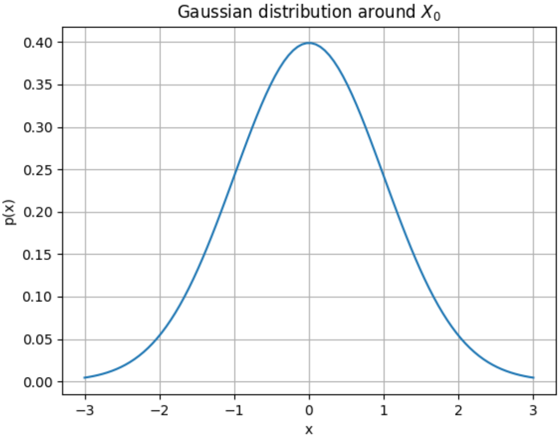
Gaussian Processes

"A GP is defined as a distribution over the infinite number of possible outputs of our function, such that the distribution over any finite number of them is a multivariate Gaussian."

- Michael A. Osborne

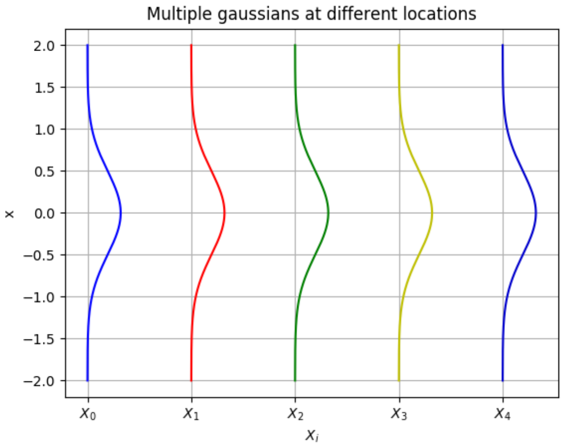
Gaussian Processes

- Random variable with distribution we can sample from



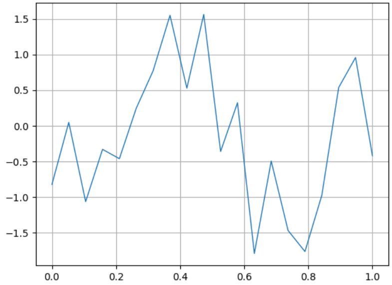
Gaussian Processes

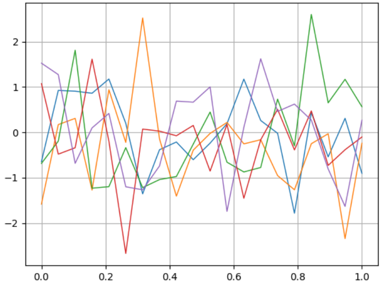
- Distributions at different locations X_i



Gaussian Processes

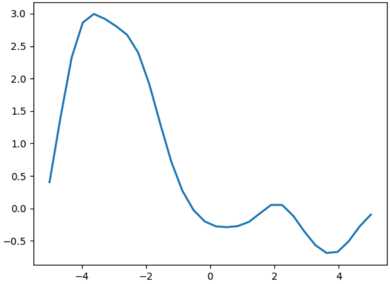
- Sample simultaneously from all distributions
- Each distribution is independent from all other distributions

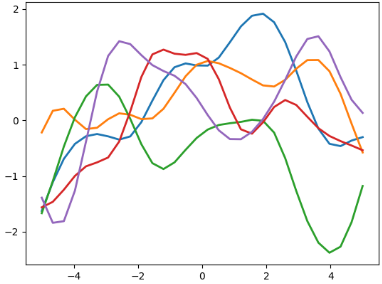




Gaussian Processes

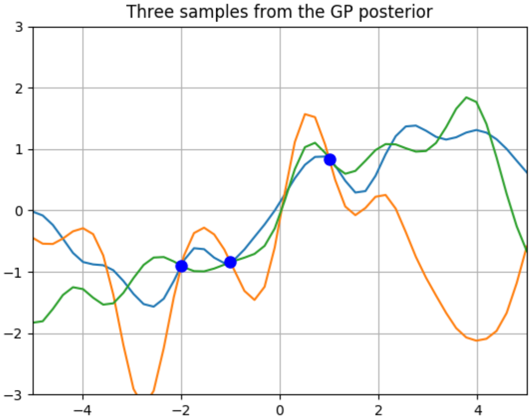
- Similar sample points should have similar values
- Introduce covariance between distributions
- Covariance determined by kernel





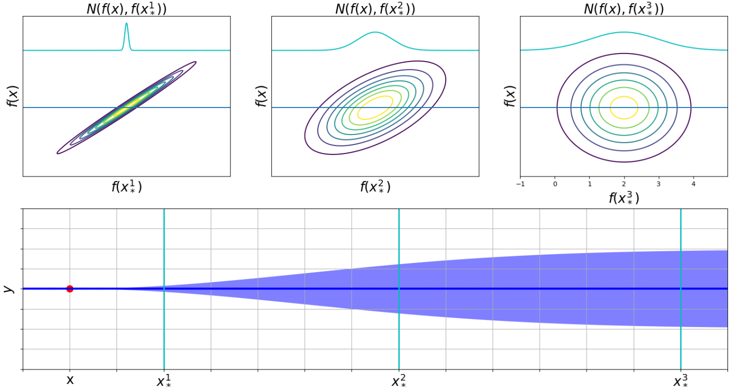
Gaussian Processes

- Condition joint distribution over all sample points on observations



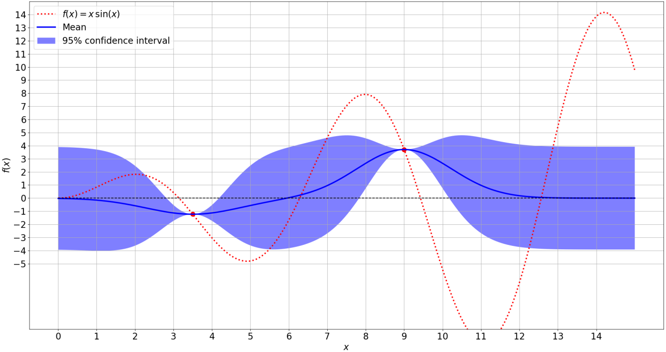
Covariance Matrix

- Variance is reduced as observations are approached



Gaussian Process in a Nutshell

- Observations $\mathcal{D} = \{(x_n, y_n)_{n=0}^{N}\} = (\mathbf{X}, \mathbf{y})$ for regression task
- Predicted y_* should be similar to y_i if x_* is similar to x_i
- Uncertainty for y_* if x_* is far away from any x_i



Gaussian Process (GP)

- Multivariate Gaussian over observations and predictions
- Kernel $k(x_i, x_j)$ measures similarity between x_i and x_j
- Kernel matrix $K_{ij} = k(x_i, x_j)$ as covariance matrix of GP

$$\begin{bmatrix} \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(\, \cdot \, | \mathbf{0}, \mathbf{K} \right)$$

- Kernel matrix $\mathbf{K}$ from observations $\mathbf{X}$ and predictions $\mathbf{x}_*$

$$\mathbf{K} = \begin{bmatrix} k_{\mathbf{y},\mathbf{y}}(\mathbf{X}, \mathbf{X}) & k_{\mathbf{y},y^*}(\mathbf{X}, x_*) \\ k_{y^*,\mathbf{y}}(x_*, \mathbf{X}) & k_{y^*,y^*}(x_*, x_*) \end{bmatrix} = \begin{bmatrix} K_{XX} & K_{Xx_*} \\ K_{x_*X} & K_{x_*x_*} \end{bmatrix}$$

Gaussian Processes

- GP's compute predictive distributions

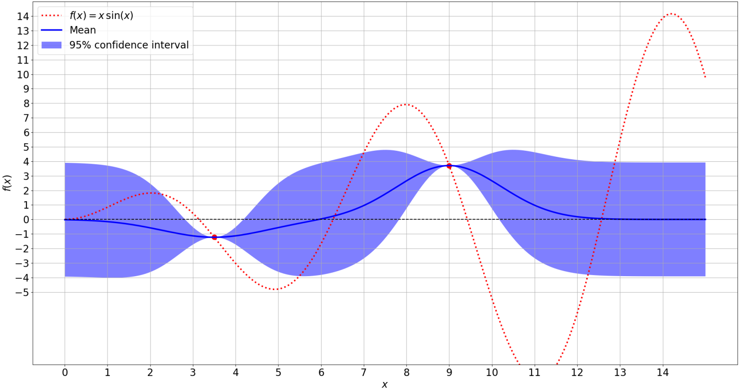
$$p(y_*|x_*, \mathbf{X}, \mathbf{y}) = \mathcal{N}\big(\underbrace{K_{x_*X}K_{XX}^{-1}\mathbf{y}}_{\mu}, \underbrace{K_{x_*x_*} - K_{x_*X}K_{XX}^{-1}K_{Xx_*}}_{\Sigma}\big)$$

- Bayesian inference for $y_*|x_*$ based on observations $(\mathbf{X}, \mathbf{y})$

$$\mu(x_*) = K_{x_*X}K_{XX}^{-1}\mathbf{y}$$
$$\sigma^2(x_*) = \text{diag}\left[K_{x_*x_*} - K_{x_*X}K_{XX}^{-1}K_{Xx_*}\right]$$

Observations

GP with Observations

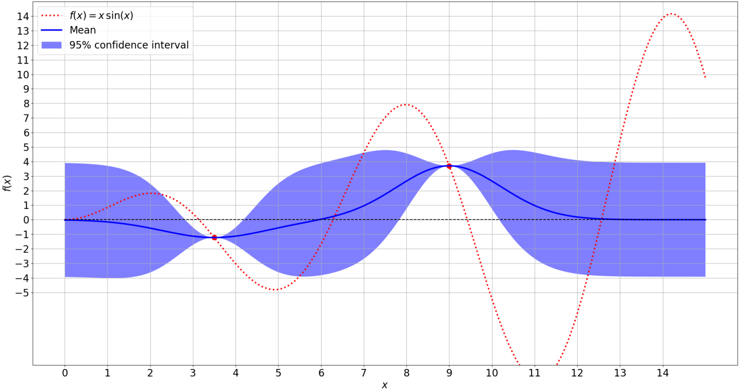


Derivative Observations

- Points close to observations should have similar derivative
- Inclusion of derivative observations
- Better predictive distributions with lower variance

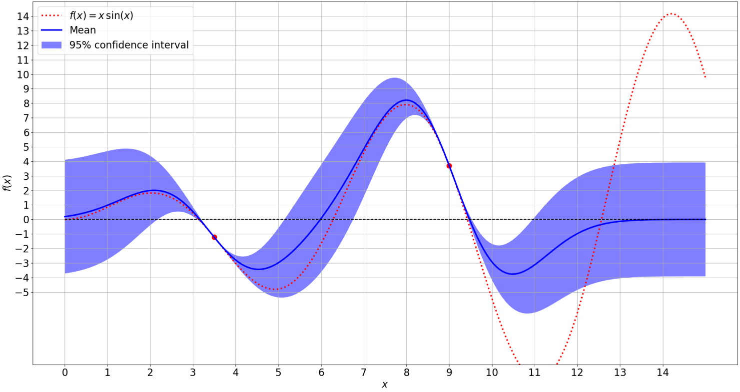
Derivative Observations

GP with Observations



Derivative Observations

GP with Derivative Observations



Derivative Observations

- GP over observations and derivative observations

$$\begin{bmatrix} \mathbf{y} \\ \nabla \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(\cdot \, | \mathbf{0}, \mathbf{K}^{\nabla} \right)$$

- Expanded covariance matrix with derivative observations

$$\mathbf{K}^{\nabla} = \begin{bmatrix} K_{XX}^{\nabla,\nabla\nabla} & K_{Xx_*}^{\nabla} \\ K_{x_*X}^{\nabla} & K_{x_*x_*} \end{bmatrix}$$

Derivative Observations

- Expanded kernel matrices with derivative observations

$$K_{XX}^{\nabla,\nabla\nabla} = \begin{bmatrix} k_{\mathbf{y},\mathbf{y}}(\mathbf{X},\mathbf{X}) & k_{\mathbf{y},\nabla\mathbf{y}}(\mathbf{X},\mathbf{X}) \\ k_{\nabla\mathbf{y},\mathbf{y}}(\mathbf{X},\mathbf{X}) & k_{\nabla\mathbf{y},\nabla\mathbf{y}}(\mathbf{X},\mathbf{X}) \end{bmatrix}$$

$$K_{Xx_*}^{\nabla} = \begin{bmatrix} k_{\mathbf{y},y_*}(\mathbf{X},x_*) \\ k_{\nabla\mathbf{y},y_*}(\mathbf{X},x_*) \end{bmatrix}$$

$$K_{x_*X}^{\nabla} = \begin{bmatrix} k_{y_*,\mathbf{y}}(x_*,\mathbf{X}) & k_{y_*,\nabla\mathbf{y}}(x_*,\mathbf{X}) \end{bmatrix}$$

- Modified kernels for kernel matrix

$$\mathrm{cov}[y, \nabla_{x'} y'] = k_{y,\nabla y'}(x, x')$$

$$\mathrm{cov}[\nabla_x y, y'] = k_{\nabla y, y'}(x, x')$$

$$\mathrm{cov}[\nabla_x y, \nabla y'] = k_{\nabla_x y, \nabla y'}(x, x')$$

Derivative Observations

- Modified kernels for covariance with derivative observations

$$\mathrm{cov}[y, y'] = \frac{1}{N}\sum_{i=0}^{N} y_i \cdot y_i' = k(x, x')$$

$$\begin{aligned}\mathrm{cov}[y, \nabla_{x'} y'] &= \frac{1}{N}\sum_{i=0}^{N} y_i \cdot \nabla_{x'} y_i' = \nabla_{x'} \frac{1}{N}\sum_{i=0}^{N} y_i \cdot y_i' \\ &= \nabla_{x'} \mathrm{cov}[y, y'] = \nabla_{x'} k(x, x')\end{aligned}$$

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Derivative Observations

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$$= \begin{bmatrix} K_{XX}^{\nabla,\nabla\nabla} & K_{Xx_*}^{\nabla} \\ K_{x_*X}^{\nabla} & K_{x_*x_*} \end{bmatrix}$$

Optimization

- Best element x^* w.r.t. to some criterion from set of elements $\mathcal{X}$
- Minimization/maximization of objective function $f(x)$

$$f(x^*) = \min_{x \in \mathcal{X}} f(x) = \max_{x \in \mathcal{X}} -f(x)$$

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- Succesive queries $x_1, x_2, \ldots \in \mathcal{X}$
- Leverage existing information to optimally select query x_i
- Maximization used as exemplary optimization

Optimization with GP

- Optimization problem as GP over set $\mathcal{X}$
- Select next query x_{n+1} from GP with previous queries $x_1, \ldots, x_n$

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- Acquisition function $\Lambda(x \mid x_1, \ldots, x_n)$ as improvement criterion

$$x_{n+1} = \underset{x \in \mathcal{X}}{\operatorname{argmax}} \; \Lambda(x \mid x_1, \ldots, x_n)$$

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$$x^+ = \underset{x_i \in x_{1:n}}{\operatorname{argmax}} f(x_i)$$

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$$x^+ = \underset{x_i \in x_{1:n}}{\operatorname{argmax}} f(x_i)$$

- Rescaling with respect to optimal solution x^+

$$z(x) = \frac{\mu(x) - f(x^+)}{\sigma(x)}$$

Acquisition Function

- Upper confidence bound

$$\mathbb{UCB}[x] = \mu(x) + \kappa\sigma(x) - f(x^+)$$

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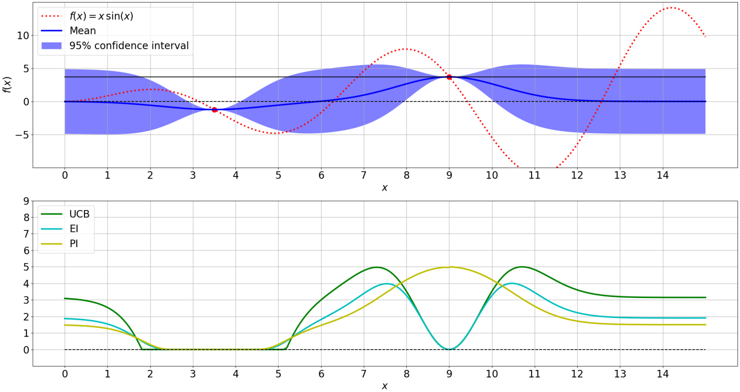
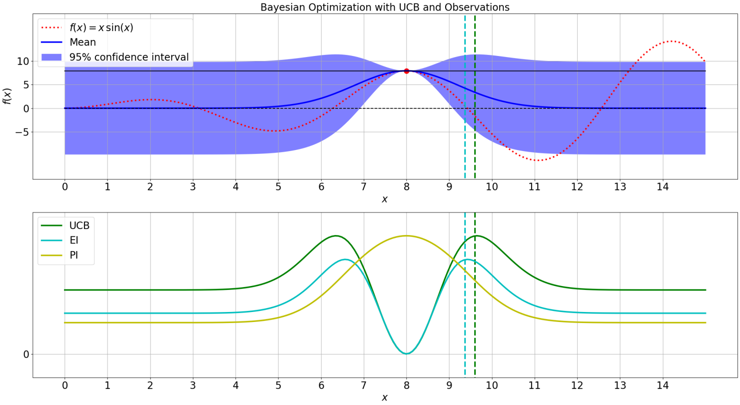
- Expected improvement

$$\mathbb{EI}[x] = \sigma(x)\left(\frac{\mu(x) - f(x^+)}{\sigma(x)}\Phi\left(\frac{\mu(x) - f(x^+)}{\sigma(x)}\right) + \mathcal{N}_{0,1}\left(\frac{\mu(x) - f(x^+)}{\sigma(x)}\right)\right)$$

Acquisition Function



Bayesian Optimization



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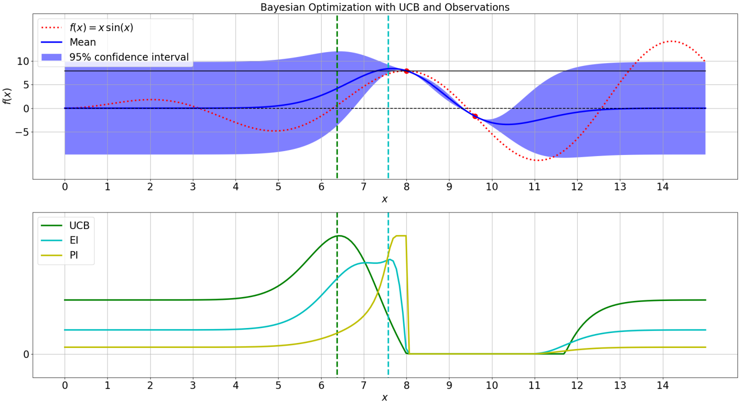

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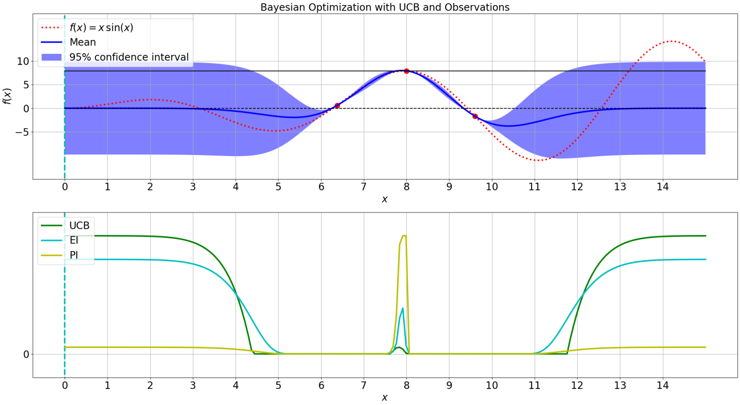

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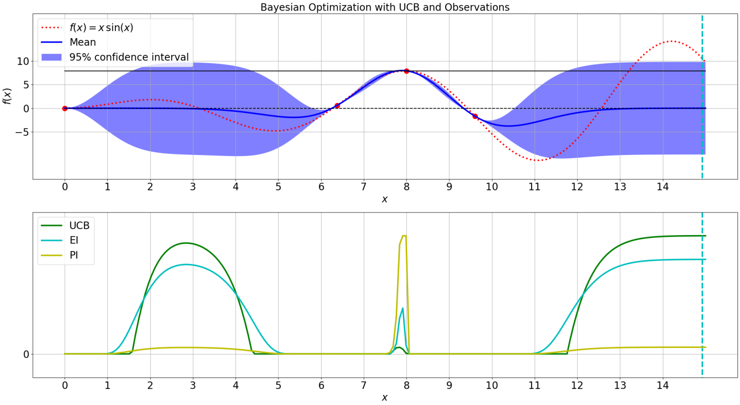

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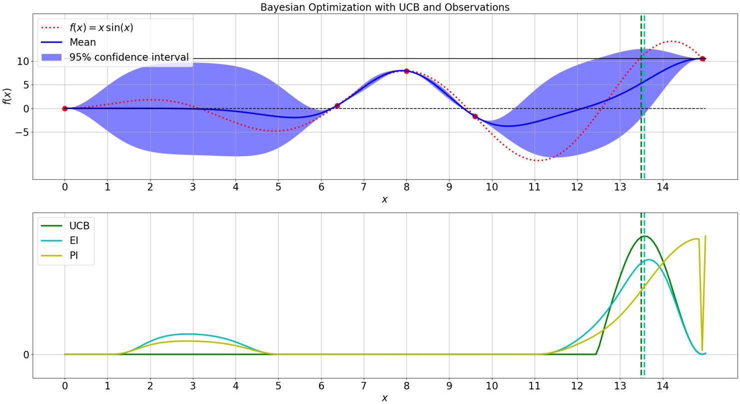

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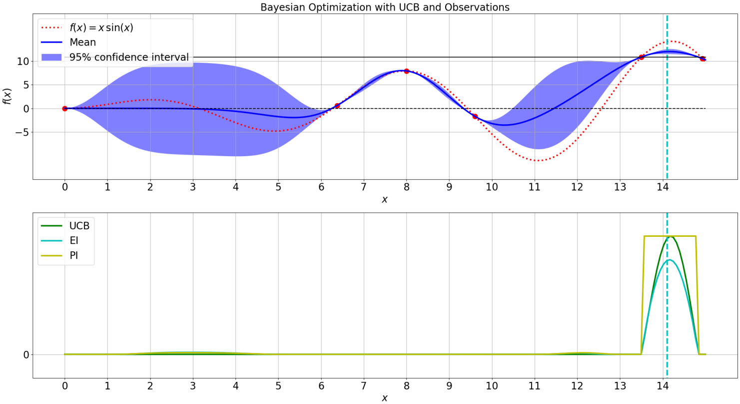

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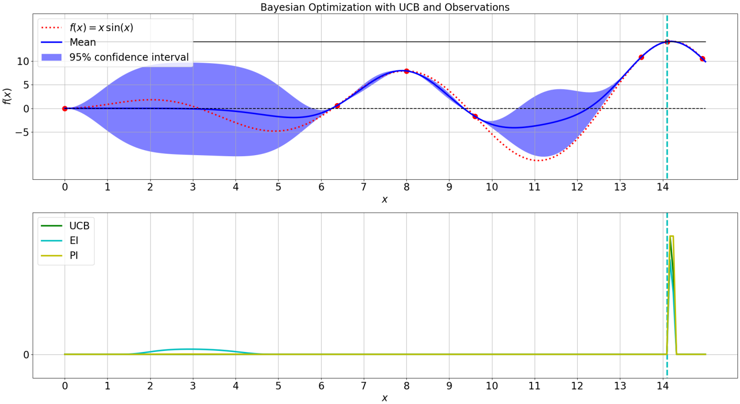

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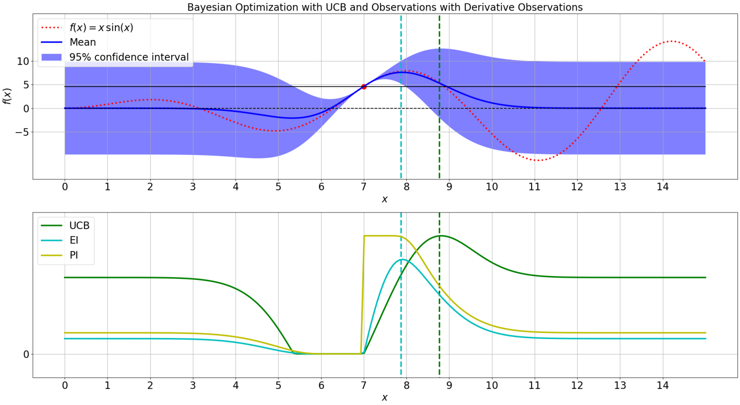

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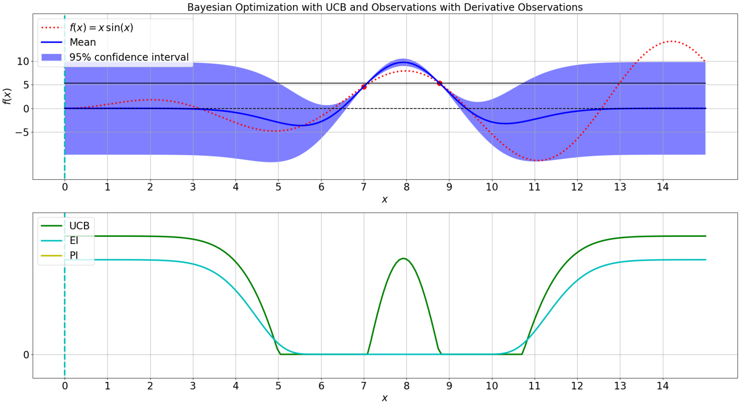

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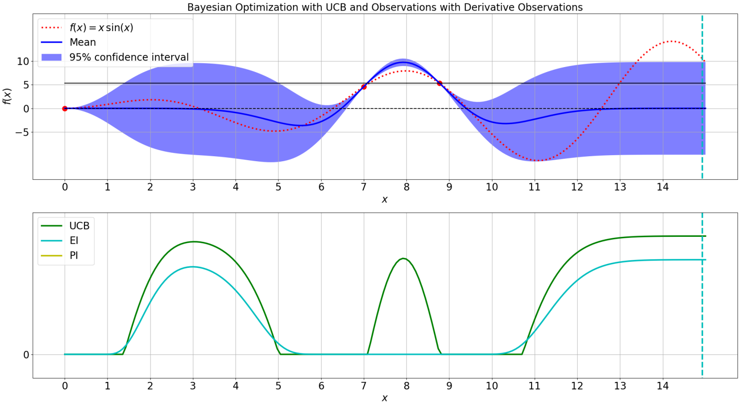

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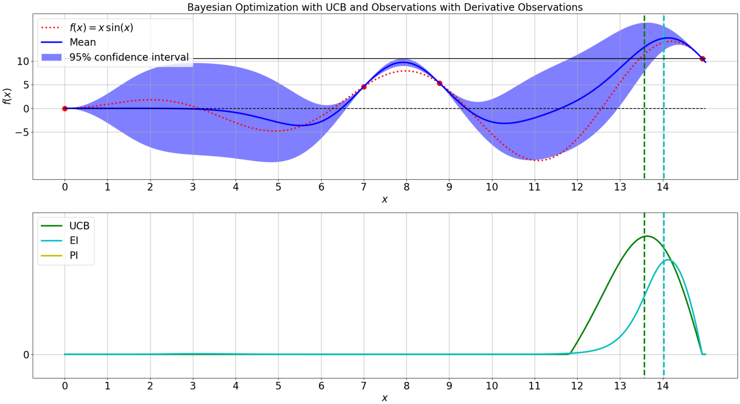

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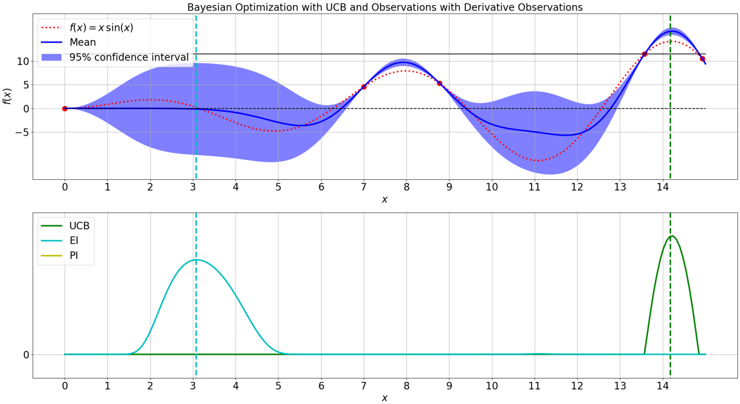

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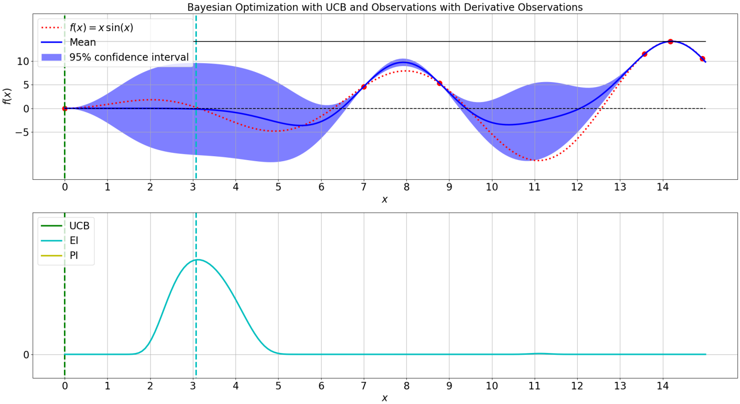

Outlook

- Multi-dimensional input feature space
- Noisy observations
- Multi-Step search
- Kernel hyperparameter optimization
- Bayesian Optimization for hyperparameter search

Thank you

Sources

- Osborne et al. - Gaussian Processes for Global optimization
- Brochu et al. - A Tutorial on Bayesian Optimization of Expensive Cost Functions, with Application to Active User Modeling and Hierarchical Reinforcement Learning
- Wu et al. - Exploiting gradients and Hessians in Bayesian optimization and Bayesian quadrature
- Solak et al. - Derivative observations in Gaussian Process Models of Dynamic Systems