Efficient High Dimensional Bayesian Optimization with Additivity and Quadrature Fourier Features

Mojmír Mutný Andreas Krause

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Learning & Adaptive Systems group
Institute of Machine Learning
ETH Zürich

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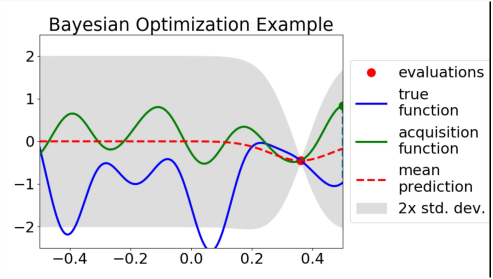

- **Metric**: cumulative regret: $R_T = \sum_{t=1}^{T} g(x_t) - g(x^*)$
- **Challenge**: exploration vs. exploitation $\implies$ Bayesian Optimization.

Challenges of high dimensions

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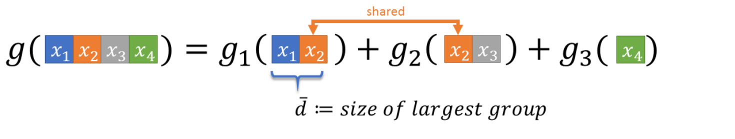

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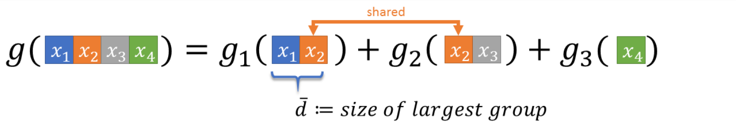

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  - Kernel inversion $\mathcal{O}(T^3) \rightarrow \mathcal{O}(T \log T)$
  - Optimization of the acquisition function $\rightarrow$ coordinate optimization

Main tool: Quadrature Fourier Features (QFF)

$$k(x-y) \overset{\text{Bochner}}{=} \int_{\Omega} p(\omega) \begin{pmatrix} \cos(\omega^\top x) \\ \sin(\omega^\top x) \end{pmatrix}^\top \begin{pmatrix} \cos(\omega^\top y) \\ \sin(\omega^\top y) \end{pmatrix} d\omega$$

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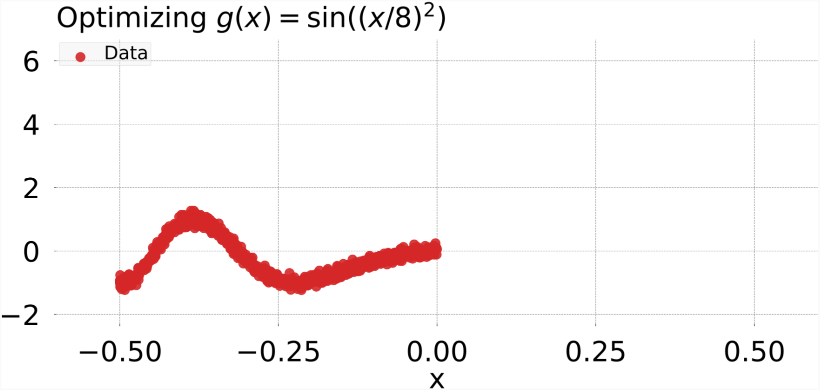
- This work: **Gaussian Quadrature**.
- (generalized) additivity $\implies$ favorable scaling with $\bar{d}$,

$$\left\| k(x, y) - \Phi(x)^\top \Phi(y) \right\|_\infty = \mathcal{O}\left(2^{\bar{d}} \rho^m\right) \;\; \rho < 1$$

Example



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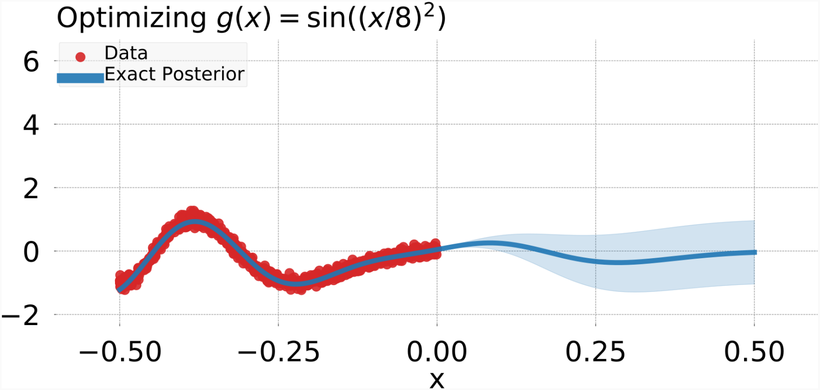
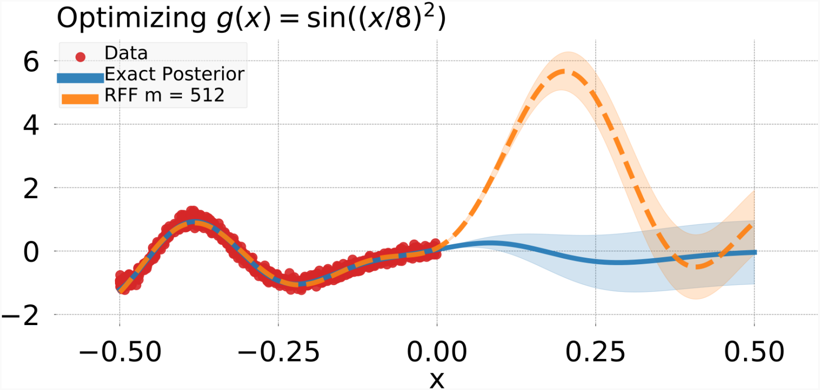


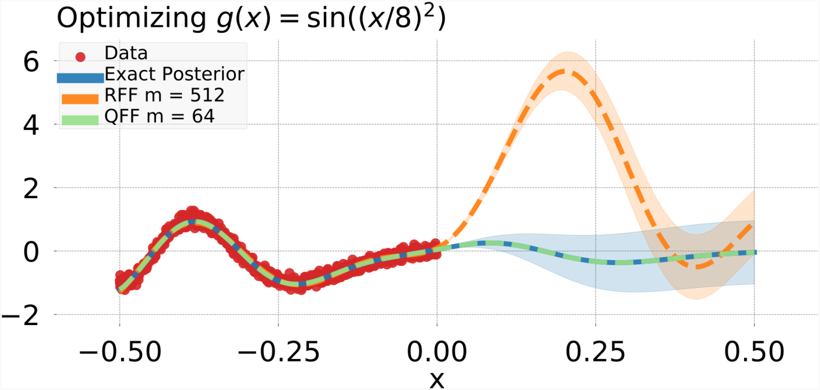
Optimizing $g(x) = \sin((x/8)^2)$
Data
Exact Posterior
6
4
2
0
−2
−0.50
−0.25
0.00
0.25
0.50
x

Example



Optimizing $g(x) = \sin((x/8)^2)$
Data
Exact Posterior
RFF m = 512
6
4
2
0
−2
−0.50
−0.25
0.00
0.25
0.50
x

Example


Optimizing $g(x) = \sin((x/8)^2)$
Data
Exact Posterior
RFF m = 512
QFF m = 64
6
4
2
0
−2
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Algorithm

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Please come to the poster #23.

Room 210 & 230 AB

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