Finding Global Minima via Kernel Approximations

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Global optimization

- **Zero-th order minimization**

$$\min_{x \in \Omega} f(x)$$

  - $\Omega \subset \mathbb{R}^d$ simple compact subset (e.g., $[-1, 1]^d$)
  - f with some bounded derivatives
  - access to function values

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- **Many applications**

  - Hyperparameter optimization in machine learning
  - Industry

Optimal algorithms

- **Goal**: Find $\hat{x} \in \Omega$ such that $f(\hat{x}) - \min_{x \in \Omega} f(x) \leqslant \varepsilon$
  - Lowest number of function calls
  - Worst-case guarantees over all functions f in some convex set $\mathcal{F}$

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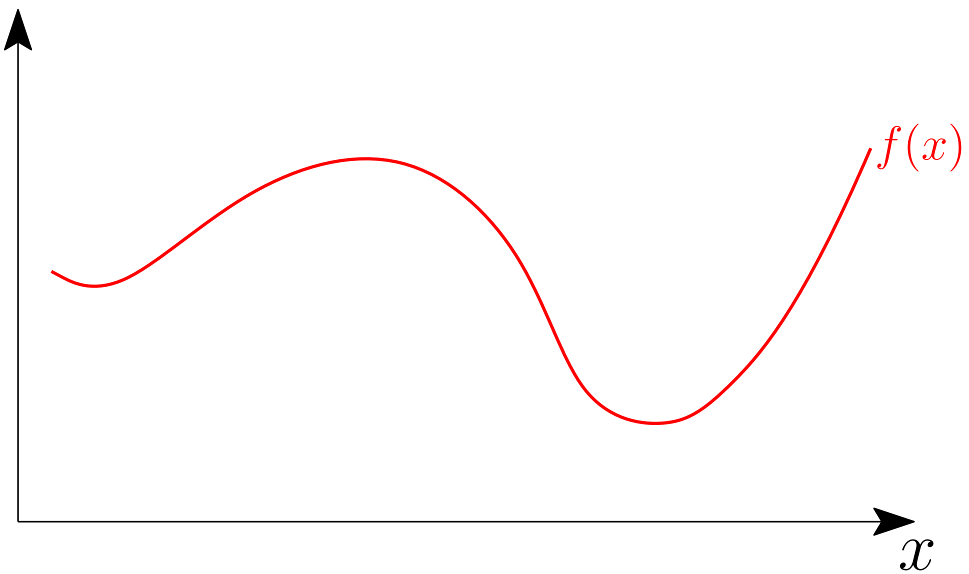
  - Simplest algorithm: approximate f by $\hat{f}$ and minimize $\hat{f}$



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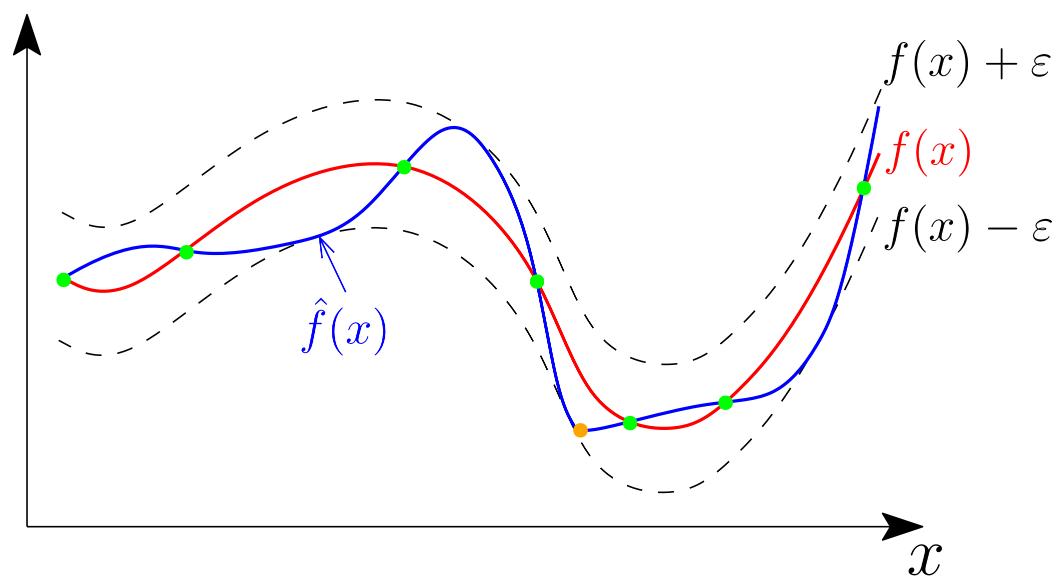

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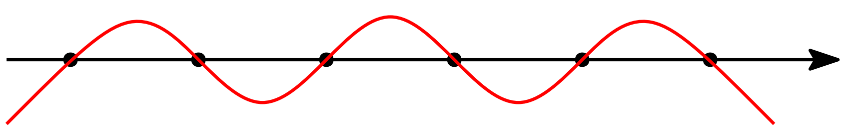

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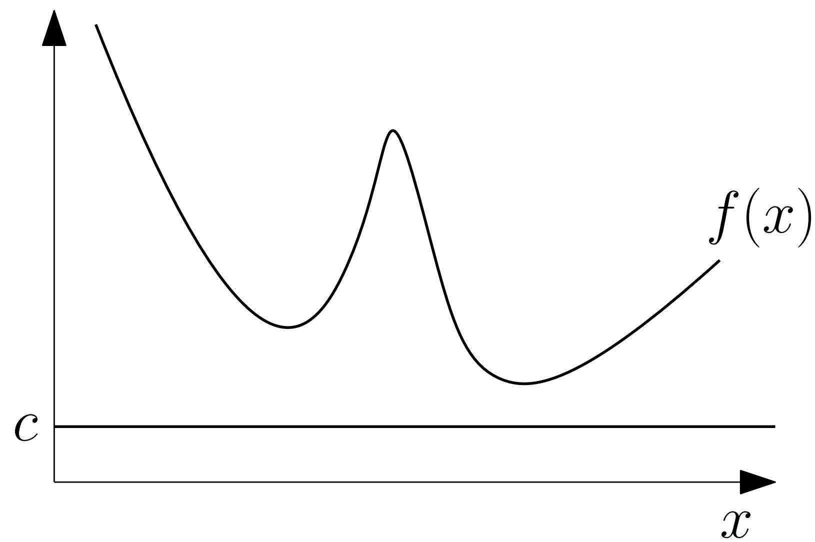
- **Algorithms with polynomial-time complexity in n?**
  - "Approximate and optimize"

Reformulations

- **Equivalent convex problem**

$$\min_{x \in \Omega} f(x) = \sup_{c \in \mathbb{R}} c \quad \text{such that} \quad \forall x \in \Omega,\ f(x) - c \geqslant 0$$



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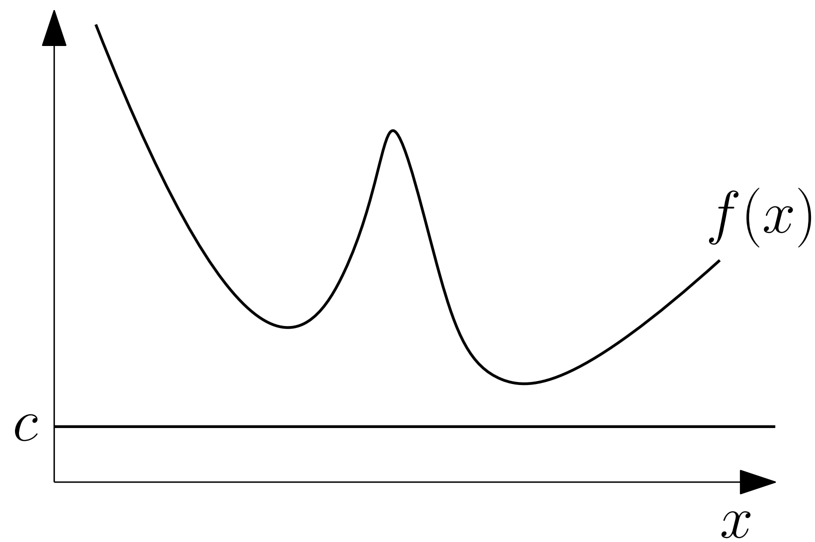

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- **Need to represent non-negative functions** (such as $f(x) - c$)

Representing non-negative functions

- **Assumption**: $g(x)$ can be represented as $g(x) = \langle \phi(x), G\phi(x) \rangle$
  - with G symmetric operator
  - Assume constant function can be represented as $1 = \langle u, \phi(x) \rangle$
  - Example: set of polynomials of degree $2r$
    with $\phi(x)$ composed of monomials of degree r, of dimension $\binom{d+r}{r}$

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- **Positivity through "sums-of-squares"**
  - If $G \succcurlyeq 0$, then $\forall x \in \Omega,\; g(x) = \langle \phi(x), G\phi(x) \rangle \geqslant 0$
  - Then, $g(x) = \sum_{i \in I} \lambda_i \langle \phi(x), (h_i \otimes h_i)\phi(x) \rangle = \sum_{i \in I} \lambda_i \langle \phi(x), h_i \rangle^2$

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- **Are all non-negative functions sums-of-squares?**
  - Polynomials: no if $d > 1$ (see, e.g., Rudin, 2000)

Global optimization with sums of square polynomials

- **Replace** $f(x) - c \geqslant 0$ by $f(x) = c + \langle \phi(x), A\phi(x) \rangle$ with $A \succcurlyeq 0$
  - represented as $F = c \cdot u \otimes u + A$

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- **Sum-of-squares optimization** (Lasserre, 2001; Parrilo, 2003)

$$\sup_{c \in \mathbb{R},\ A \succcurlyeq 0} c \quad \text{such that} \quad \forall x \in \mathbb{R}^d,\ f(x) = c + \langle \phi(x), A\phi(x) \rangle$$

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  - Equivalent to original problem if $f(x) - f_*$ is a sum-of-squares
  - If not, and if localization set $\Omega = \{x, \|x\|^2 \leqslant R^2\}$ is known,

$$\forall x \in \Omega,\ f(x) \geqslant 0 \quad \Leftrightarrow \quad \forall x \in \mathbb{R}^d,\ f(x) = q(x) + (R^2 - \|x\|^2)p(x)$$

    with p and q sums-of-squares polynomials (of unknown degree)
  - Needs "hierarchies"

Representing more general functions with RKHSs

- **Reproducing Kernel Hilbert Space (RKHS)** :
  - Hilbert space of functions $g \in \mathcal{H},\ g : \mathbb{R}^d \to \mathbb{R}$
  - Representation as linear form : $g(x) = \langle g, \phi(x) \rangle$
  - Kernel : $k(x, x') = \langle \phi(x), \phi(x') \rangle$ (computable)

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- **Example : Sobolev spaces** (Berlinet and Thomas-Agnan, 2011)
  - Sobolev spaces $H^s(\Omega)$ with $\Omega \subset \mathbb{R}^d$, $s > d/2$

$$\langle f, g \rangle = \sum_{|\alpha| \leq s} \int_{\Omega} \partial^\alpha f(x) \cdot \partial^\alpha g(x) dx$$

  - Example $s = d/2 + 1/2$: $k(x, y) = \exp(-\|x - y\|)$

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- **Everything can be expressed using only the kernel function k**
  - Useful when dealing with function evaluations
  - Representer theorem (Kimeldorf and Wahba, 1971): Minimizing $L(g(x_1), \ldots, g(x_n)) + \frac{\lambda}{2}\|g\|^2$ can be done by restricting to

$$g(x) = \sum_{i=1}^{n} \alpha_i k(x, x_i)$$

  - Then $g(x_j) = \sum_{i=1}^{n} \alpha_i k(x_j, x_i)$ and $\|g\|^2 = \sum_{i,j=1}^{n} \alpha_i \alpha_j k(x_i, x_j)$

Going infinite-dimensional (Rudi, Marteau-Ferey, and Bach, 2020)

$$\sup_{c \in \mathbb{R},\ A \succcurlyeq 0} \ c \quad \text{such that} \quad \forall x \in \Omega,\ f(x) = c + \langle \phi(x), A\phi(x) \rangle$$

- $\phi(x) \in \mathcal{H}$ Hilbert space so that $\langle w, \phi(x) \rangle$ spans a Sobolev space
  - $s > d/2$ squared-integrable derivative
  - Reproducing kernel Hilbert space (RKHS)
  - $k(x,y) = \langle \phi(x), \phi(y) \rangle = \exp(-\|x-y\|)$ for $s = d/2 + 1/2$.
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- **Theorem**: $\exists A_* \succcurlyeq 0$ such that $\forall x \in \Omega,\ \ f(x) = f_* + \langle \phi(x), A_*\phi(x) \rangle$
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$\Rightarrow$ Equivalent to original problem, but infinite-dimensional

Controlled approximation through sampling

- **Subsample n points $x_1, \dots, x_n \in \Omega$ and solve**

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- **Approximation guarantees** (Rudi, Marteau-Ferey, and Bach, 2020)
  - With random samples, $n \approx \varepsilon^{-d/(m-d/2-3)}$ (up to logarithmic terms)
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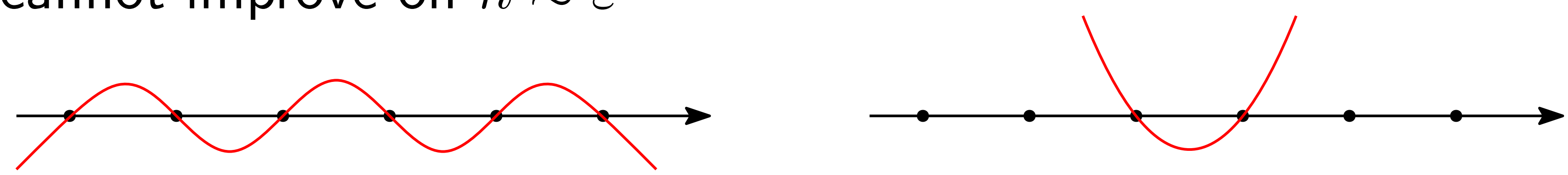
- **Subsampling inequalities as $f(x_i) \geqslant c$ directly?**
  - cannot improve on $n \approx \varepsilon^{-d}$



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- **Finite-dimensional algorithm through representer theorem**
  - Marteau-Ferey, Bach, and Rudi (2020)
  - Restrict optimization to $A = \sum_{i,j=1}^{n} C_{ij} \phi(x_i) \otimes \phi(x_j)$ with $C \succcurlyeq 0$

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- **Semi-definite programming problem**
  - Complexity $O(n^{3.5} \log \frac{1}{\varepsilon})$ by interior point method
  - More efficient Newton algorithm in $O(n^3)$

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2. **Feature computation**

   – Compute $K_{ij} = k(x_i, x_j)$ for k Sobolev kernel of smoothness s
   – Compute square root of $K = R^\top R \in \mathbb{R}^{n \times n}$
   – Set $\Phi_j = j$-th column of R, $\forall j \in \{1, \dots, n\}$
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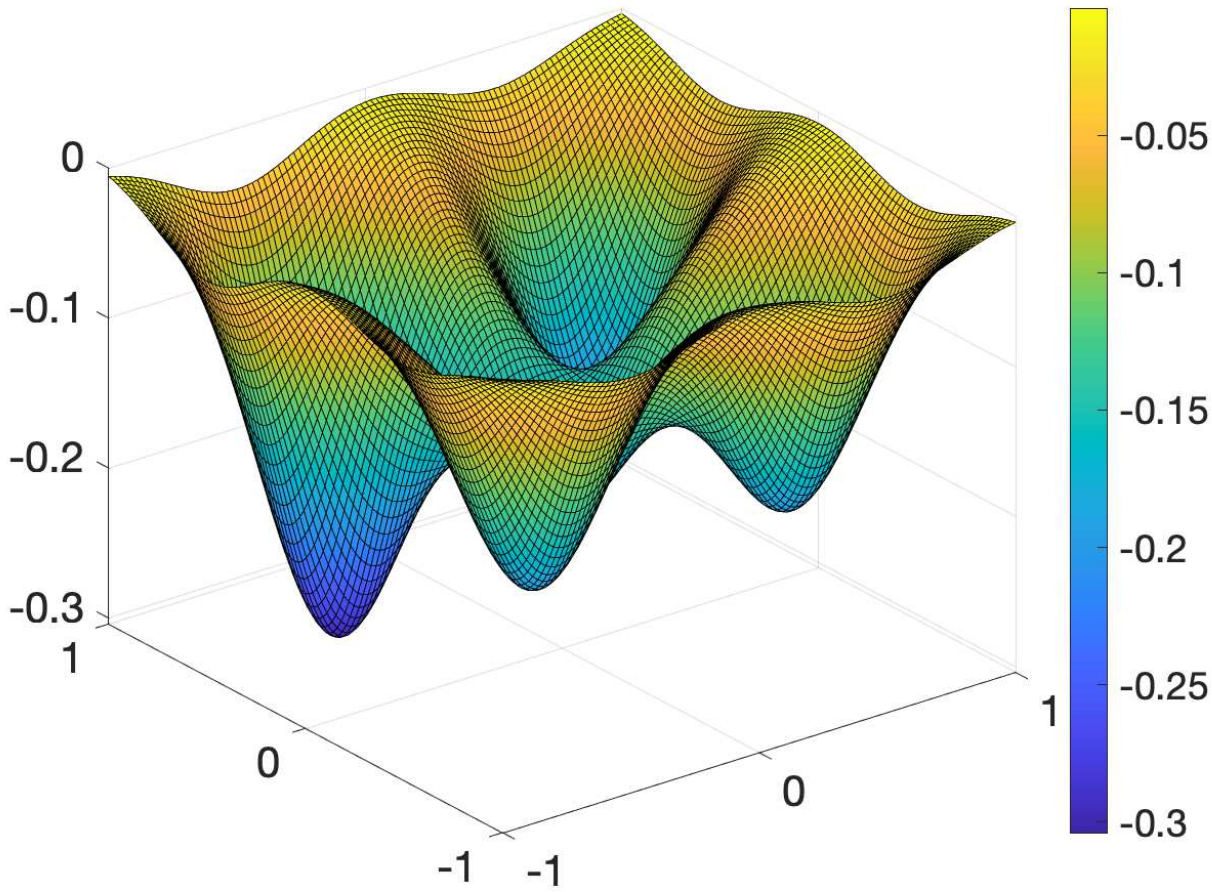
- **Output:** c and $\hat{x} = \sum_{j=1}^n \alpha_j x_j$

Illustration

- **Minimization of two-dimensional function**



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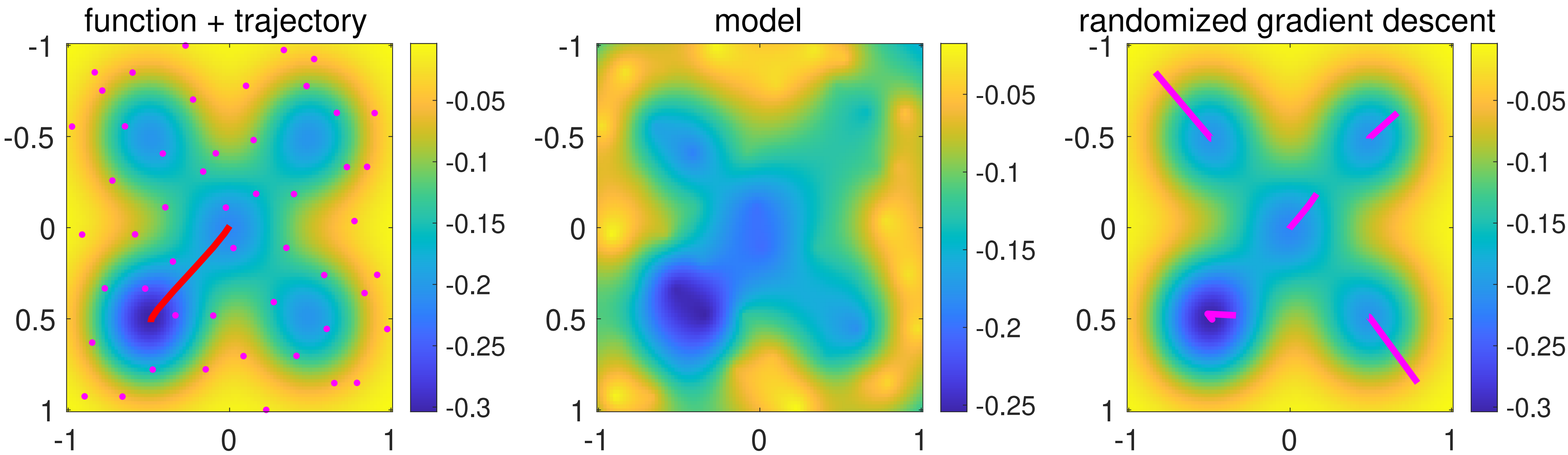

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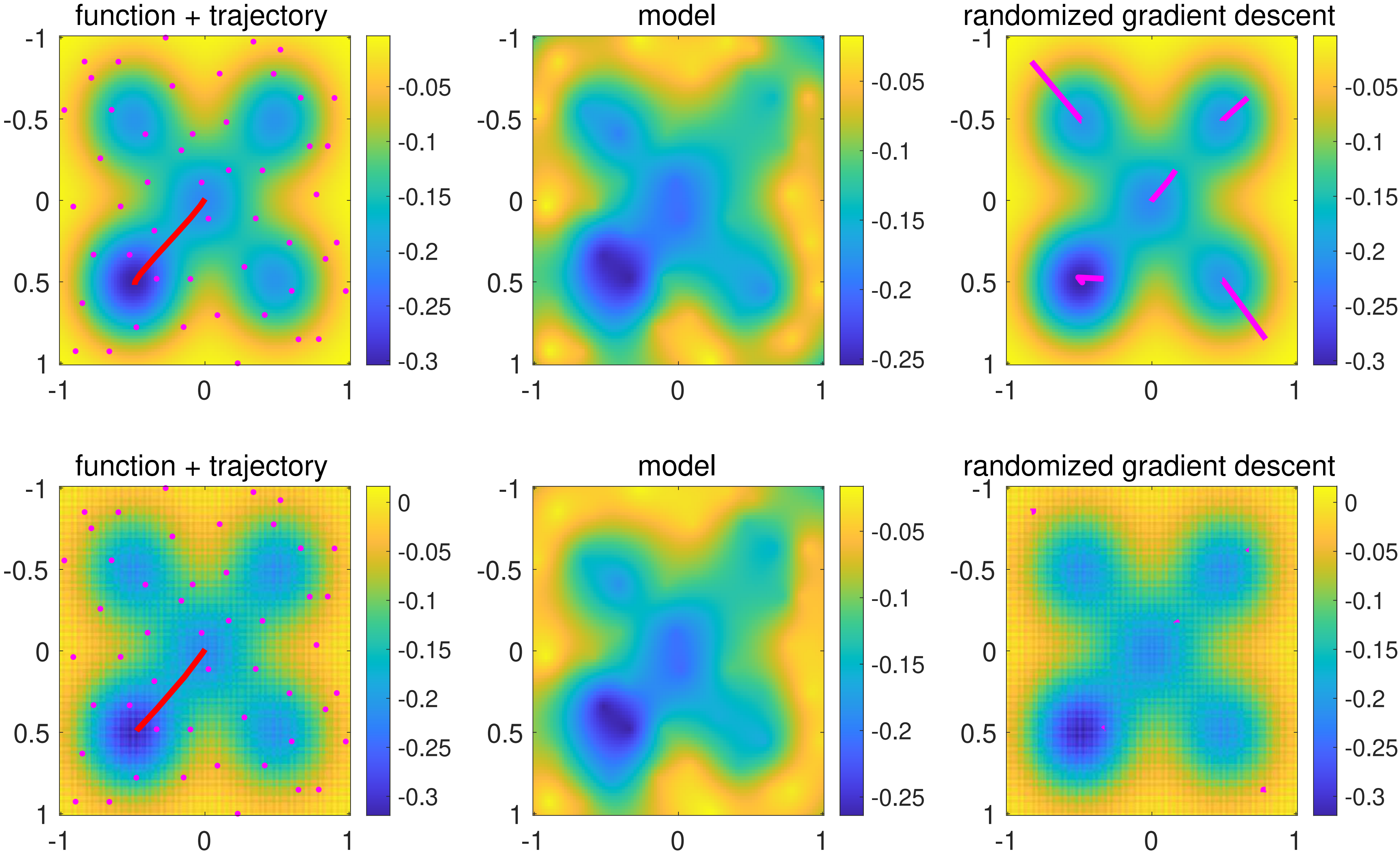
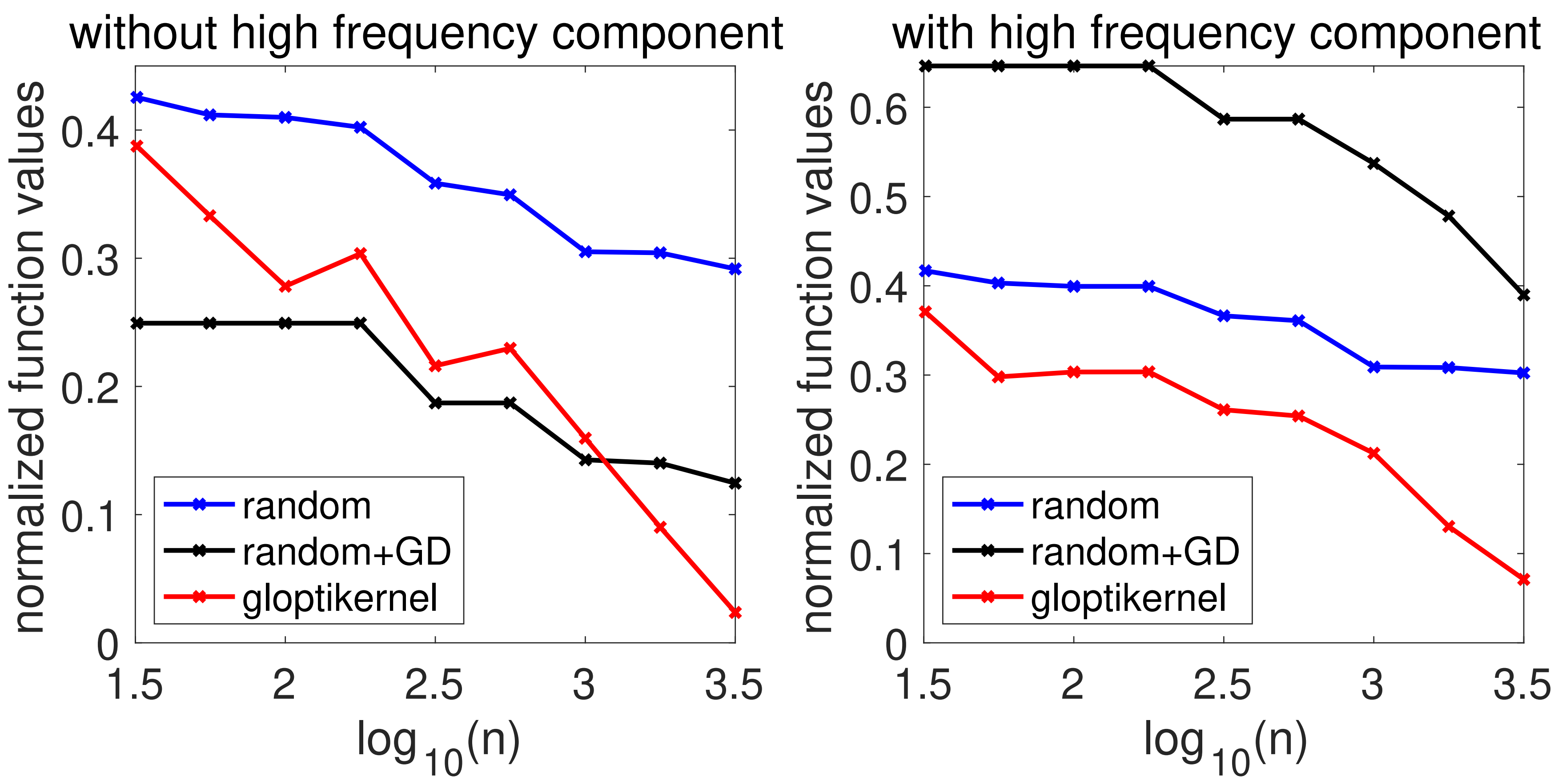


Illustration

- **Minimization of eight-dimensional function**



Duality

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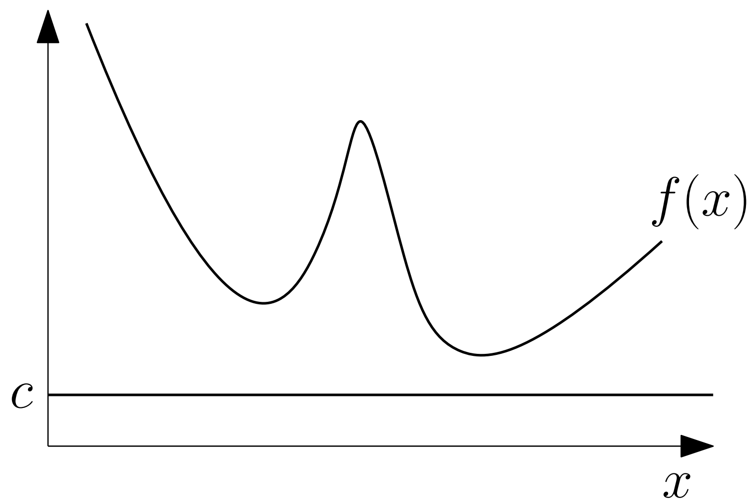

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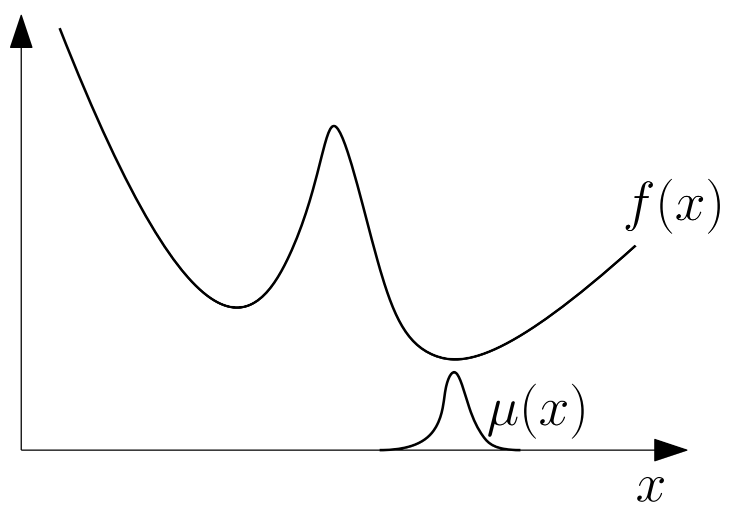
- **Dual problem on probability measures**

$$\inf_{\mu \in \mathbb{R}^{\Omega}} \int_{\Omega} \mu(x) f(x) dx \quad \text{such that} \quad \int_{\Omega} \mu(x) dx = 1,\ \forall x \in \Omega,\ \mu(x) \geqslant 0$$



Duality with sums-of-squares

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- **Dual problem on signed measures**

$$\inf_{\mu \in \mathbb{R}^\Omega} \int_\Omega \mu(x) f(x) dx \ \text{ s. t. } \ \int_\Omega \mu(x) dx = 1,\ \int_\Omega \mu(x) \phi(x) \otimes \phi(x) \succcurlyeq 0$$

– Extension of results on polynomials (Lasserre, 2020)

Extension - I

- **Generic constrained optimization problem**

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- **Sums-of-squares reformulation**

$$\inf_{\theta \in \Theta,\ A \succcurlyeq 0} F(\theta) \quad \text{such that} \quad \forall x \in \Omega,\ g(\theta, x) = \langle \phi(x), A\phi(x) \rangle$$

  – Requires penalization by $\mathrm{tr}(A)$ and subsampling
  – Need representation as sums-of-squares to benefit from smoothness
  – Can be done in the primal or the dual

Extension - I

- **Generic constrained optimization problem**

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  – Requires penalization by $\mathrm{tr}(A)$ and subsampling
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- **Application to optimal transport** (Vacher, Muzellec, Rudi, Bach, and Vialard, 2021)

Smooth optimal transport (Vacher et al., 2021)

- **Primal formulation**: $\inf_{\gamma \in \Gamma(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x,y) d\gamma(x,y)$
  - $\Gamma(\mu,\nu)$ set of probability distributions with marginals μ and ν
- **Dual formulation**: $\sup_{u,v \in C(\mathbb{R}^d)} \int_{\mathcal{X}} u(x) d\mu(x) + \int_{\mathcal{Y}} v(y) d\mu(y)$

  such that $\quad \forall (x,y) \in \mathcal{X}\times\mathcal{Y},\ c(x,y) \geqslant u(x) + v(y)$

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  - Rate: from $O(n^{-1/d})$ to $O(n^{-m/d})$ (Weed and Berthet, 2019)
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- **Kernel sums of squares**: replace inequality constraint by:

$$\forall (x,y) \in \mathcal{X}\times\mathcal{Y},\ c(x,y) = u(x) + v(y) + \langle \phi(x,y), A\phi(x,y) \rangle$$

Extension - II

- **Constrained optimization problem**

$$\inf_{x \in \mathbb{R}^d} f(x) \quad \text{such that} \quad \forall x \in \Omega,\ g(x) \geqslant 0$$

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$$\inf_{x \in \mathbb{R}^d} f(x) \quad \text{such that} \quad \forall x \in \Omega, \; g(x) \geqslant 0$$

- **Sums-of-squares reformulation**

$$\sup_{c \in \mathbb{R}, \; A \succcurlyeq 0, \; B \succcurlyeq 0} \quad c$$

$$\text{such that} \quad \forall x \in \Omega, \; f(x) = c + \langle \phi(x), A\phi(x) \rangle + g(x) \langle \phi(x), B\phi(x) \rangle$$

  – Extension of results on polynomials (Lasserre, 2001)

Conclusion

- **Global optimization through kernel approximations**
  - Joint optimization and approximation
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- **See** `arxiv.org/abs/2012.11978` and `francisbach.com/`

- See talk by Ulysse Marteau-Ferey (Wednesday at 11am)

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