Conception de systèmes à partir d'expériences numériques coûteuses

(mots-clés : planification d'expériences, modélisation de systèmes par processus aléatoires gaussiens, optimisation)

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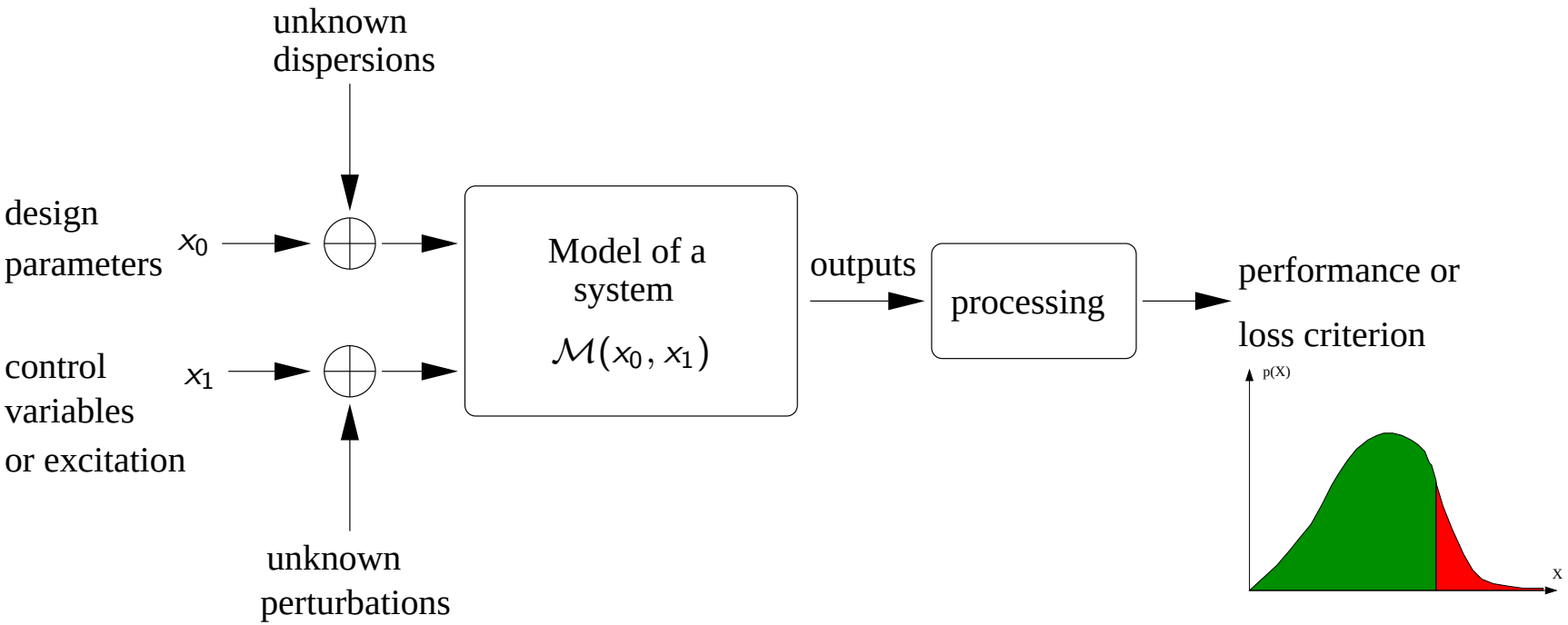
Outline

1. Computer models in engineering

Context overview



Model implemented under the form of a computer program
(e.g., a finite element model).
A single run of the program may be time- and resource-consuming.

Computer models in engineering

- $\mathbb{X} \subseteq \mathbb{R}^d \quad \rightsquigarrow$ factor/parameter space of the system
- $f : \mathbb{X} \to \mathbb{R} \rightsquigarrow$ performance or cost function (function of the outputs of the system)

- Main classes of problems:
  1. Approximation of the performance of a system, from expensive evaluations $x_i \mapsto f(x_i)$, $1 \leq i \leq N$, on a domain of interest
  2. Optimization of the performance of a system, cost minimization...

$$x^\star = \underset{x \in \mathbb{X}}{\operatorname{argmax}} f(x) \qquad \text{or} \qquad x^\star = \underset{x \in \mathbb{X}}{\operatorname{argmin}} f(x)$$

  3. In presence of uncertain factors, estimation of a probability of failure

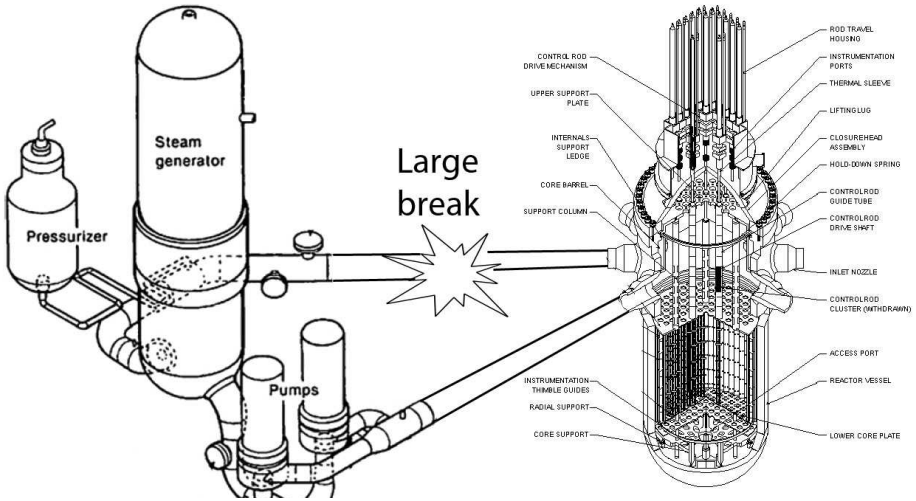
$$\alpha^u(x) \quad := \quad \mathrm{P}_{\mathbb{X}}\{x \in \mathbb{X} : f(x) > u\}$$

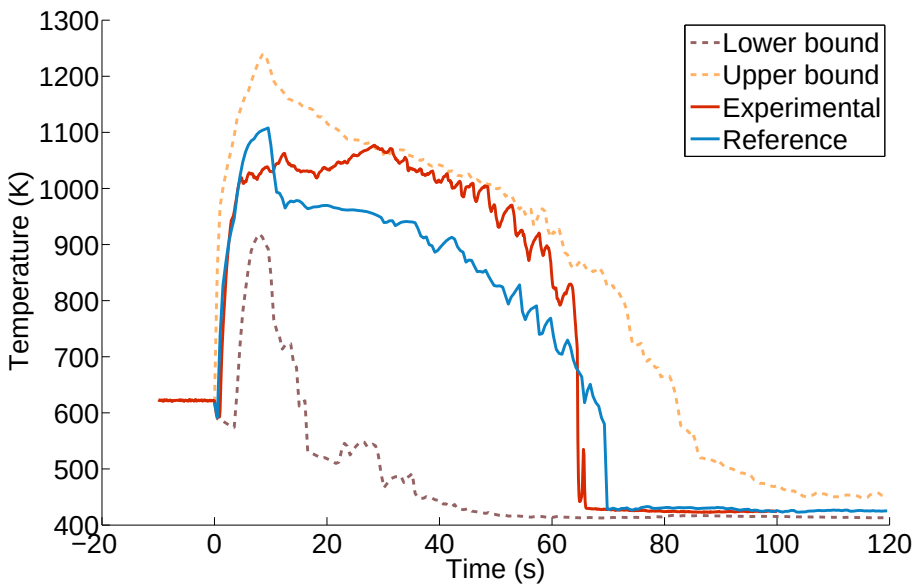
  where $\mathrm{P}_{\mathbb{X}}$ is some probability distribution on $(\mathbb{X}, \mathcal{B}(\mathbb{X}))$

NB: this is a simplified view $\to$ most real problems have several performance functions, and mix different objectives

Example 1/2 – Risk analysis

- Computer simulations to assess the probability of undesirable events





(Courtesy of CEA)

- A serious accident: loss of coolant in a pressurized water nuclear reactor
- Under these conditions, temperature of fuel rods can be described by $\sim$ 50 dimensioning factors, which are not known accurately
- Peak temperature can be estimated using complex and time-consuming simulations
- $f : \mathbb{X} \to \mathbb{R}$ peak temp. as a function of dim. factors
- Objective: estimate a probability of exceeding a critical value

$$\alpha = \mathrm{P}_{\mathbb{X}}\{f \geq u\}$$

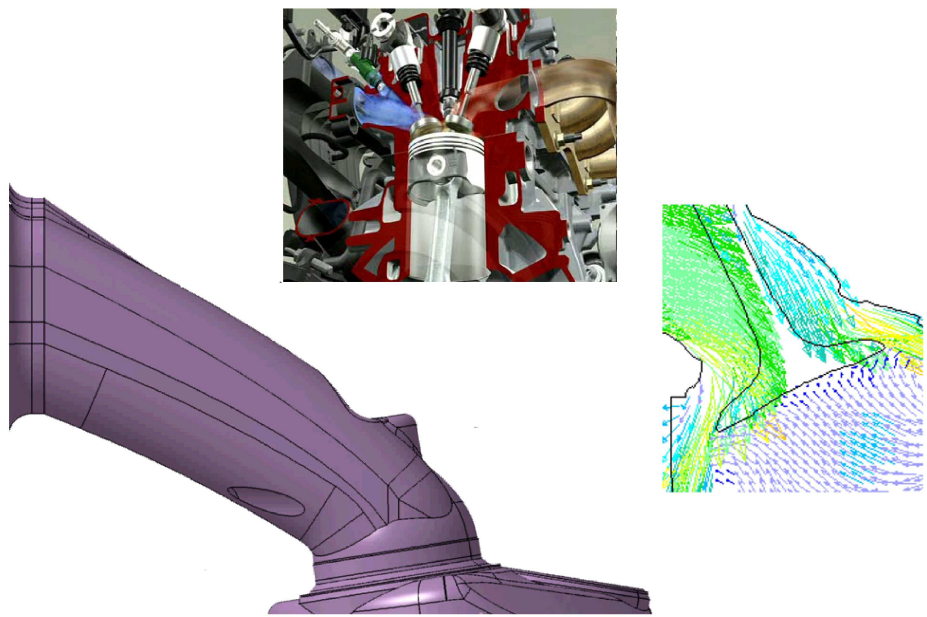
or a worst-case

$$M = \sup_{x \in \mathbb{X}} f(x)$$

Example 2/2 – Design optimization

- Computer simulations to design a product or a process, in particular
  - to find the best feasible values for design parameters (optimization problem)
  - to minimize the probability of failure of a product

- To comply with European emissions standards, the design parameters of combustion engines have to be carefully optimized
- The shape of intake ports controls airflow characteristics, which have direct impact on
  - the performances of the engine
  - emissions of NO_x and CO
- $f : \mathbb{X} \subset \mathbb{R}^d \to \mathbb{R}$ performance as a function of design parameters ($d = 20 \sim 100$)
- Computing $f(x)$ is time-consuming
- Objective: estimate $x^\star = \mathrm{argmax}_x\, f(x)$, or $x^\star = \mathrm{argmax}_x\, f(x)$ subject to $\mathrm{P}\{\text{pollutant emissions} \leq \text{threshold}\} > \gamma$



Simulation of an intake port (Navier-Stokes equations) (courtesy of Renault, Julien Villemonteix)

Distinct properties of computer experiments

- The performance/cost function $f : \mathbb{X} \subseteq \mathbb{R}^d \to \mathbb{R}$ is only known through pointwise evaluations
- An evaluation of f is called a computer experiment. It consists in
  - choosing an $x \in \mathbb{X}$
  - running one or several deterministic computer programs to obtain the value $f(x)$
- ∇f may also be known in rare cases
- The factor space $\mathbb{X}$ may be high-dimensional (typically $10 \sim 100$)
- Evaluation of f may be expensive (e.g., several hours) ➠ budget of experiments is limited (typically < 1000)

2. How to construct a good estimation procedure?

Estimation from computer experiments

- Let $f : \mathbb{X} \to \mathbb{R}$ be a continuous function defined on a compact domain $\mathbb{X}$ with non-empty interior

  (f corresponds to a computer program whose output is not a closed-form expression of the inputs.)

- Objective: from a set of computer experiments, obtain an approximation of

$$f : \mathbb{X} \to \mathbb{R}$$

$$\text{or} \quad m(f) = \min_{x \in \mathbb{X}} f(x) = f(x^\star)$$

$$\text{or} \quad \alpha^u(f) = \mathrm{P}_{\mathbb{X}}\{f > u\} = \int_{\mathbb{X}} \mathbb{1}_{f>u} \mathrm{dP}_{\mathbb{X}}$$

$$\ldots$$

- The result of a pointwise evaluation of f carries information about f and quantities depending on f (in particular, $m(f)$, $\alpha^u(f) \ldots$)
- Expensive computer experiments: the number of evaluations is limited $\to$ $m(f)$, $\alpha^u(f)$, etc. must be estimated using a fixed number, say N, of evaluations of f.

The case of optimization

- In the context of rare events estimation and risk analysis, it is often desirable to assess the worst-case performance of a system, that is, to determine

$$M = \sup_{x \in \mathbb{X}} f(x)$$

or

$$m = \inf_{x \in \mathbb{X}} f(x)$$

  - ➟ f may be non-convex
  - ➟ this is a global optimization problem

- How to design a good optimization algorithm?
- In a context of risk analysis, and also in difficult economic environments, we want to use an optimization algorithm that will provide a robust estimation of the global optimum

Why local optimization methods may not be satisfactory in the domain of computer experiments?

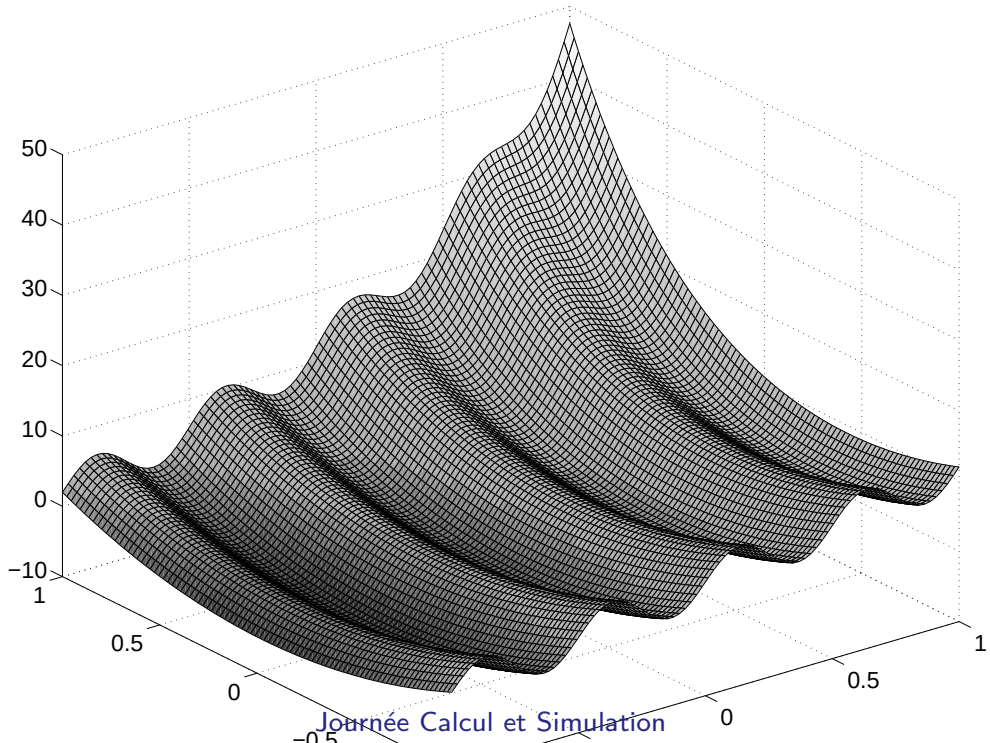
- An illustrative example: consider

$$\begin{array}{rccl} f: & \mathbb{R}^2 & \to & \mathbb{R} \\ & x & \mapsto & f(x) = \exp\left(1.8\left(x_{[1]} + x_{[2]}\right)\right) + 5x_{[1]} + 6{x_{[2]}}^2 + 3\sin\left(4\pi x_{[1]}\right) \end{array}$$

- Objective: find an approximation of

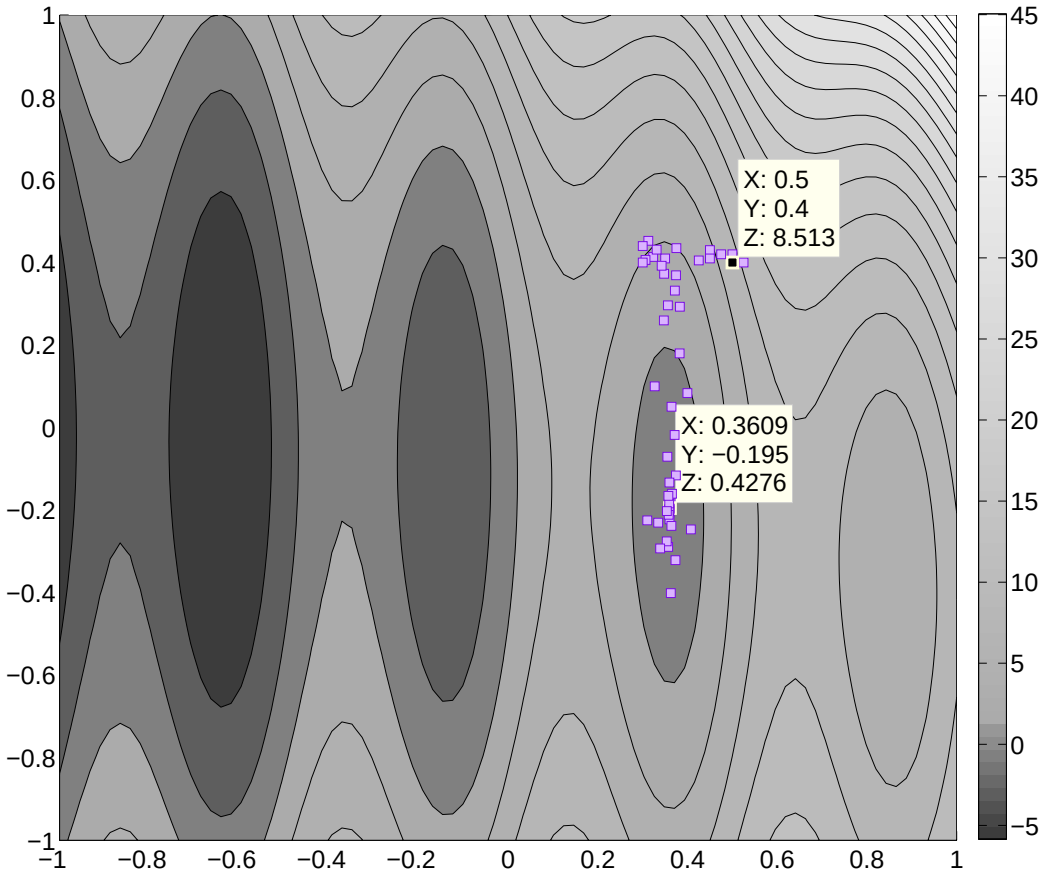
$$x^\star = \underset{x\in[-1,1]^2}{\operatorname{argmin}}\ f(x)\,.$$

with a budget of $N = 60$ experiments



Illustrative example (continued)

Evaluations points using a Nelder-Mead algorithm



$\rightarrow$ the algorithm converges to a local minimum (≈ 0.427)

This comes as no surprise (local search algorithm). But above all...

- after having spent the budget of (possibly expensive) evaluations, the behavior of the function is only known in a small region of the search domain
- the global behavior of the function is unknown
- potentially interesting regions have not been explored

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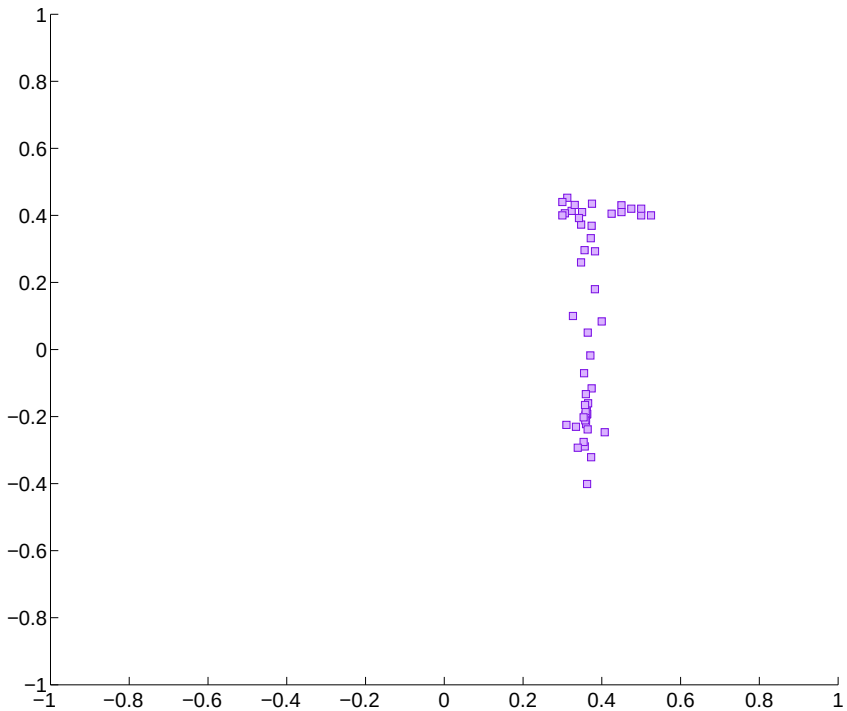

- the global behavior of the function is unknown
- potentially interesting regions have not been explored

- In a context of expensive-to-evaluate functions and a small budget of evaluations, it seems "safer" to achieve a balance between local search and exploration of the search domain
- Uniform random sampling:

$\rightarrow$ minimum of evaluation results is ≈ -5.823 (global minimum is ≈ -5.845)

- What is a robust optimization strategy? How to obtain such a strategy?

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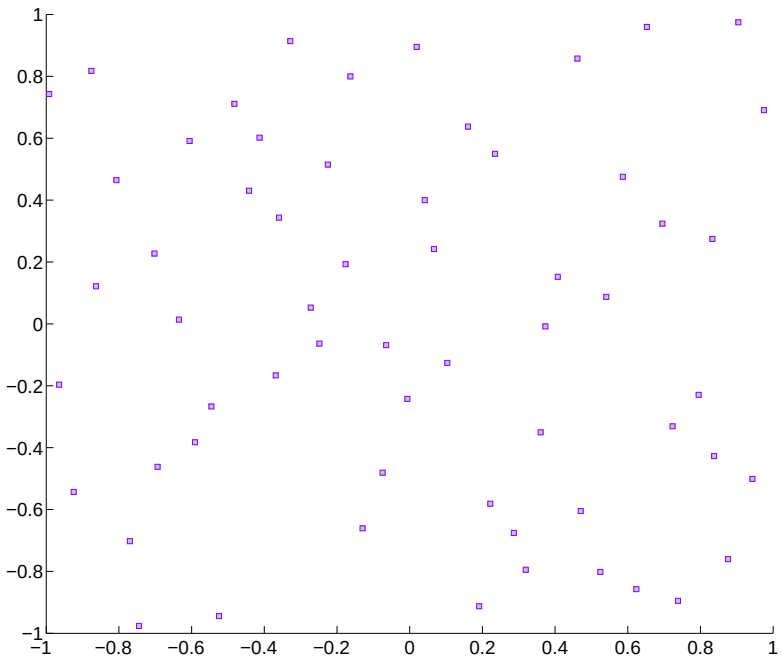

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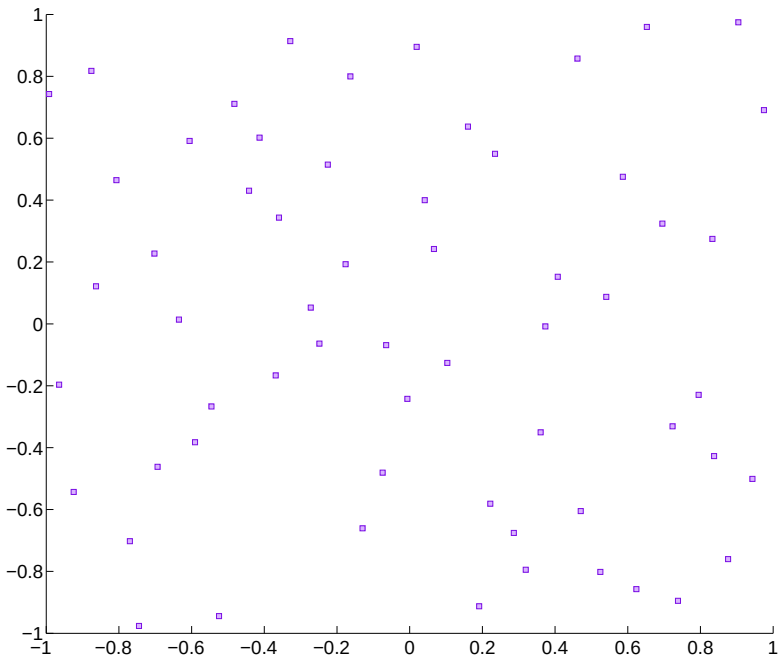

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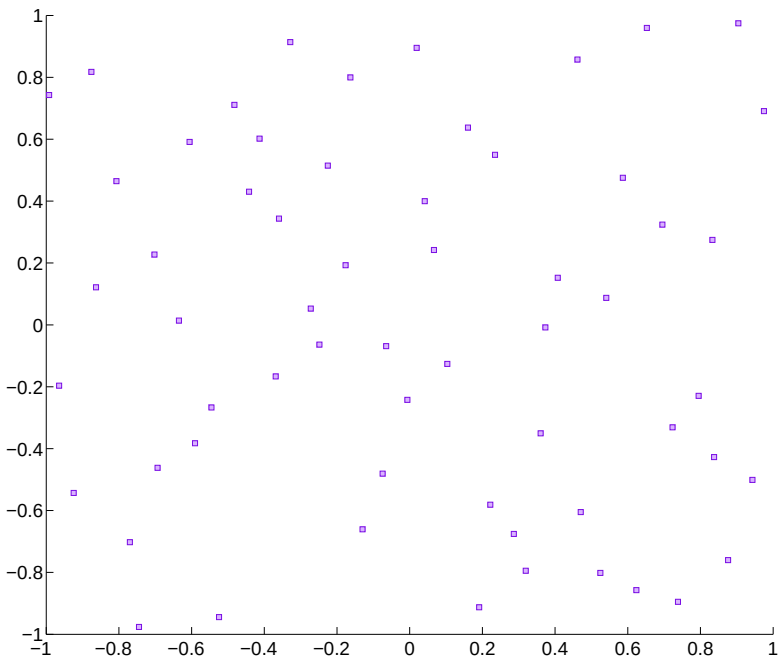

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The worst-case approach

- Let $\mathcal{A}_N$ be the class of all optimization strategies $\underline{X}_N$ that query sequentially N evaluations of f at points $X_1, \ldots, X_N$.
- Define the error of approximation of a strategy $\underline{X}_N \in \mathcal{A}_N$ on f as

$$\varepsilon(\underline{X}_N, f) = \widehat{m}_N(f) - m(f)$$

with $\widehat{m}_N(f) = f(X_1) \wedge \cdots \wedge f(X_N)$

- Assume that f belongs to a class of functions $\mathcal{F} \rightarrow$ prior information

➜ A first idea to define a notion of a good strategy is to consider robustness with respect to a worst case

- Define the minimax risk

$$r_{\mathrm{minimax}}(\mathcal{F}) = \inf_{\underline{X}_N \in \mathcal{A}_N} \sup_{f \in \mathcal{F}} \varepsilon(\underline{X}_N, f)$$

- A strategy ${\underline{X}_N}^\star$ that attains $r_{\mathrm{minimax}}(\mathcal{F})$ is called an (optimal) minimax strategy
- ${\underline{X}_N}^\star$ has the best worst-case performance on $\mathcal{F}$

Example of a minimax strategy: case of Lipschitz functions

- Recall that a function $f : \mathbb{X} \to \mathbb{R}$ is Lipschitz continuous if there exists $K \geq 0$ such that, for all x_1 and x_2 in $\mathbb{X}$,

$$|f(x_1) - f(x_2)| \leq K\|x_1 - x_2\|.$$

  (Any such K is referred to as a Lipschitz constant for the function f.)

- Let $\mathcal{F}$ be the class of all Lipschitz continuous functions $\mathbb{X} \to \mathbb{R}$, with Lipschitz constant K

Example of a minimax strategy: case of Lipschitz functions

- For any strategy $\underline{X}_N$, define the fill distance as

$$h_N = \sup_{x \in \mathbb{X}} \min_{i=1,\ldots,N} |x - X_i|$$

- For any $\underline{X}_N \in \mathcal{A}_N$ and any $f \in \mathcal{F}$,

$$\varepsilon(\underline{X}_N, f) = f(X_1) \wedge \cdots \wedge f(X_N) - f(x^\star) \leq f(X_{i^\star}) - f(x^\star) \leq K h_N \,,$$

  where $X_{i^\star}$ is the nearest point to $x^\star$
- Thus, for any $\underline{X}_N \in \mathcal{A}_N$, $\sup_{f \in \mathcal{F}} \varepsilon(\underline{X}_N, f) \leq K h_n$
- For any $\underline{X}_N$, there exists a function $f \in \mathcal{F}$ such that

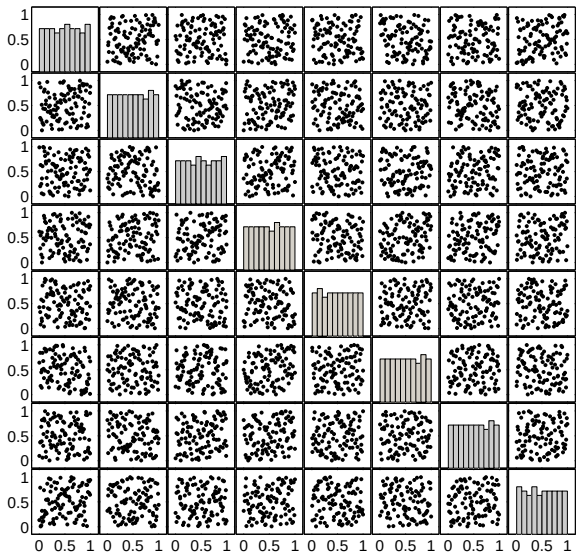
$$\varepsilon(\underline{X}_N, f) = K h_N$$

  Thus,

$$\sup_{f \in \mathcal{F}} \varepsilon(\underline{X}_N, f) = K h_N$$

Example of a minimax strategy: case of Lipschitz functions

- Consequence: a minimax strategy minimizes h_N
  $\rightarrow$ sample points have to be uniformly distributed over the search domain
- For $d = 1$, $\forall\, \underline{X}_N$, $h_N \geq \frac{|X|}{(N+1)} \implies$ the optimal strategy is the uniform sampling: $r_{\text{minimax}}(\mathcal{F}) = K\frac{|X|}{(N+1)}$
- For $d > 1$, use a *space-filling* design, *e.g.*., Maximin Latin Hypercube Sampling [McKay, Conover and Beckman (1979)] is an easy procedure that will generally provide good suboptimal designs



Example of a maximin Latin hypercube sampling of size $n = 100$ in dimension $d = 8$

The worst-case approach

- Consequence: for Lipschitz continuous functions, the minimax strategy consists in having sample points uniformly distributed over the search domain
- Here, the optimal strategy is non-adaptive!
- It may be more satisfying to achieve a balance between exploration of the search domain and local search in promising regions (good performance on worst cases and good convergence rate)
- Worst-case setting: appropriate framework to assess the performance of an optimization algorithm?
- We need to know how an optimization algorithm performs for "typical" functions f not corresponding to worst cases
- A classical approach is to adopt an average-case point of view

3. Average-case approach to the problem of optimization

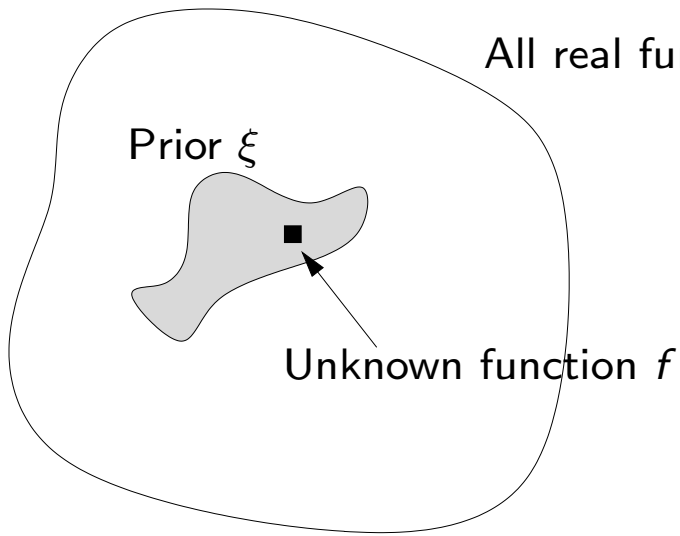
Average-case approach

- Average-case $\rightarrow$ introduction of a probability space $(\Omega, \mathcal{B}, \mathrm{P}_0)$
- We consider methods where f is seen as a sample path of a real-valued random process ξ defined on $(\Omega, \mathcal{B}, \mathrm{P}_0)$ with parameter in $\mathbb{X}$

  $\rightarrow$ there exists $\omega \in \Omega$ such that

$$f = \xi(\omega, \cdot)$$

- From a Bayesian decision-theoretic point of view, ξ represents prior knowledge about f



- A good strategy is a strategy that achieves, or gets close to, the optimal average risk

$$r_{\mathrm{average}} := \inf_{\underline{X}_N \in \mathcal{A}_N} \mathrm{E}_0 \left(\epsilon(\underline{X}_N, \xi) \right)$$

where E_0 denotes the expectation with respect to P_0

Expected Improvement [Mockus et al. 78, Schonlau et al. 96, Jones et al. 98]

- The optimal Bayesian one-step lookahead strategy for the problem of optimization corresponds to choosing each new evaluation point according to

$$\begin{aligned} X_{n+1} &= \operatorname*{argmin}_{x\in\mathbb{X}} \mathsf{E}_n\left(\widehat{m}_{n+1} - m \mid X_{n+1} = x\right) \\ &= \operatorname*{argmin}_{x\in\mathbb{X}} \mathsf{E}_n\left(\widehat{m}_{n+1} \mid X_{n+1} = x\right) \\ &= \operatorname*{argmin}_{x\in\mathbb{X}} \mathsf{E}_n\left(\widehat{m}_n \wedge \xi(X_{n+1}) \mid X_{n+1} = x\right) \\ &= \operatorname*{argmin}_{x\in\mathbb{X}} \mathsf{E}_n\left(0 \wedge (\xi(X_{n+1}) - \widehat{m}_n) \mid X_{n+1} = x\right) \\ &= \operatorname*{argmax}_{x\in\mathbb{X}} \rho_n(x) := \mathsf{E}_n\left((\widehat{m}_n - \xi(X_{n+1}))_+ \;\middle|\; X_{n+1} = x\right) \end{aligned}$$

  with

  - E_n conditional expectation wrt $\xi(X_1), \ldots, \xi(X_n)$
  - $\widehat{m}_n = \xi(X_1) \wedge \cdots \wedge \xi(X_n)$,
  - $z_+ = \max(z, 0)$

- The sampling criterion ρ_n is the expected improvement (EI)

  $\rightarrow$ average excursion of $\xi(x)$ below the current minimum of past evaluation results

- A well-known Bayesian optimization algorithm
  - proposed by Mockus et al.
  - popularized by the EGO algorithm of Jones et al.

Expected Improvement [Mockus 78, Schonlau et al. 96, Jones et al. 98]

- Assume ξ is a Gaussian process, with known mean and covariance functions
- Then, $\rho_n(x)$ has a closed-form expression:

$$\rho_n(x) \;=\; \gamma\left(\, m_n - \widehat{\xi}_n(x;\underline{X}_n),\, \sigma_n^2(x)\,\right),$$

where

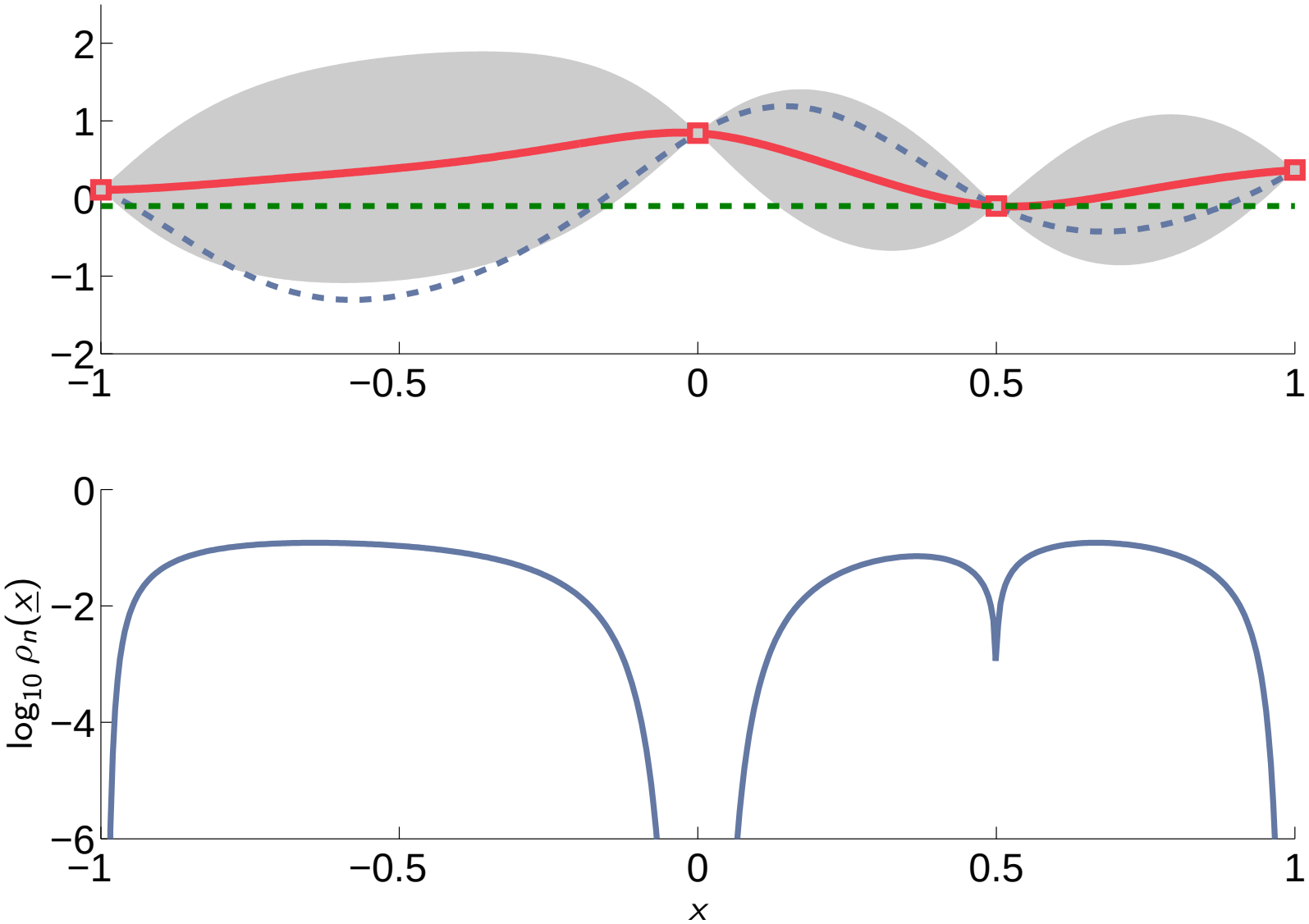
$$\gamma(z,s) \;=\; \begin{cases} \sqrt{s}\,\Phi'\left(\frac{z}{\sqrt{s}}\right) + z\,\Phi\left(\frac{z}{\sqrt{s}}\right) & \text{if } s>0, \\ \max(z,0) & \text{if } s=0. \end{cases}$$

and $\widehat{\xi}_n(x;\underline{X}_n)$ and $\sigma_n^2(x)$ are the kriging predictor and the kriging variance of $\xi(x)$ (Matheron, 1960) $\rightarrow$ see illustrating figure below.

- The EI algorithm:

$$\begin{cases} X_1 & = & x_{\text{init}}\,, \\ X_{n+1} & = & \underset{x\in\mathbb{X}}{\text{argmax}}\ \rho_n(x)\,, \quad n\geq 1\,, \end{cases}$$

Global optimization based on EI



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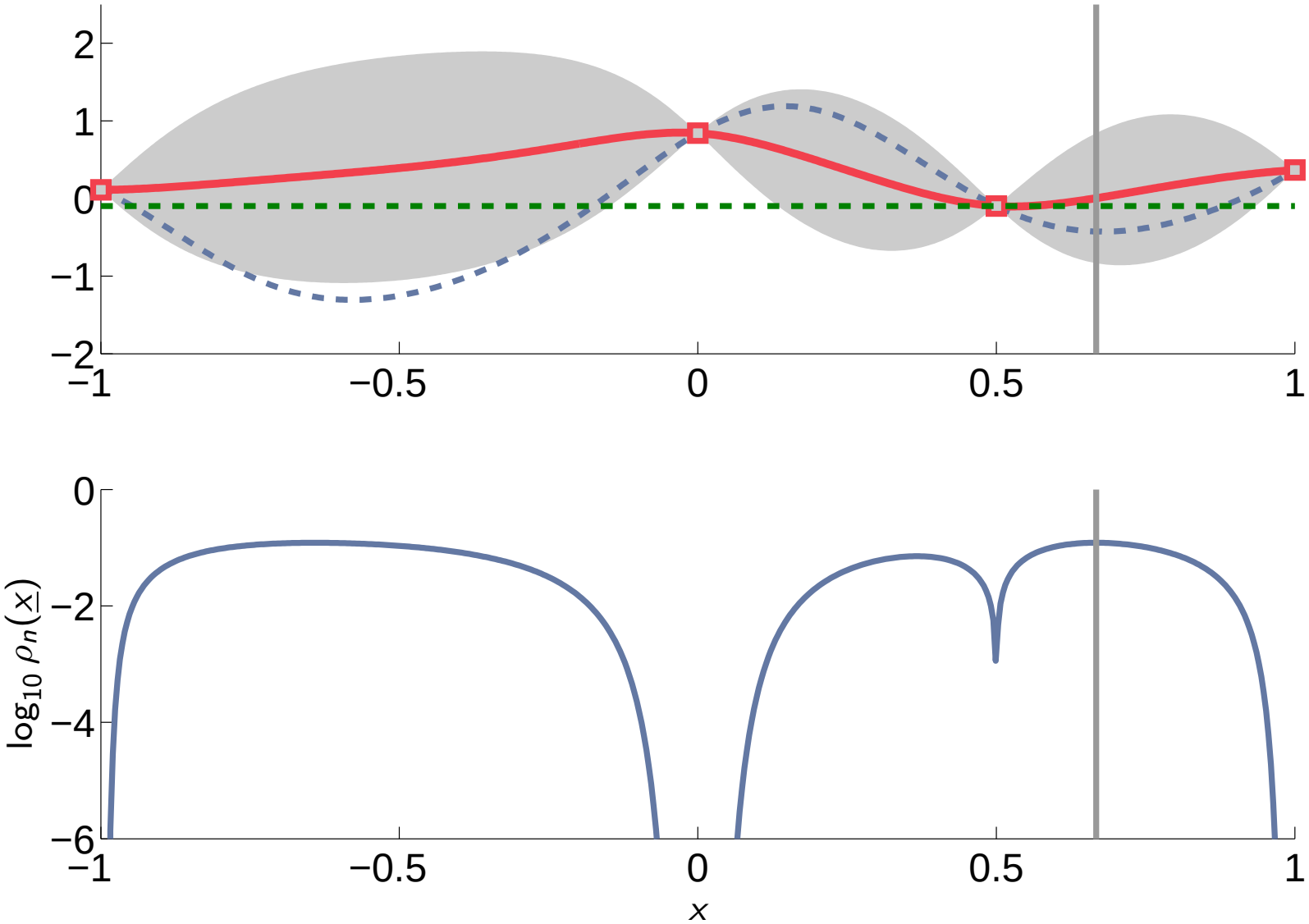

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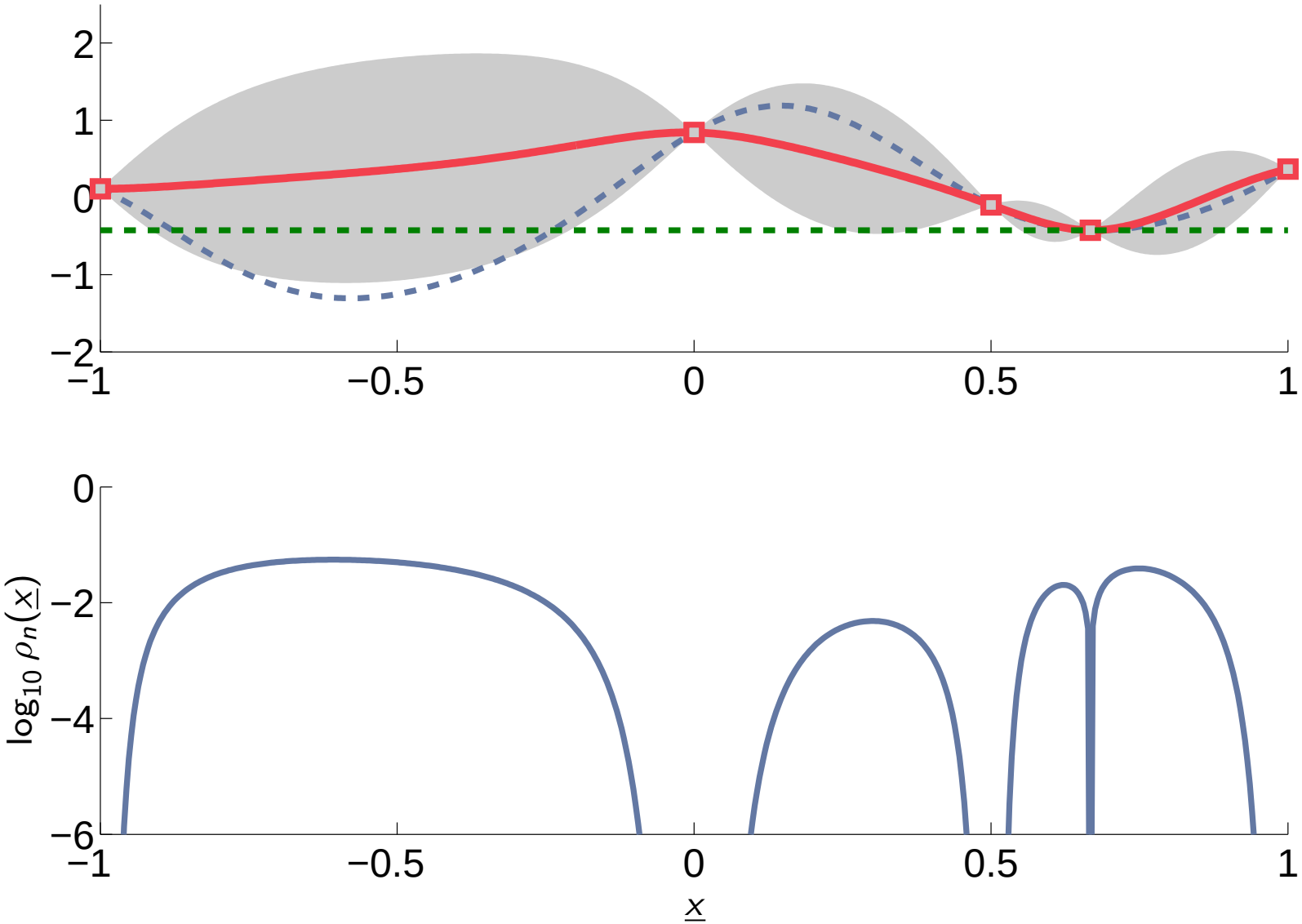

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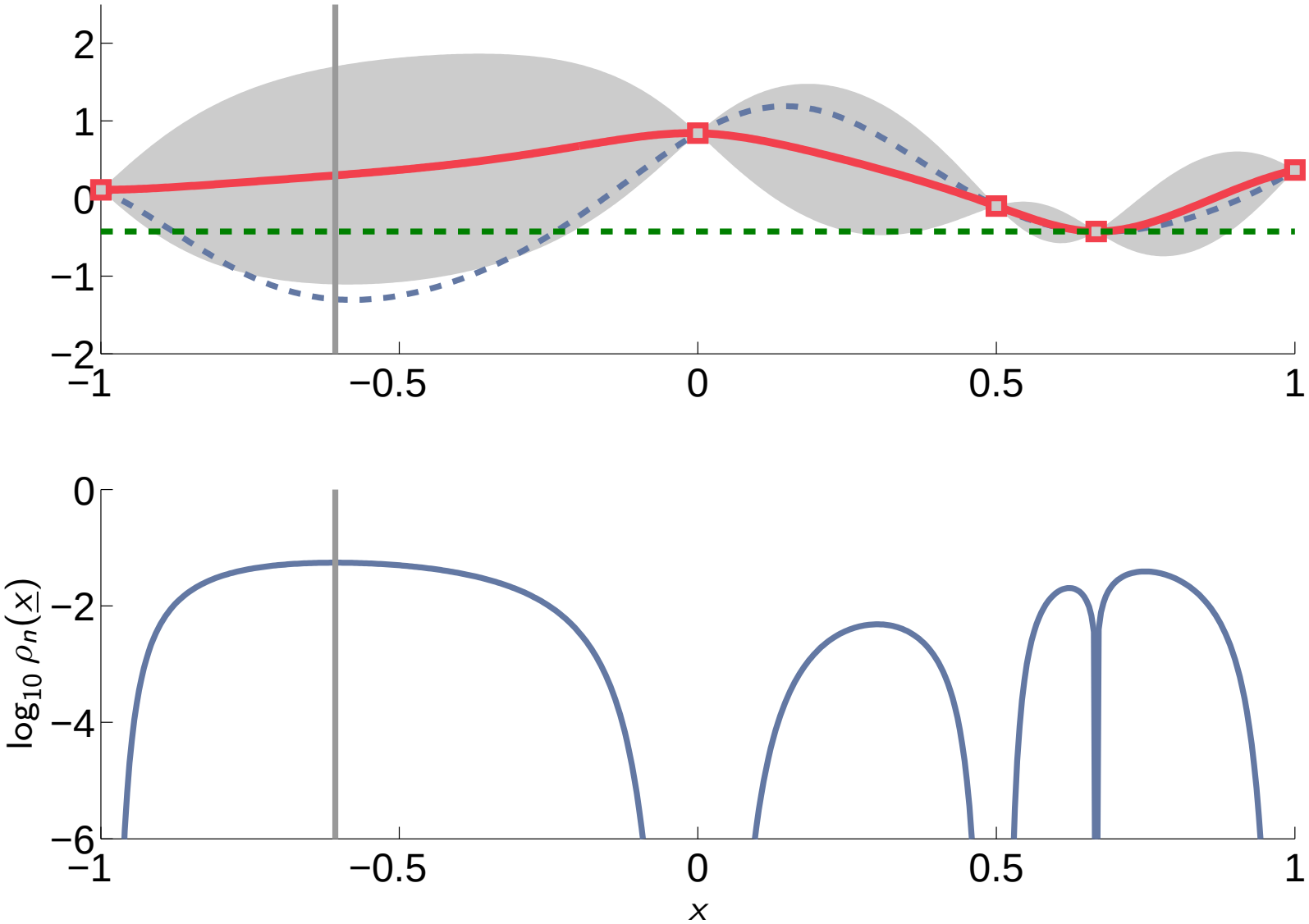

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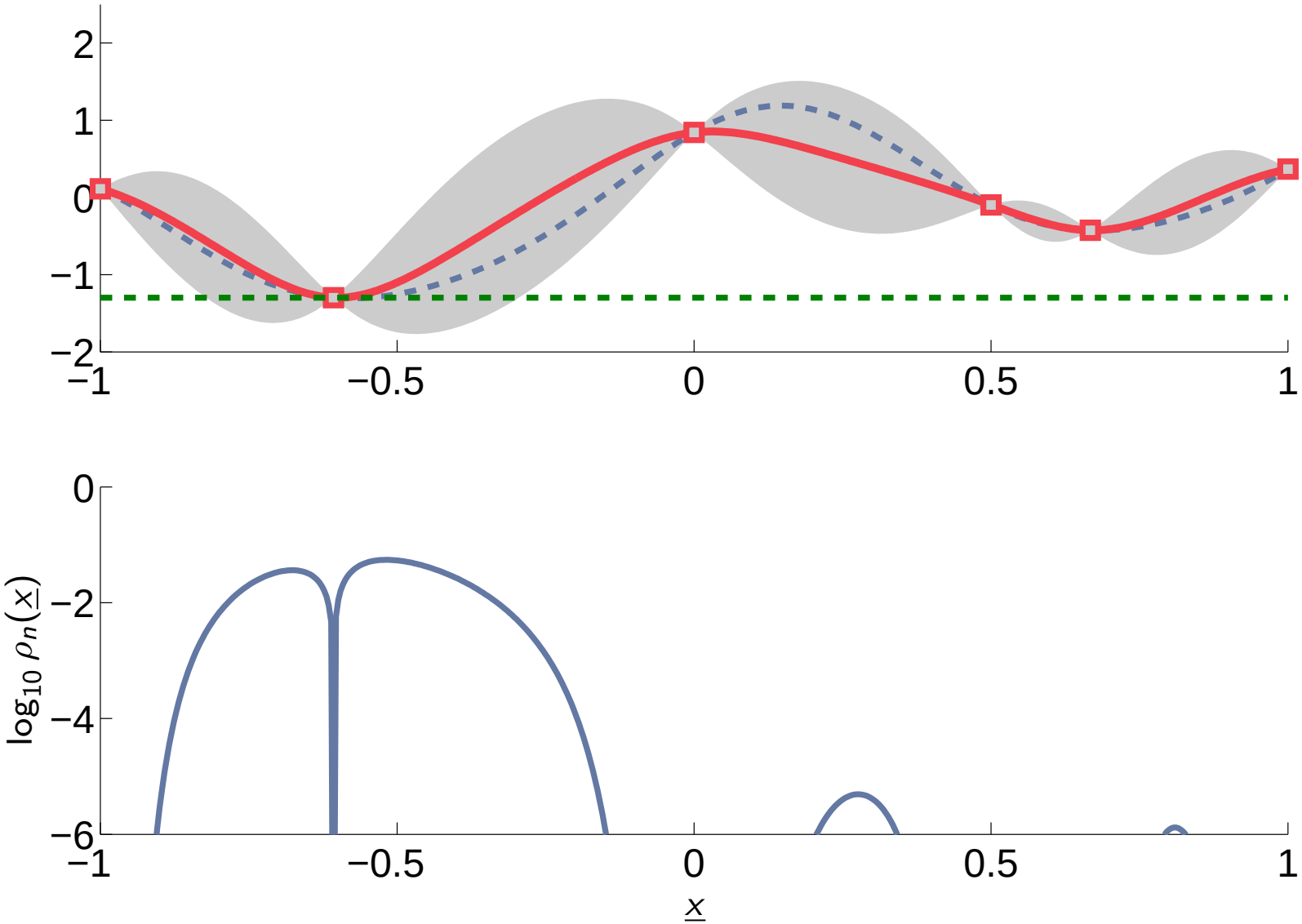

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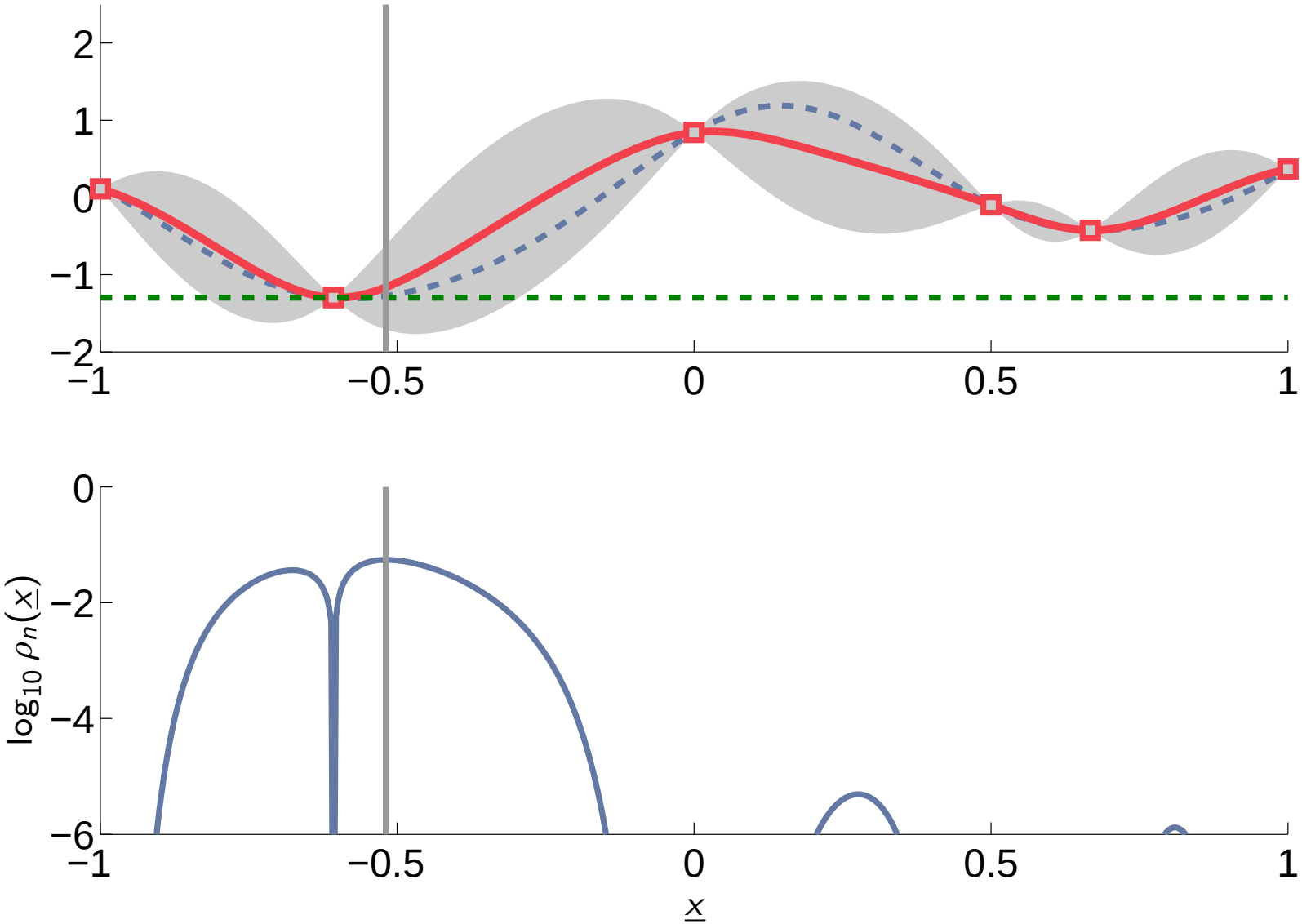

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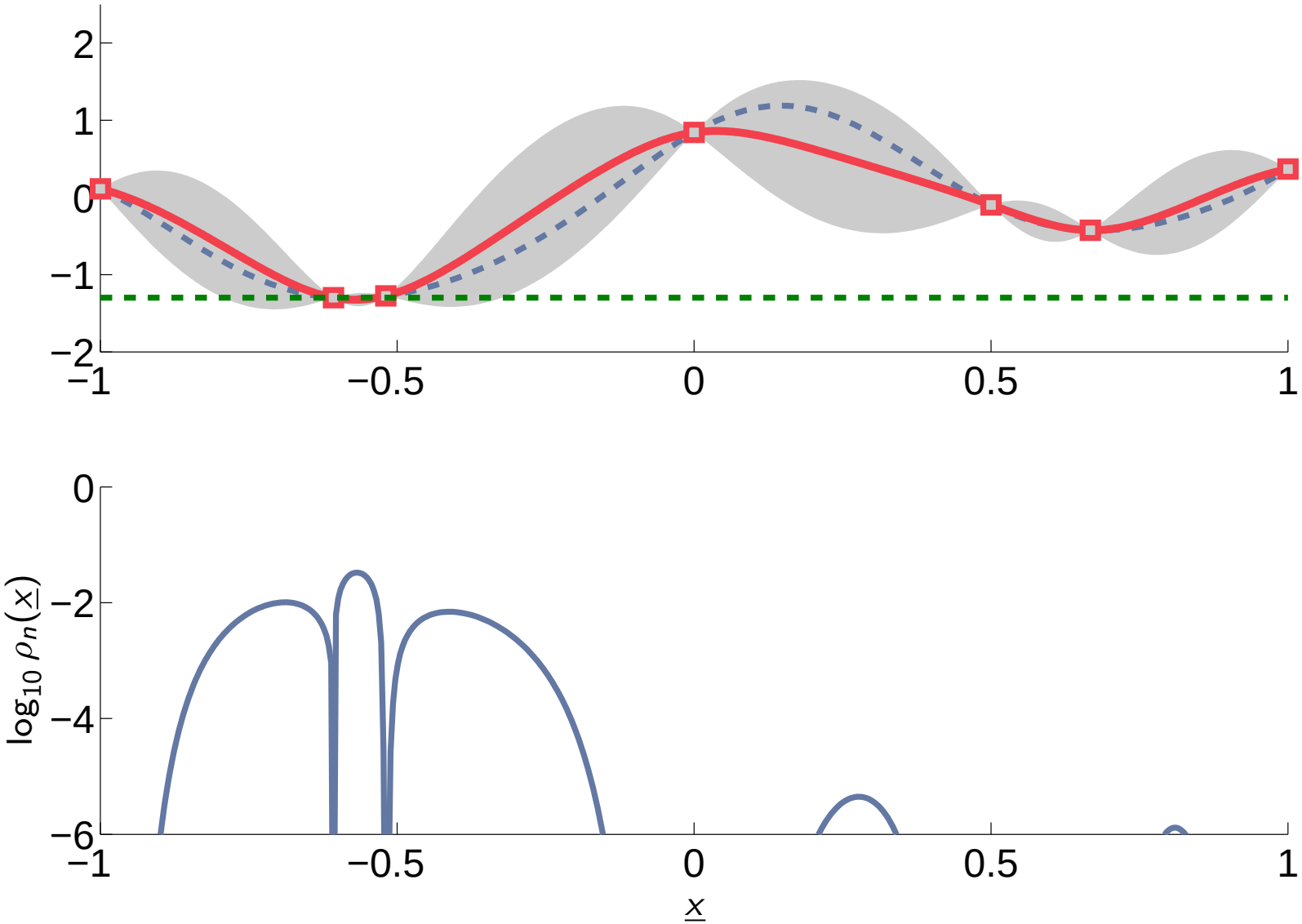

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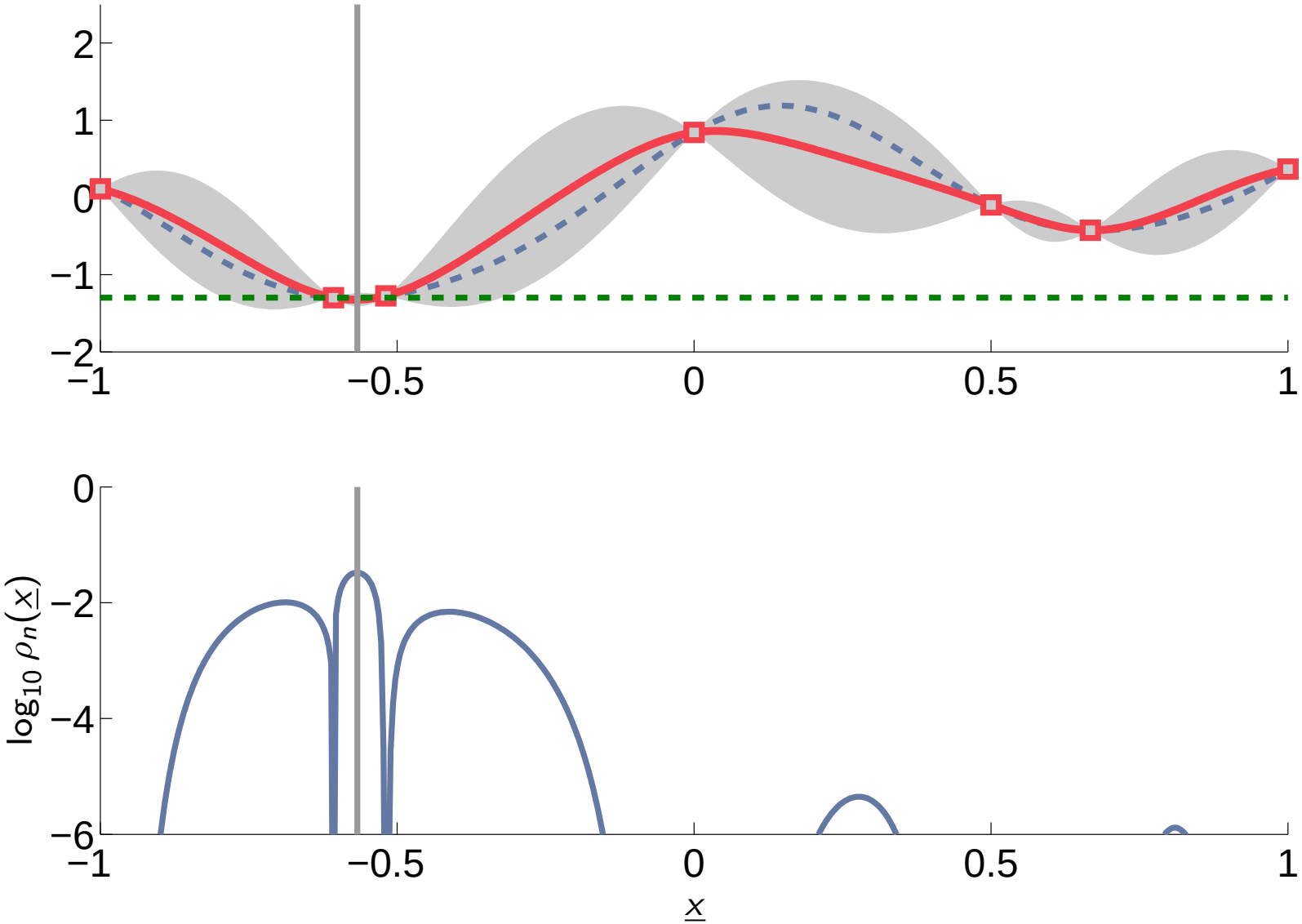

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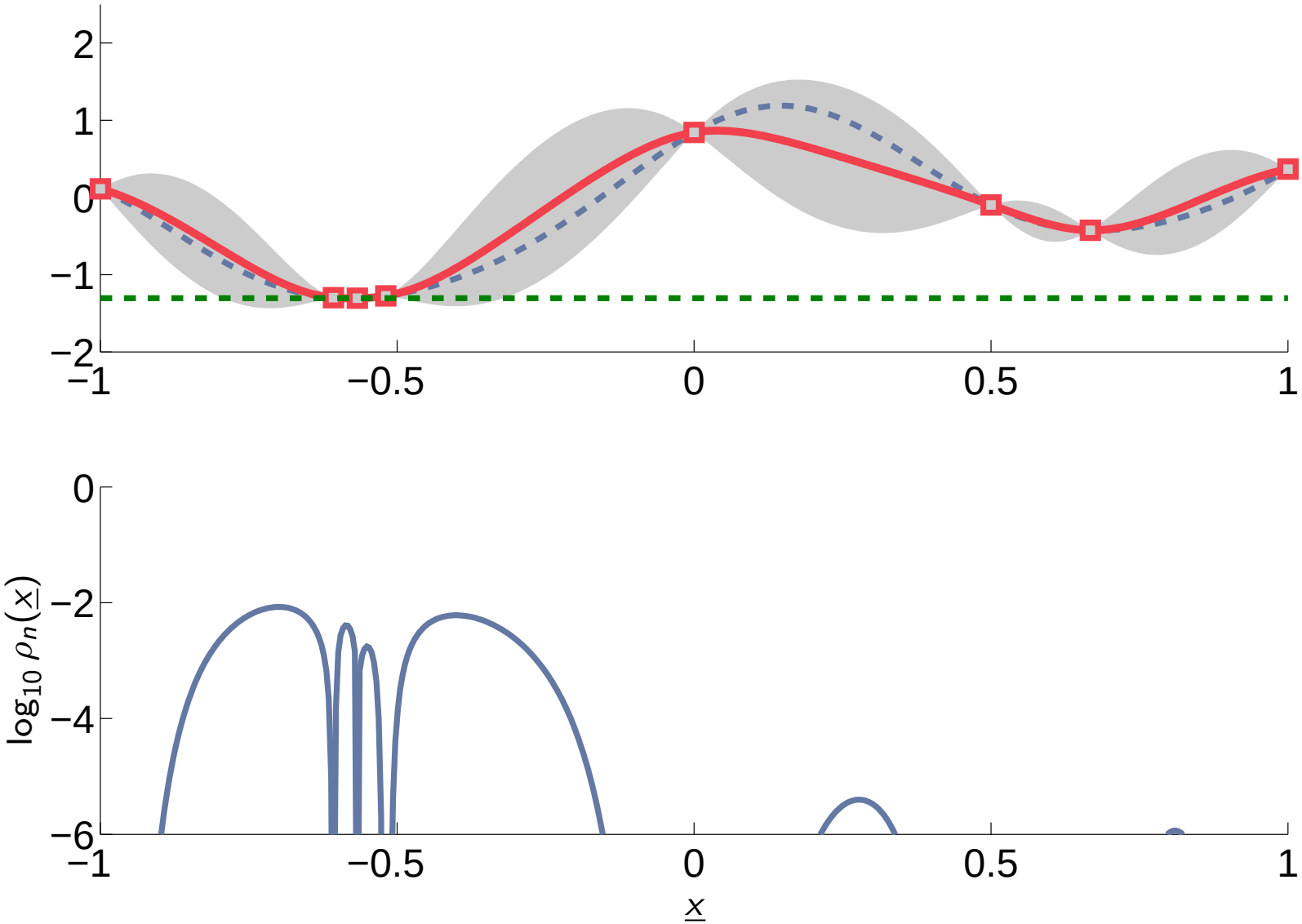

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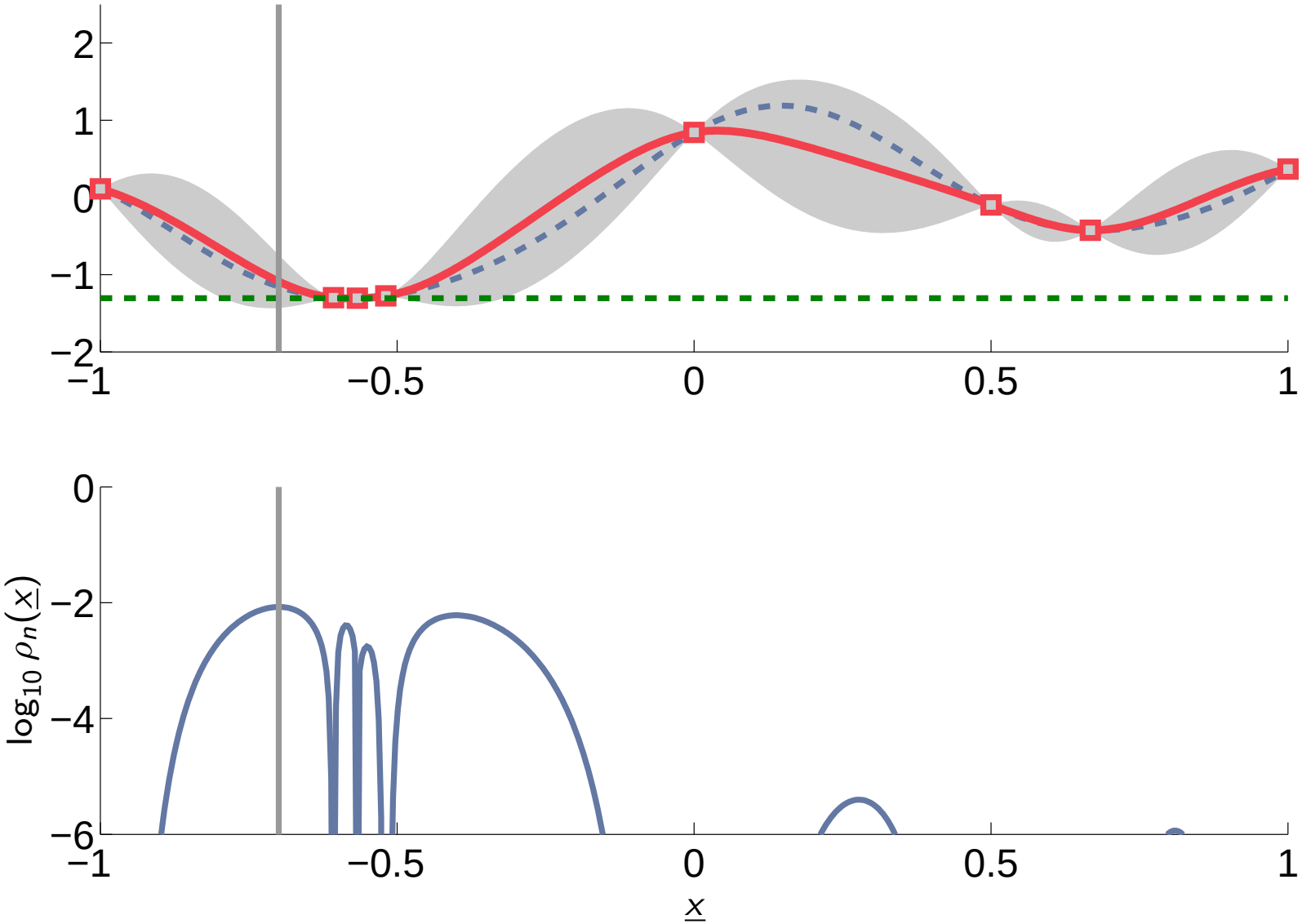

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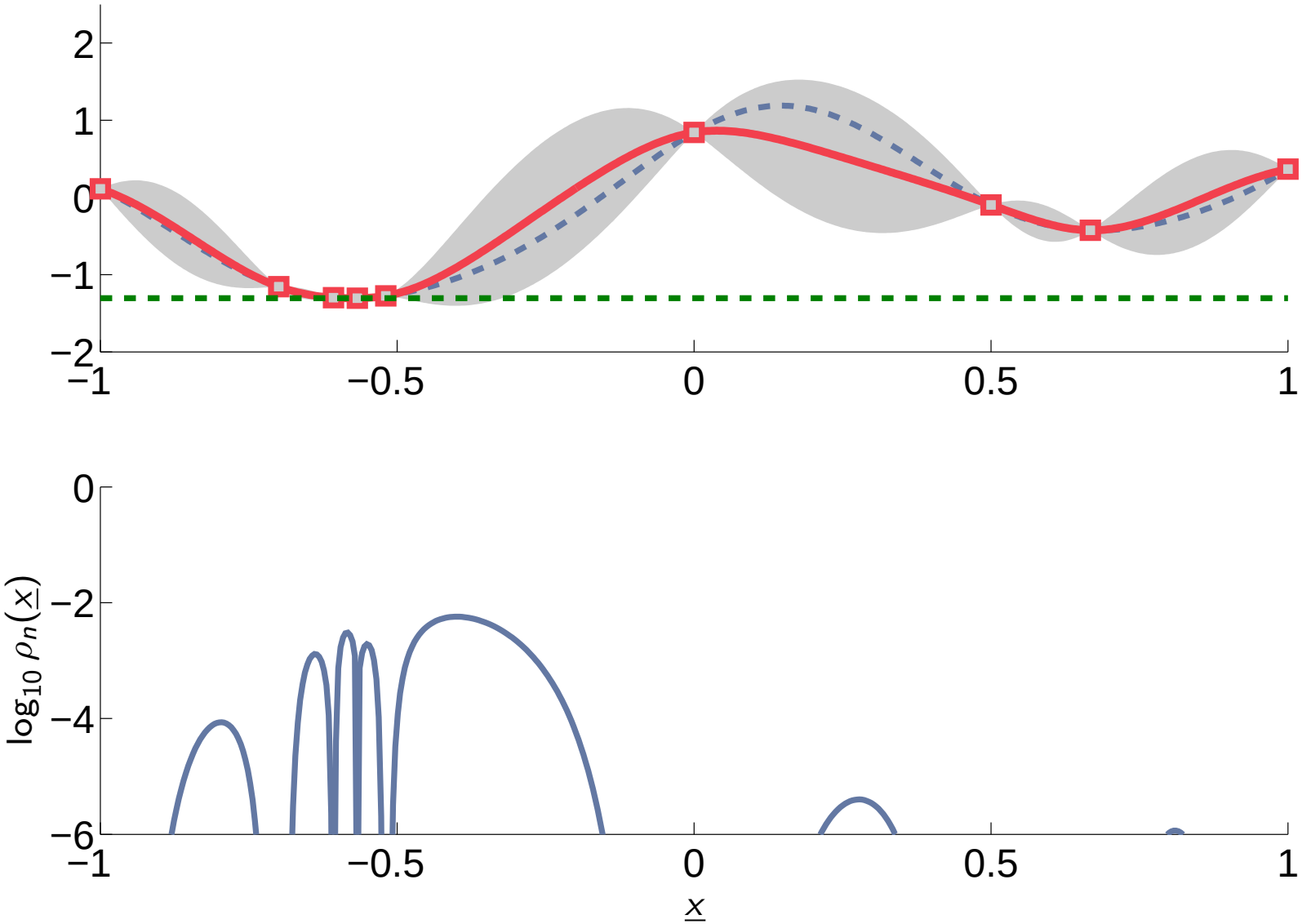

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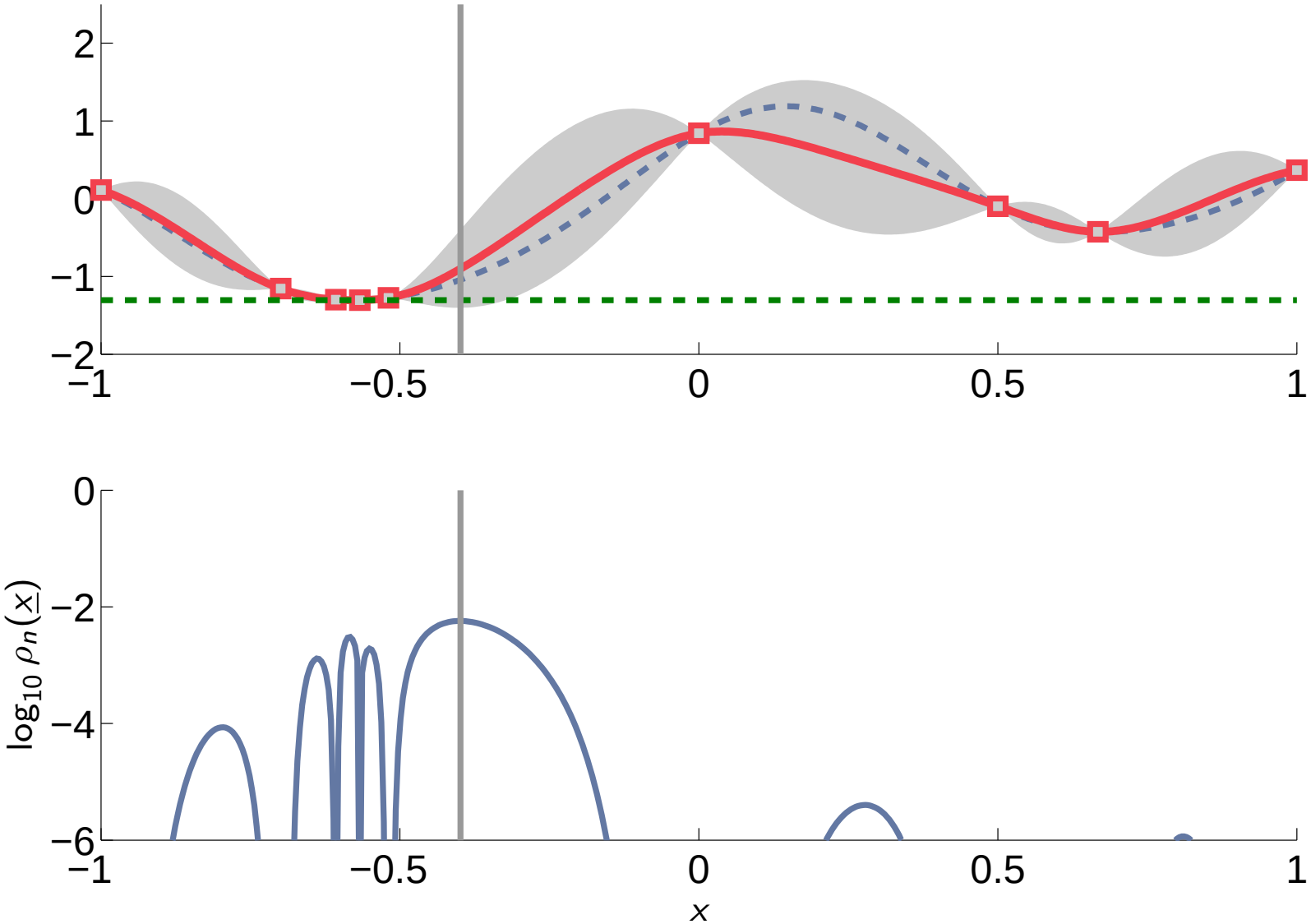

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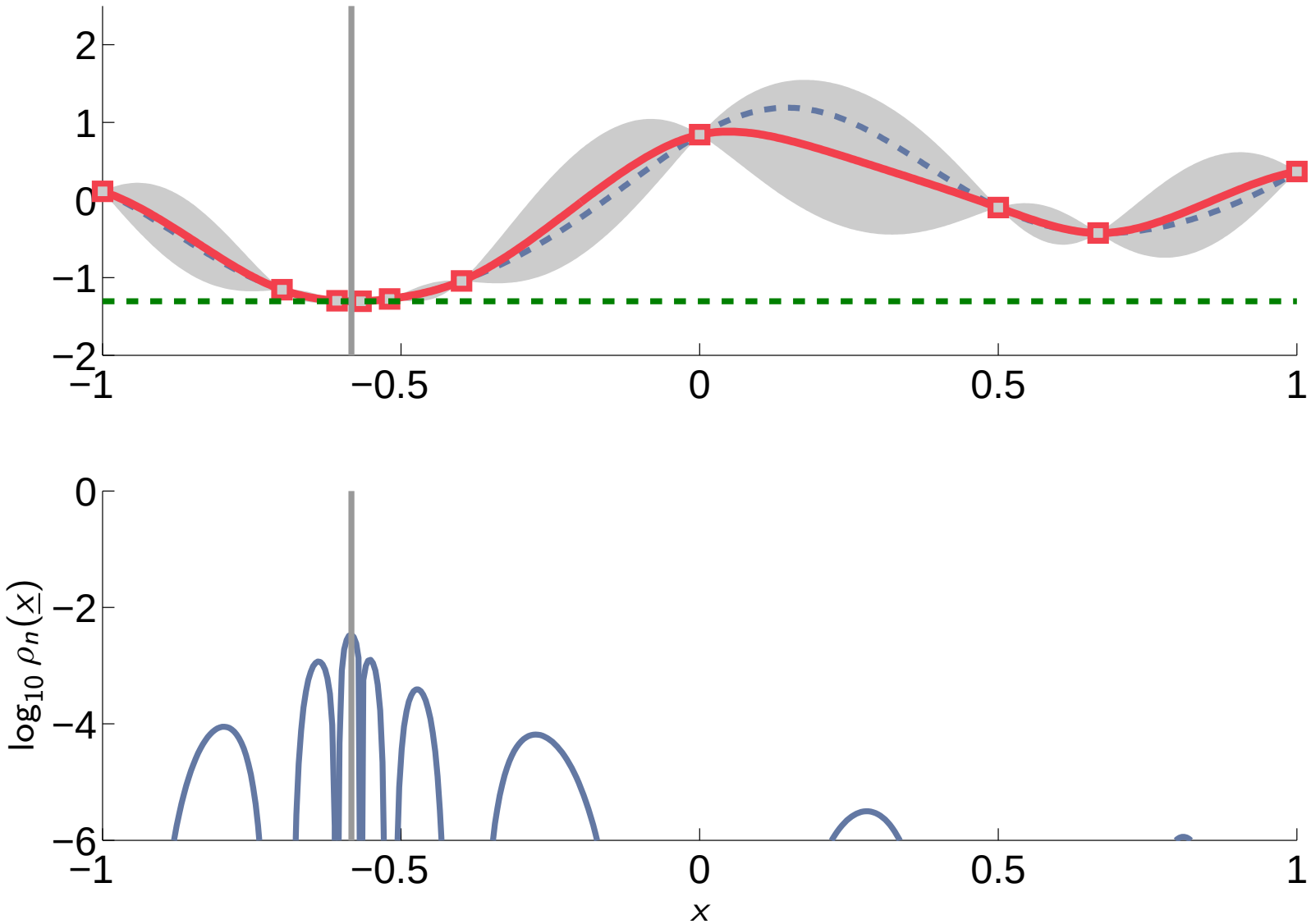
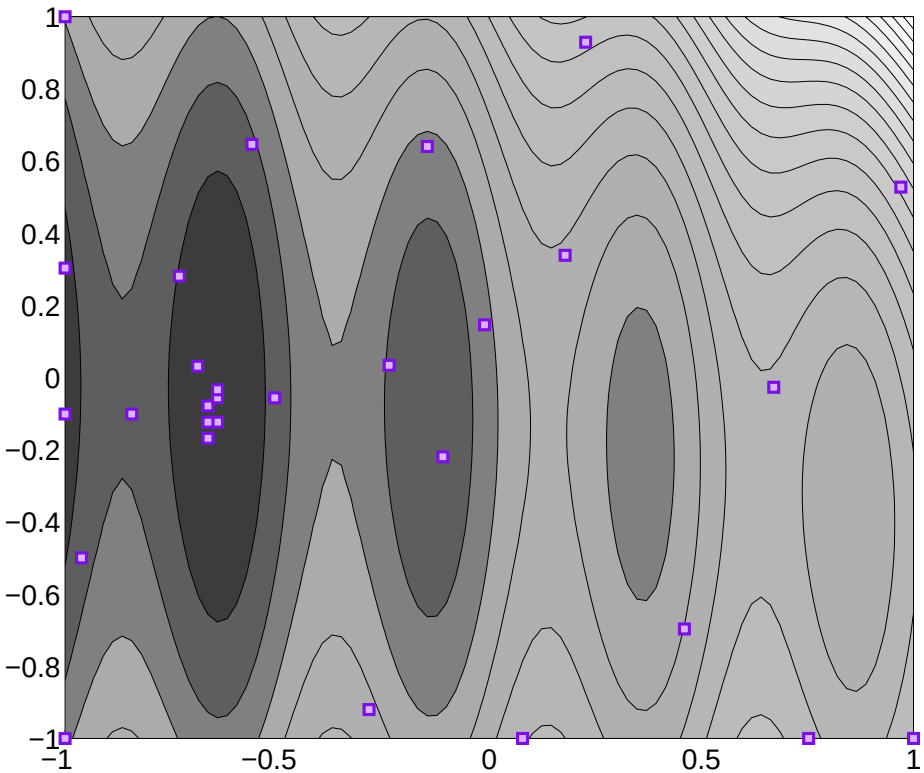


EI/EGO: 2D illustration

(f defined on Slide 12)



	$\widehat{m}_n$ with $N = 60$
LHS	-5.823
DIRECT	-5.839
EI/EGO	-5.845
Global minimum	-5.845

NB: Global minimum found by the EI algorithm in only 31 evaluations (abs. tol. 1.10^{-4})

Summing up

Global optimization based on EI

- Particularly interesting in the context of expensive-to-evaluate functions, very useful and effective in practical situations
- A great number of applications can be found in the literature (aeronautics, chemistry, energy...)
- Some theoretical results on the convergence of these algorithms: Vazquez & Bect 2010, Bull 2011...
- Efficient implementation based on SMC techniques: Benassi, Bect, Vazquez 2013

Concluding remarks

- In the context expensive simulations, Bayesian strategies show very good performances with respect to alternative approaches
- Bayesian strategies can be used for global optimization, estimation of probabilities of failure, quantile estimation...