Bayesian Methods for Simulation Optimization

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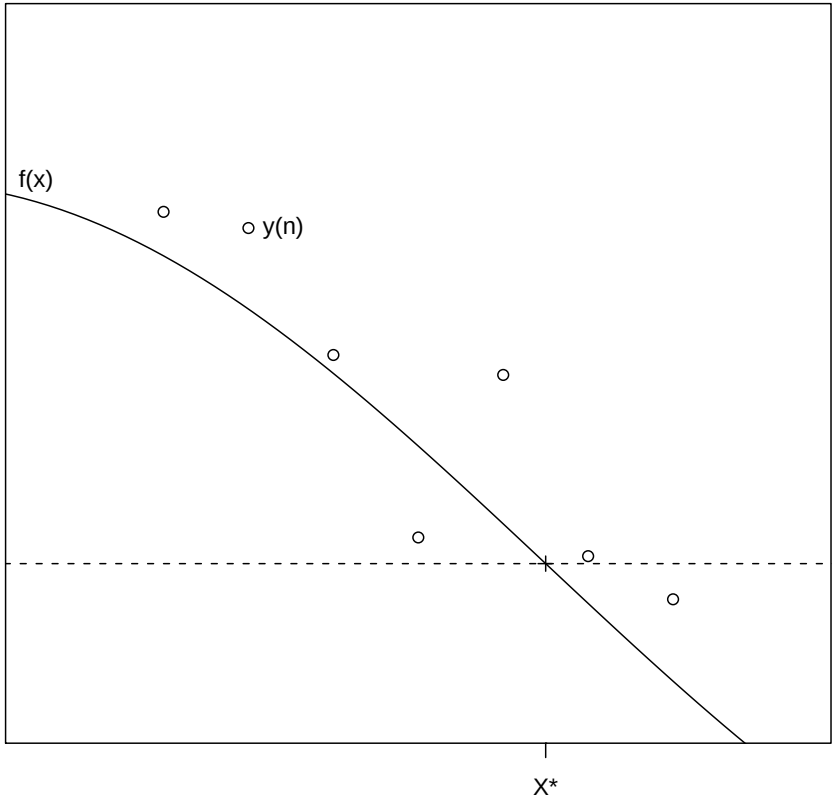
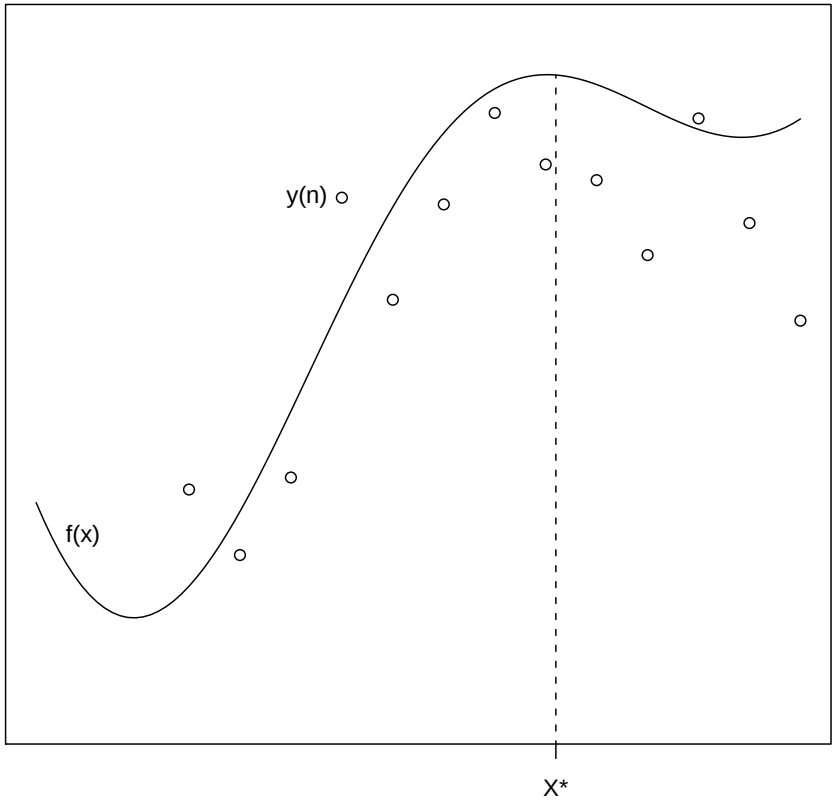
Stochastic Root Finding

Find the root of a monotone function whose values can only be measured with noise. Use as few function evaluations as possible.



Stochastic Global Optimization

Find the maximum of a non-concave function in 1 or more dimensions whose values can only be measured with noise. Use as few function evaluations as possible.



Overview

- Simulation optimization problems can be formulated as problems in sequential Bayesian design of experiments.
- When formulated in this way, they can be analyzed using dynamic programming.
- Novel results:
  - We solve the DP for an idealized version of stochastic root-finding and apply this to the real stochastic root-finding problem.
  - We present a myopic policy motivated by the DP for stochastic global optimization.

Outline

General Framework

1. Before we begin, nature fixes some true function f.
   - e.g., f is the function whose root we are trying to find.
2. For time $n = 1$ up to N, we:
   1. Choose some type of measurement x_n to perform.
   2. Observe some value y_n whose distribution depends on x_n and f.
3. After the final measurement, we make some decision $\widehat{x_*}$ based on the data $x_1, \ldots, x_N$, $y_1, \ldots, y_N$.
4. We pay some penalty $L(\widehat{x_*}, f)$.

Our goal is to choose $x_1, \ldots, x_N, \widehat{x_*}$ adaptively to minimize $L(\widehat{x_*}, f)$.

General Framework

- $\mathbb{E}^{\pi}[L(\widehat{x_*}, f) \mid f]$ is the expected loss when we use policy π and the truth is f.
  - A policy π is a method for choosing each x_{n+1} as a function of $x_{1:n}, y_{1:n}$, and choosing $\widehat{x_*}$ as a function of $x_{1:N}, y_{1:N}$.
- We cannot solve $\inf_{\pi} \mathbb{E}^{\pi}[L(\widehat{x_*}, f) \mid f]$ because the answer depends on f, which we do not know.
- In this talk, we are interested in **average case performance**.

Bayesian General Framework

- The average-case loss under a probability distribution $\mathbb{P}_0$ is

$$\int \mathbb{E}^{\pi}\left[L(\widehat{x_*}, f) \mid f\right] \mathbb{P}_0(df) = \mathbb{E}^{\pi}\left[L(\widehat{x_*}, f)\right]$$

- We call $\mathbb{P}_0$ our "prior".
- Goal: minimize the average-case loss

$$\inf_{\pi} \mathbb{E}^{\pi}\left[L(\widehat{x_*}, f)\right]$$

Bayesian General Framework

- Associated with the prior is a sequence of "posterior" distributions

$$\mathbb{P}_n(f \in \cdot) = \mathbb{P}_0\{f \in \cdot \mid x_{1:n}, y_{1:n}\}.$$

- The problem $\inf_\pi \mathbb{E}^\pi[L(\widehat{x}_*, f)]$ can be viewed as a **Markov decision process**, where the Markov process being controlled is the sequence of posterior distributions $(\mathbb{P}_n : n \geq 0)$.
- As a Markov decision process, its solution is characterized by the **dynamic programming equations**.

Dynamic Programming

- $V_n(\mathbb{P}_n)$ is the **value function**. $\mathbb{P}_n$ at time n.

$$V_n(\mathbb{P}_n) = \inf_{\pi} \mathbb{E}_n^{\pi} \left[L(\widehat{x}_*, f) \right]$$

- The value function satisfies the **dynamic programming equations**:

$$V_N(\mathbb{P}_N) = \inf_{\widehat{x}_*} \mathbb{E}_N \left[L(\widehat{x}_*, f) \right]$$

$$V_n(\mathbb{P}_n) = \inf_{x} \mathbb{E}_n \left[V_{n+1}(\mathbb{P}_{n+1}) \mid x_{n+1} = x \right].$$

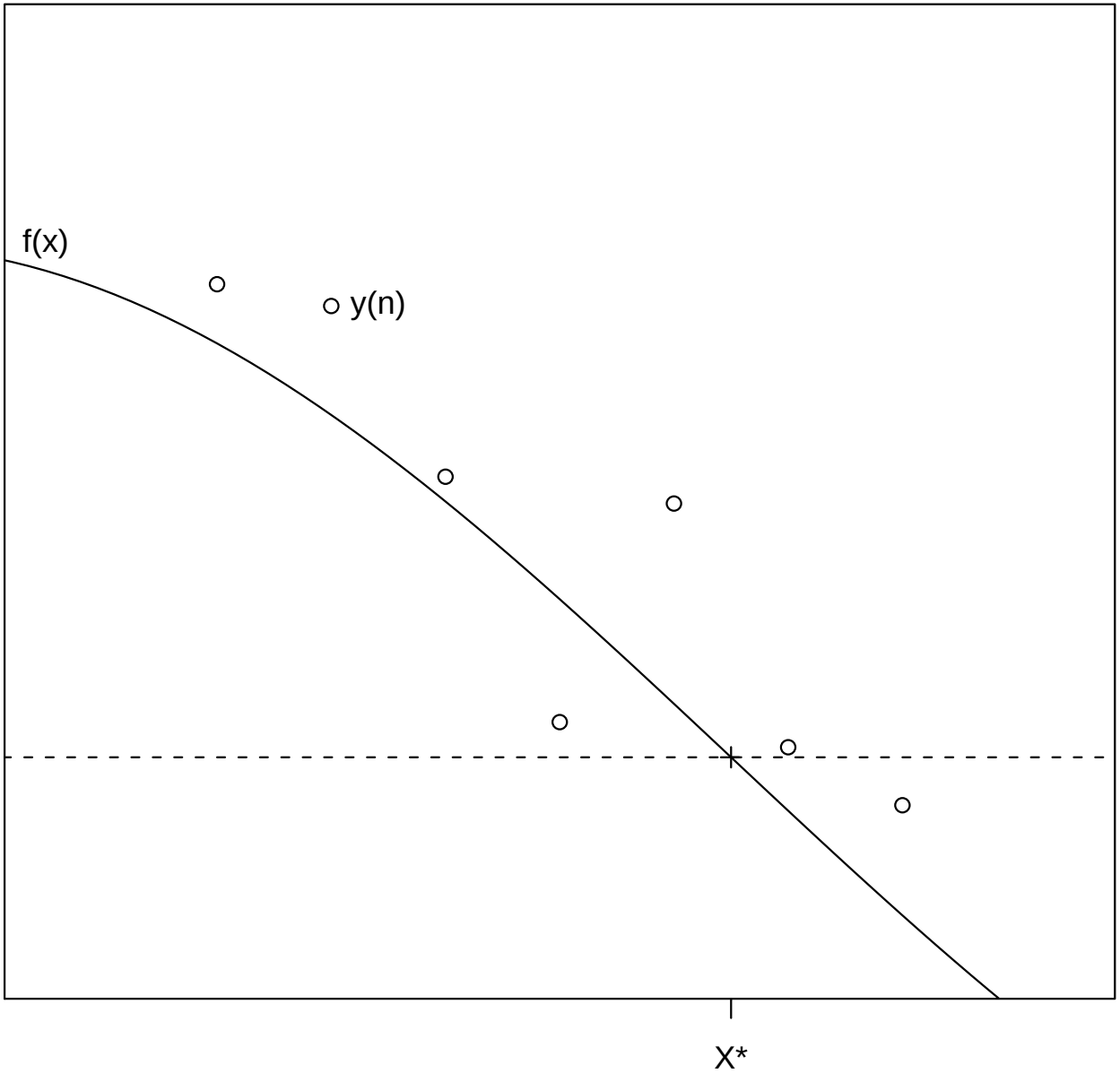
- Any policy whose decisions x_n, $\widehat{x}_*$ attain the infimum is optimal.
- **If we can find the value function, we can find the optimal policy**.

Dynamic Programming

- To find the value function numerically, we would have to compute V_n for every possible value of $(n, \mathbb{P}_n)$.
- This is usually **much too large to solve numerically**.
- Finding analytic solutions to dynamic programs is usually also difficult.
- In this talk, dynamic programming is used as a theoretical tool.
  - We solve one dynamic program analytically.
  - We solve another in a special case, motivating a heuristic solution.

Outline

Stochastic Root-Finding

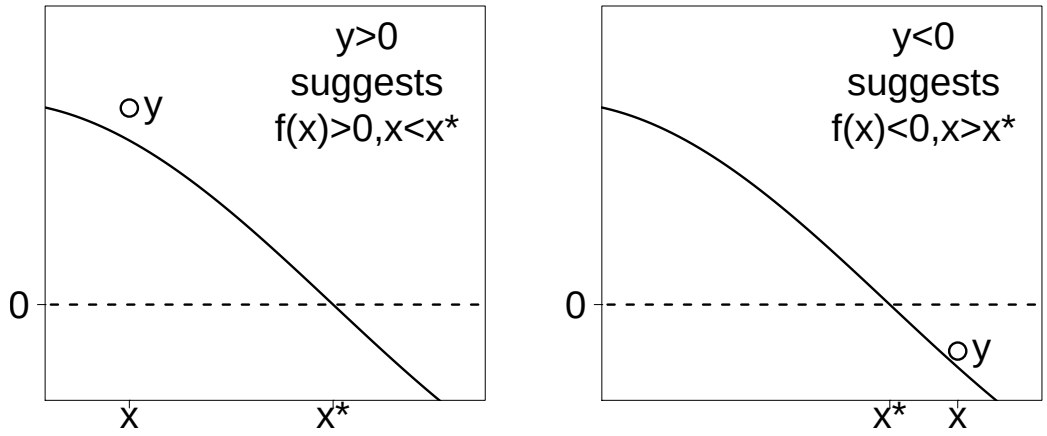


Stochastic Root-Finding

- $f : \mathbb{R} \mapsto \mathbb{R}$ is a decreasing function.
- The only way to evaluate f is via stochastic simulation.
- We observe $y_n = f(x_n) + \varepsilon_n$, where ε_n is independent noise.
- Our goal is to find a root x_*, i.e., a point x_* such that $f(x_*) = 0$.
- Central Question: Given a budget of N measurements, $x_1, \ldots, x_N$, how should we place them to find x_* as accurately as possible?

Stochastic Root-Finding: Model

- Assume we observe only whether y_n is larger or smaller than 0.



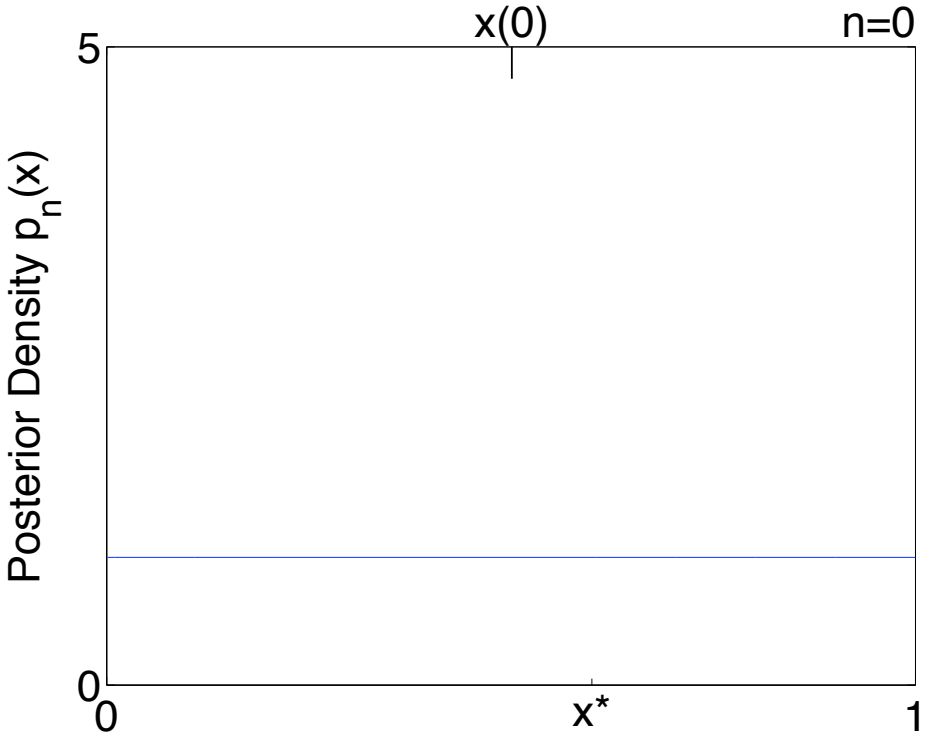
- Assume nature gives the incorrect sign with fixed known probability q:

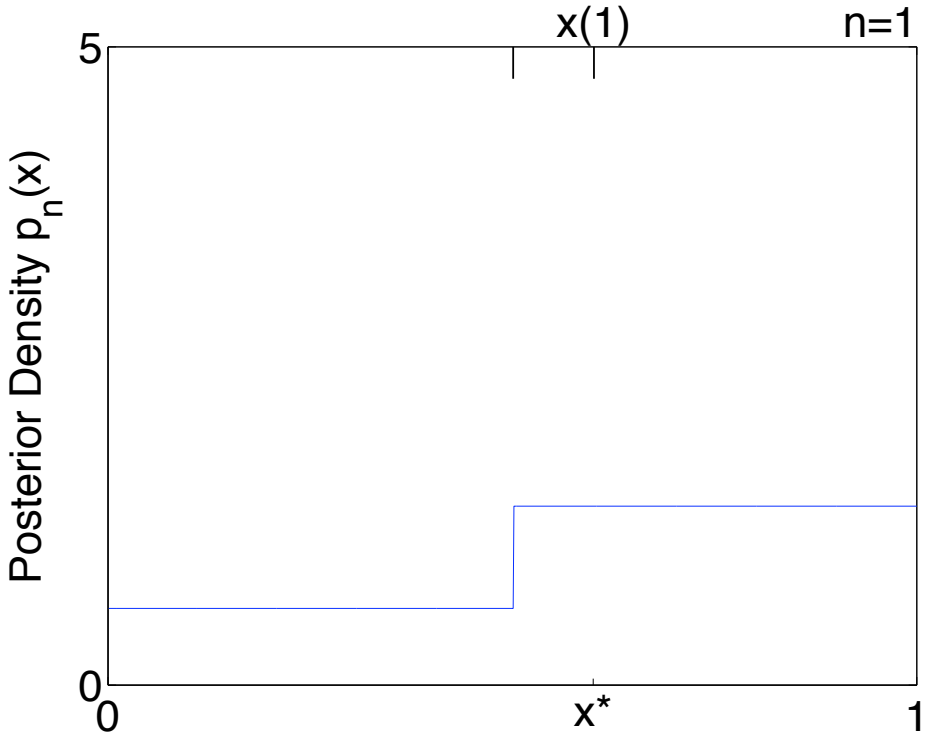
$$\operatorname{sgn}(y_n) = \begin{cases} -\operatorname{sgn}(f(x_n)), & \text{with probability } q, \\ \operatorname{sgn}(f(x_n)), & \text{with probability } 1-q \end{cases}$$

Posterior Distributions

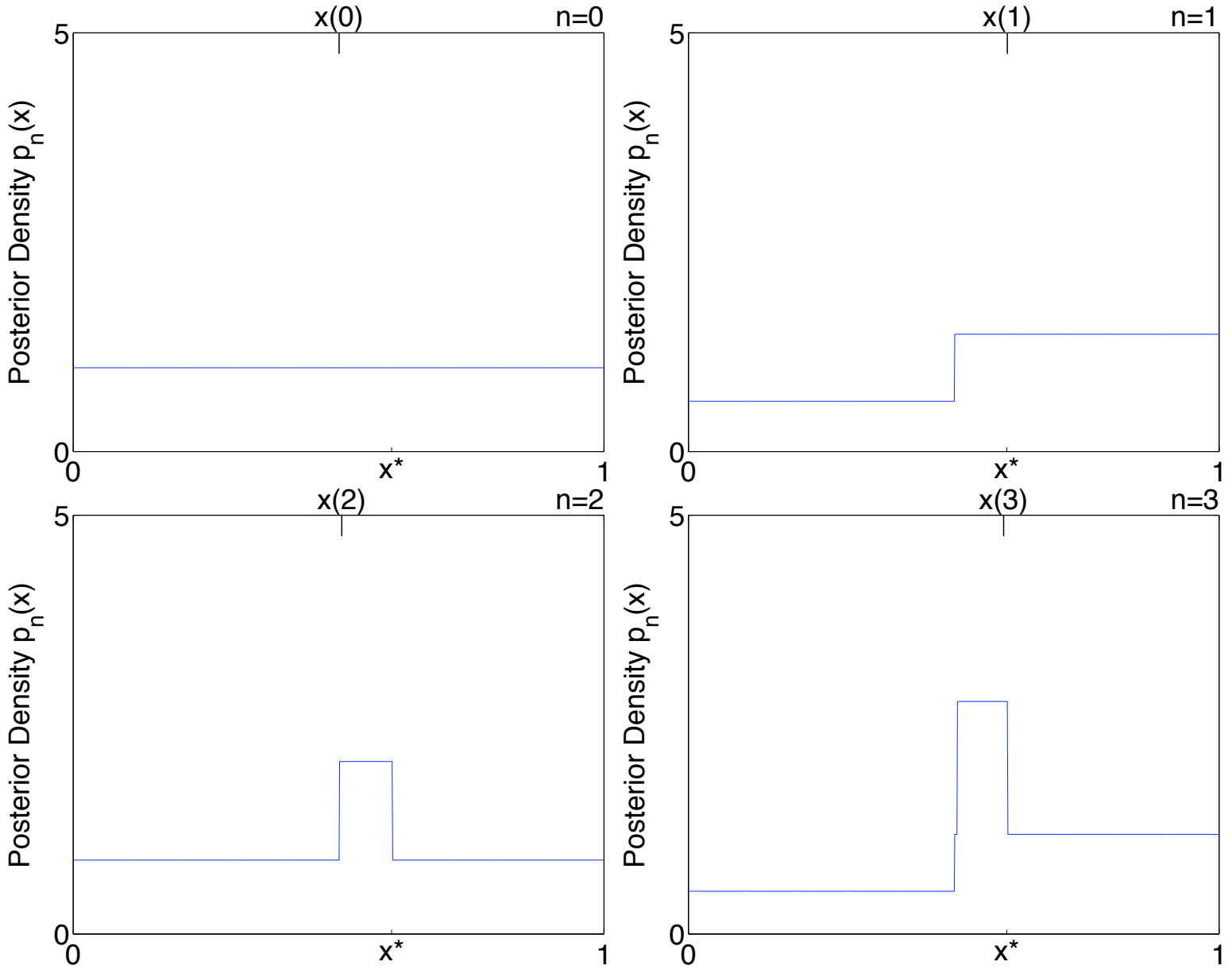
- Place a prior density p_0 on the root x_*, e.g., uniform on $[0,1]$.
- Each measurement x_n produces a new posterior density p_n on x_*:

$$p_n(x) = \mathbb{P}\{X_* \in dx \mid x_{1:n-1}, y_{1:n-1}\}$$





Posterior Distributions



Stochastic Root-Finding

- Our goal is to minimize the final entropy

$$H(p_N) = -\int p_N(x) \log p_N(x)\, dx.$$

- The value function is

$$V_n(p_n) = \inf_{\pi} \mathbb{E}^{\pi} \left[H(p_N) \mid p_n \right],$$

  and the stochastic optimization problem we need to solve is to find the policy π that attains the infimum defining $V_0(p_0)$.
- Bellman's recursion can be written,
  $V_n(p_n) = \inf_{x_n \in [0,1]} \mathbb{E}\left[V_{n+1}(p_{n+1}) \mid p_n \right]$.

Main Result: Bayes Optimality

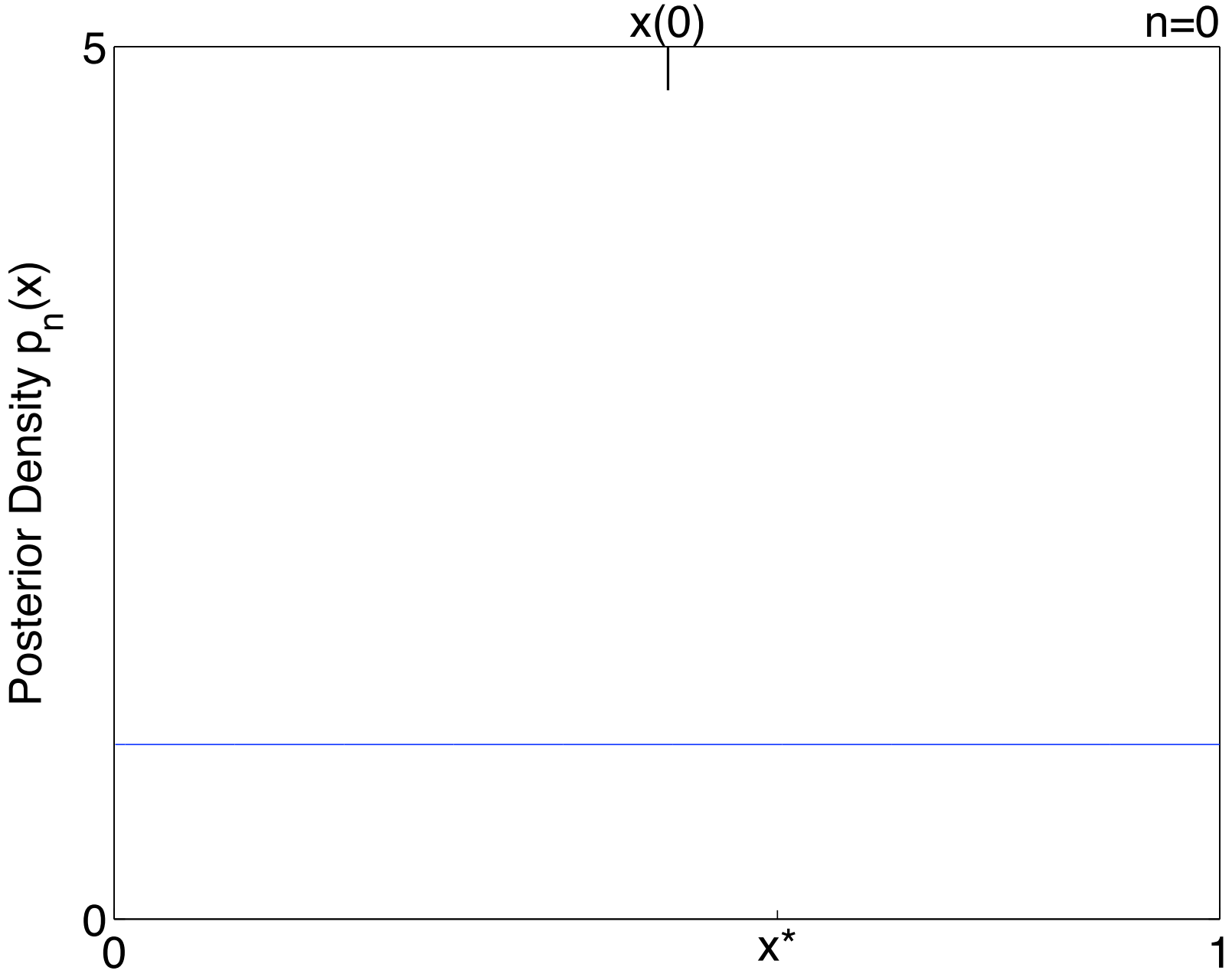
Theorem

The value function can be written explicitly as

$$V(p_n) = H(p_n) - (N-n)\left[-q\log_2(q) - (1-q)\log_2(1-q)\right],$$

and **the policy that chooses x_n at the median of p_n is optimal**.

Example



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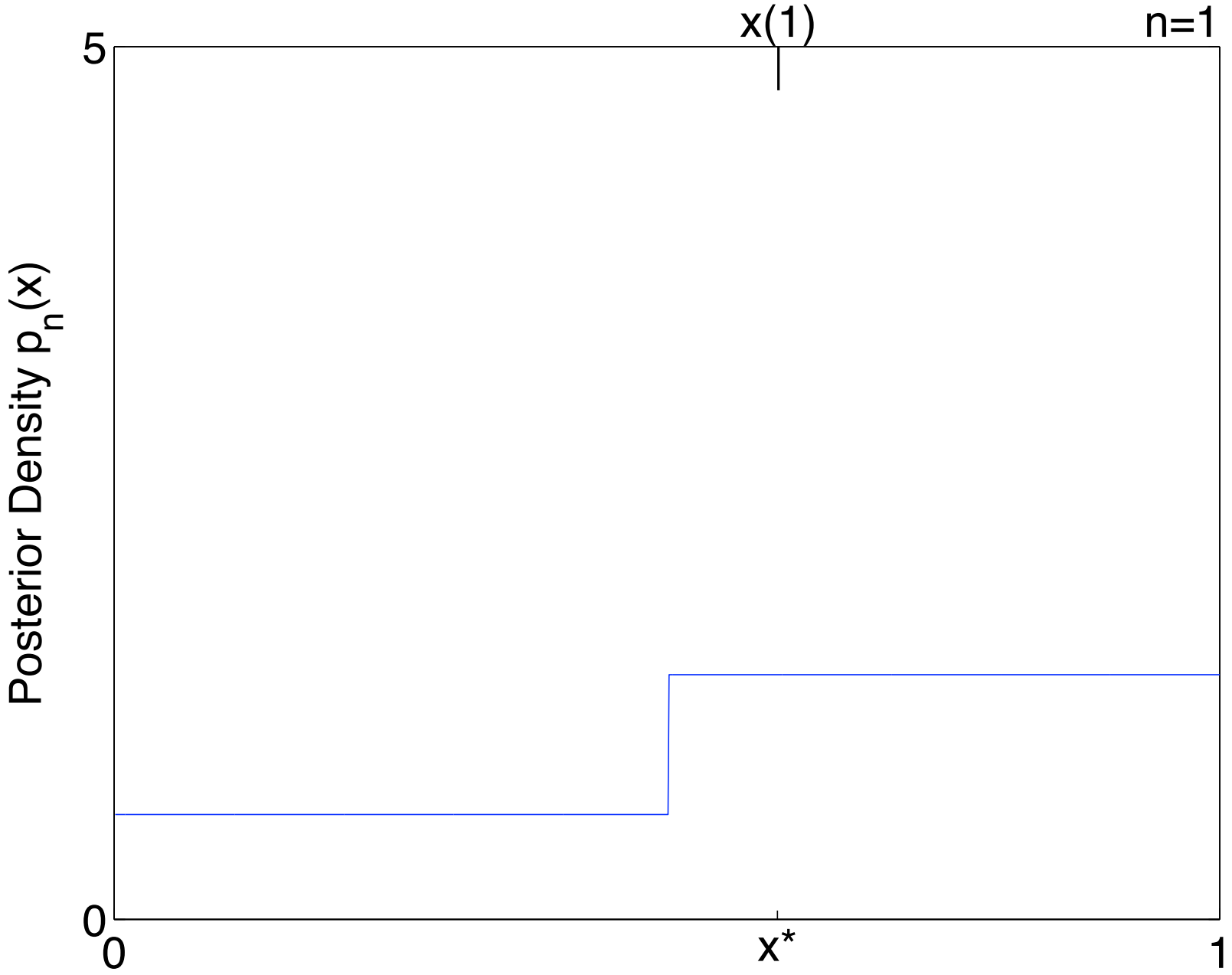

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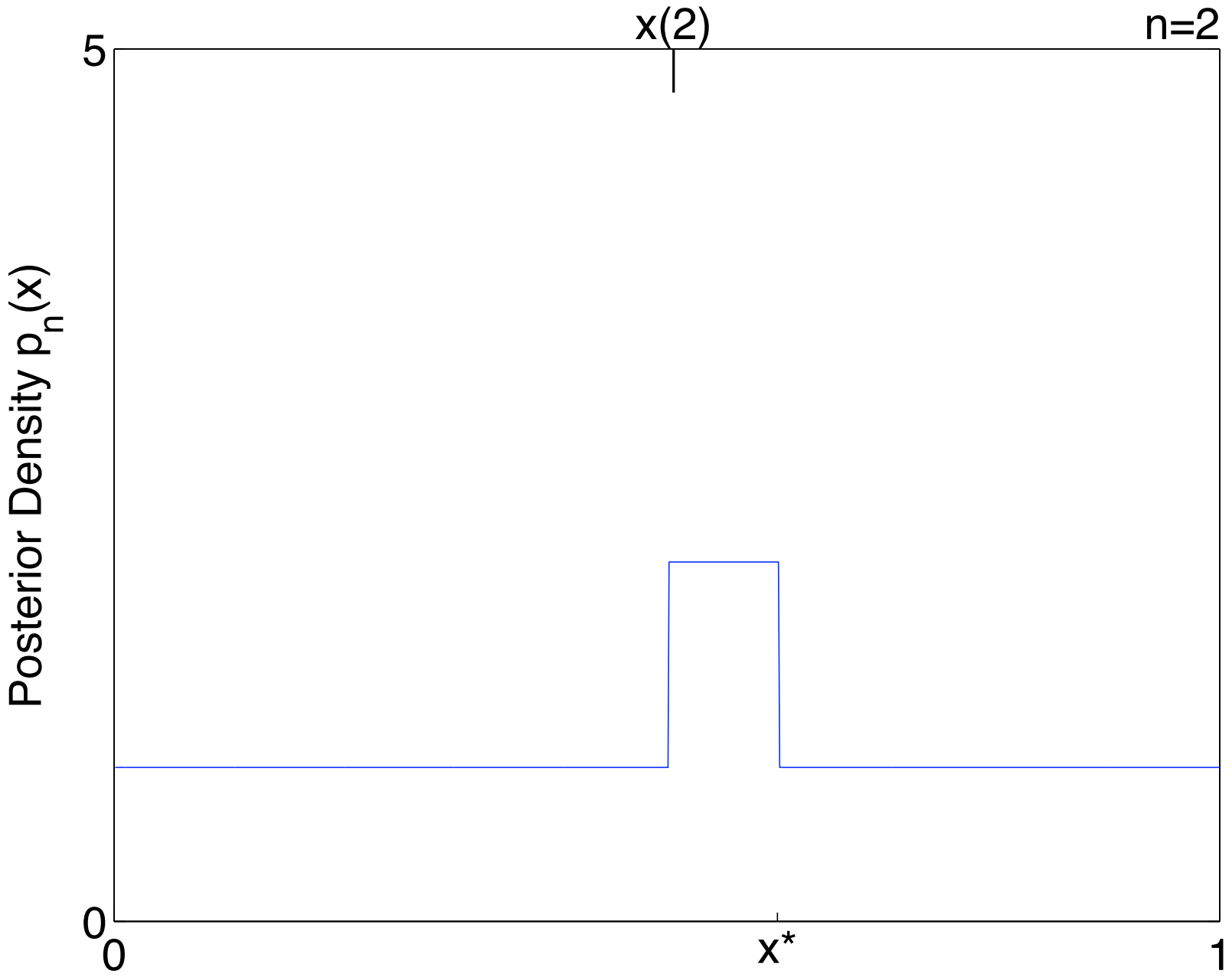

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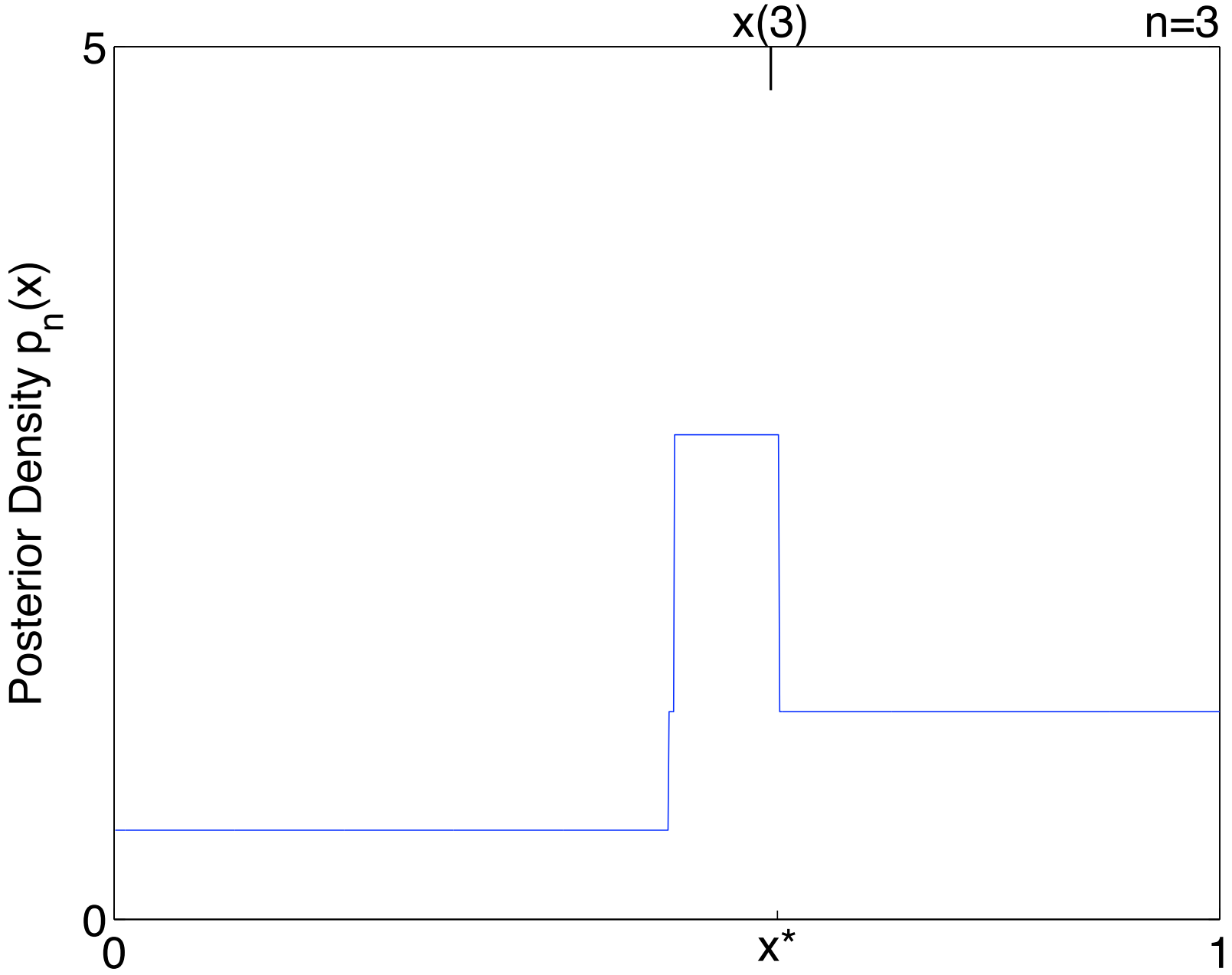

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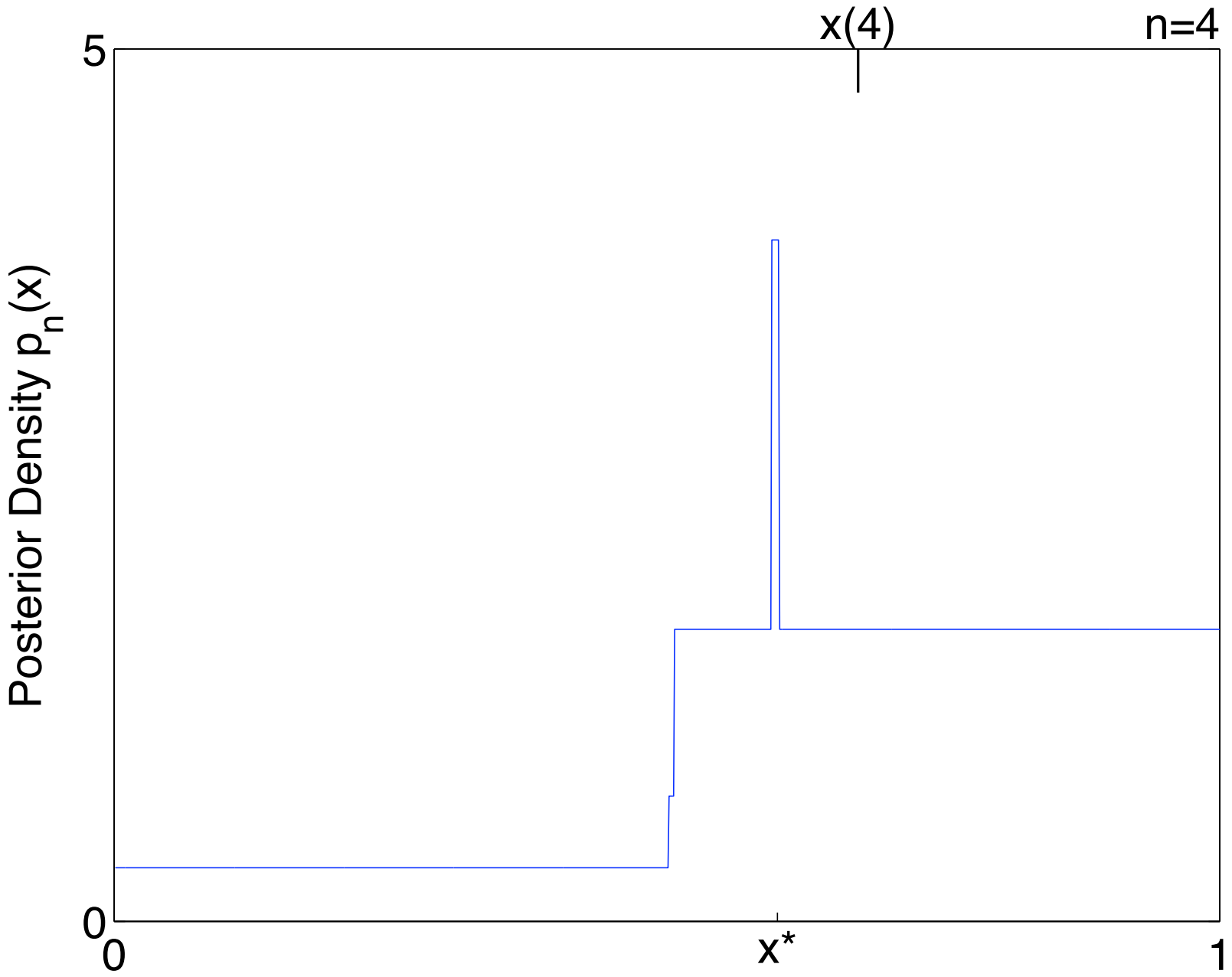

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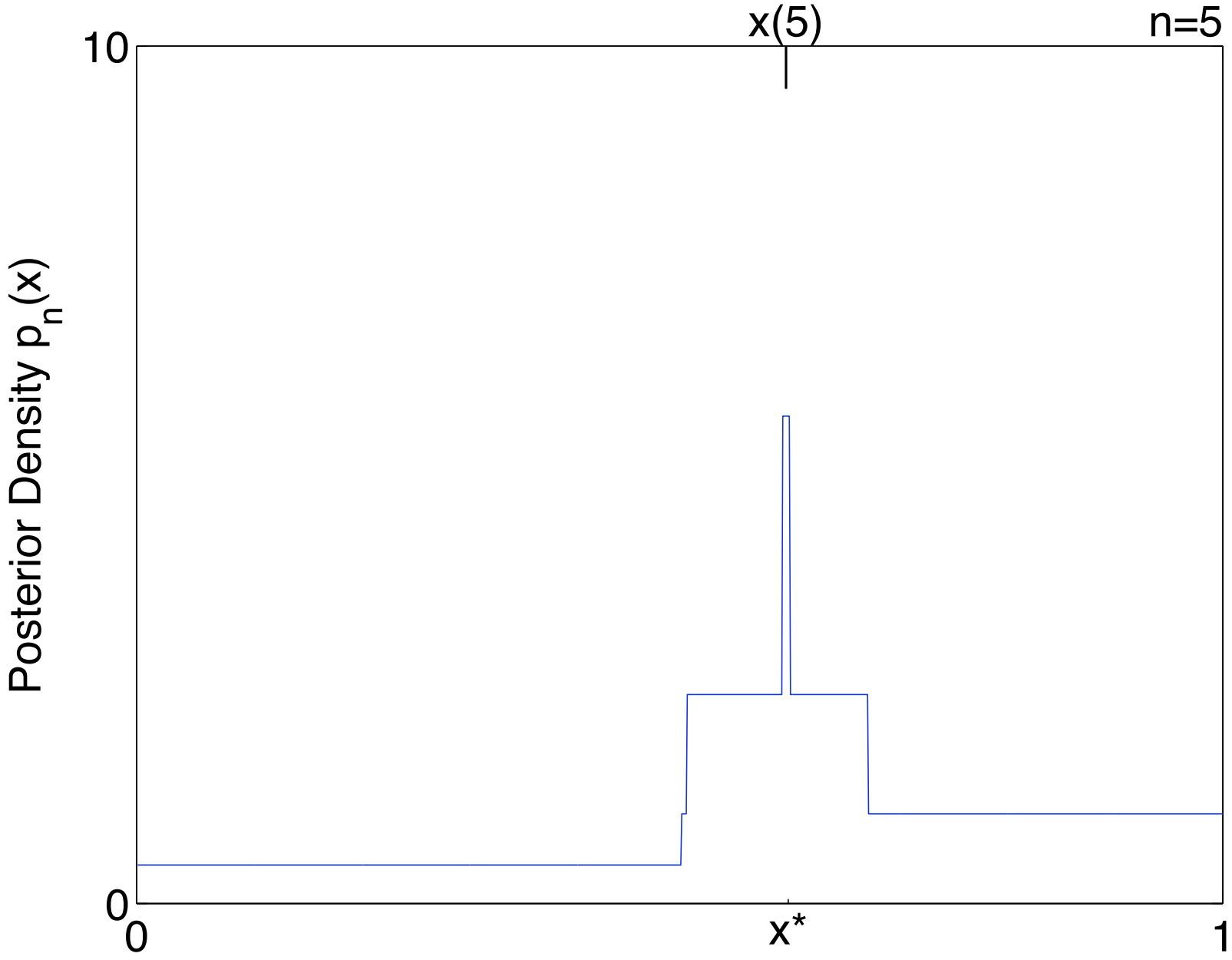

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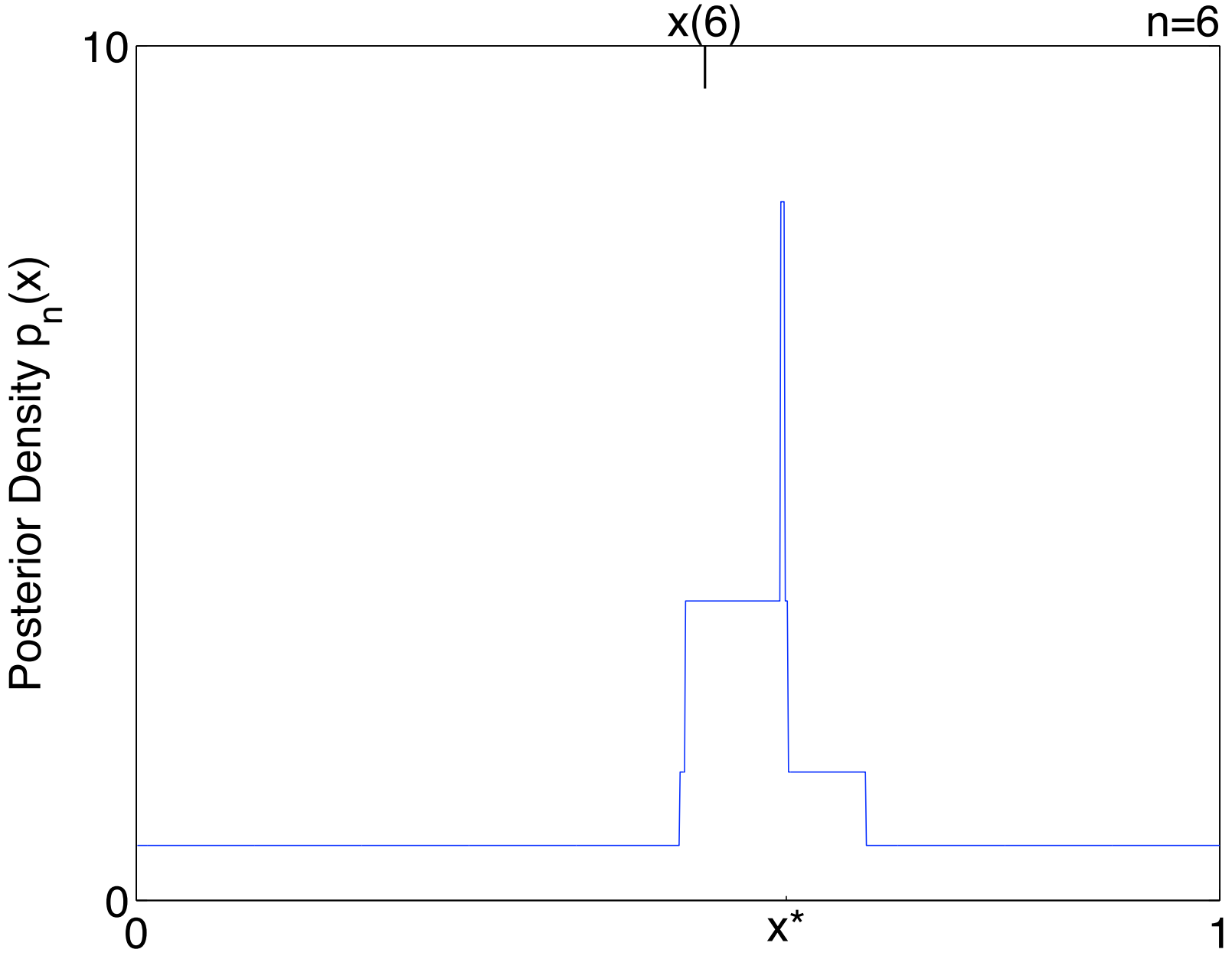

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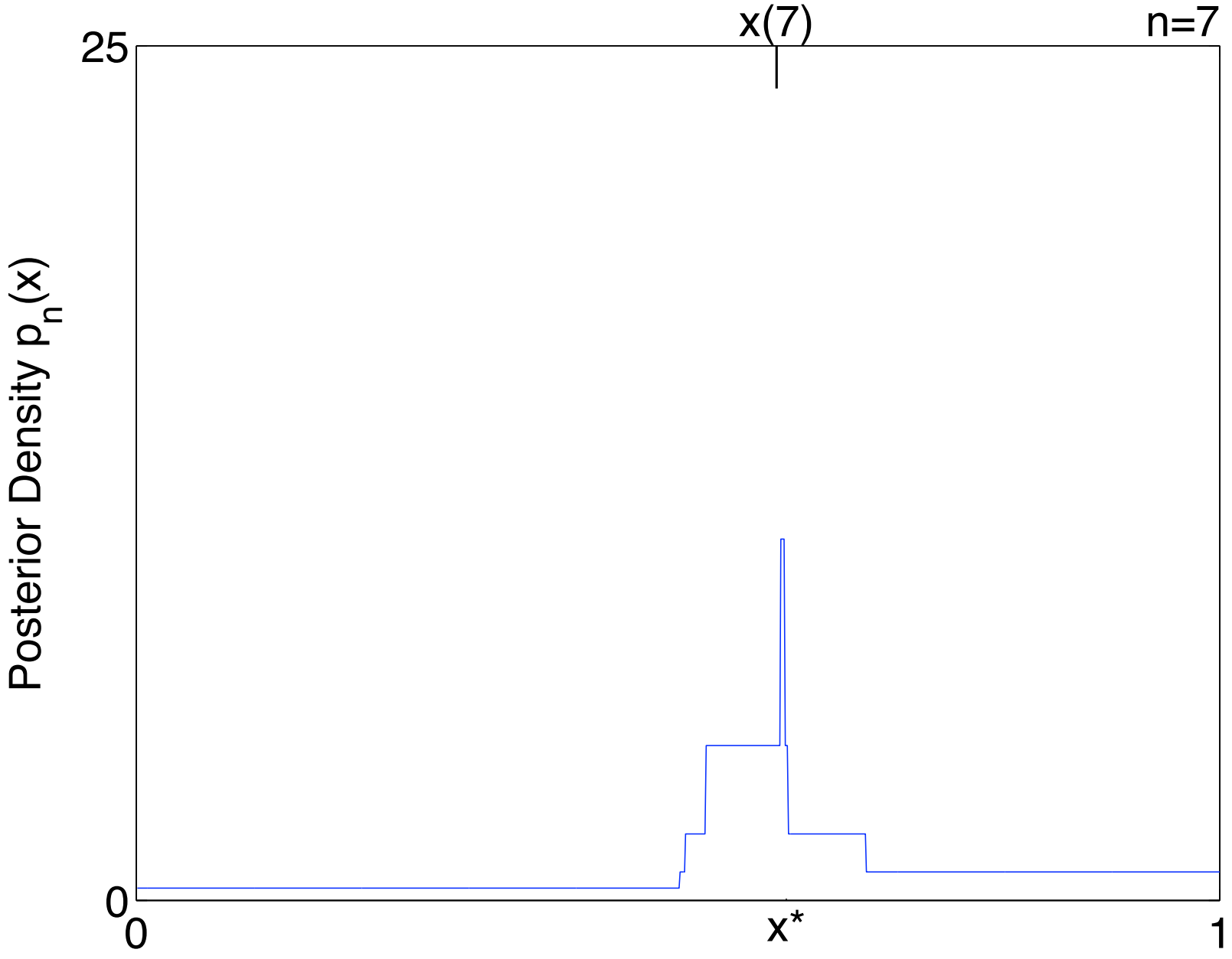

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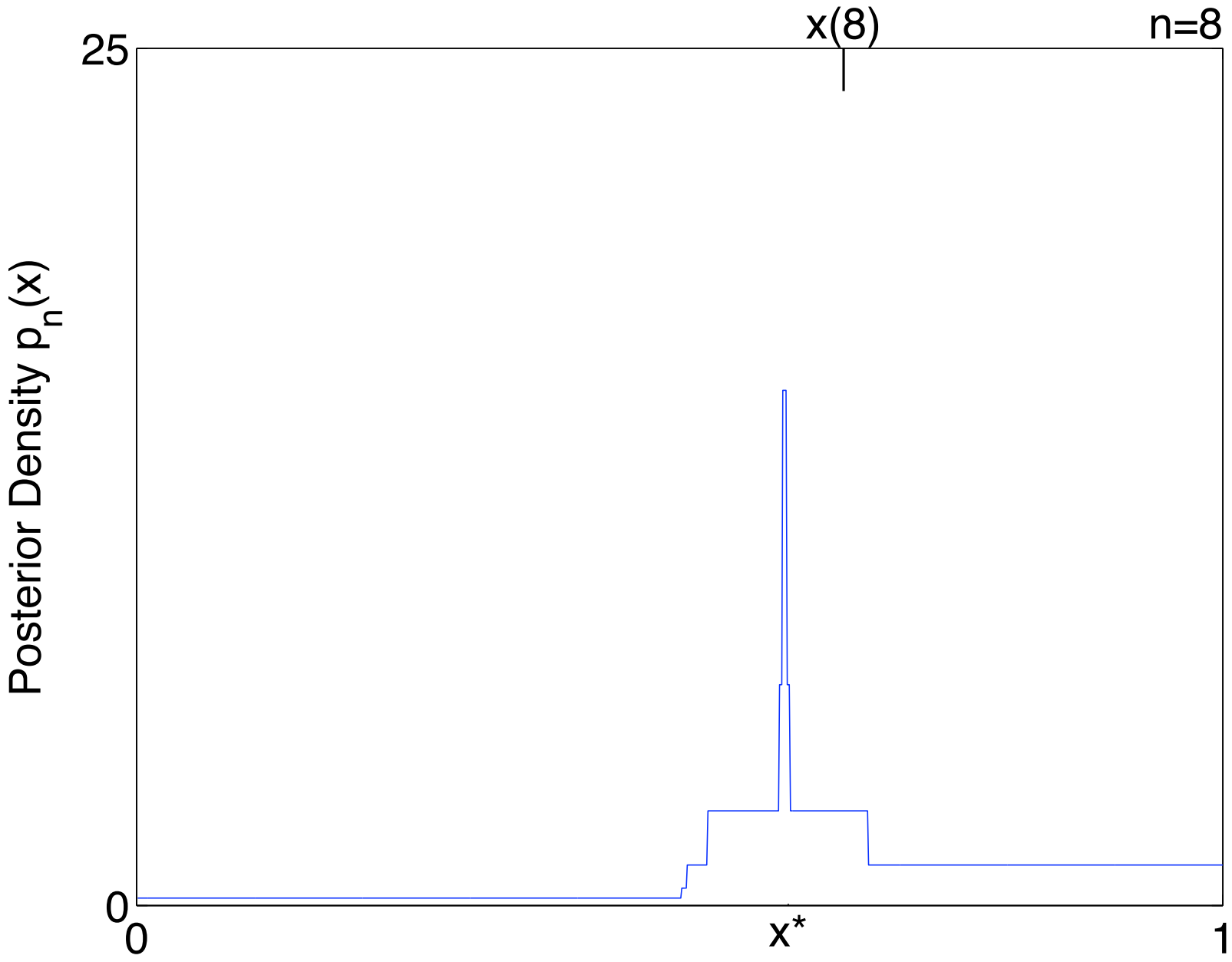

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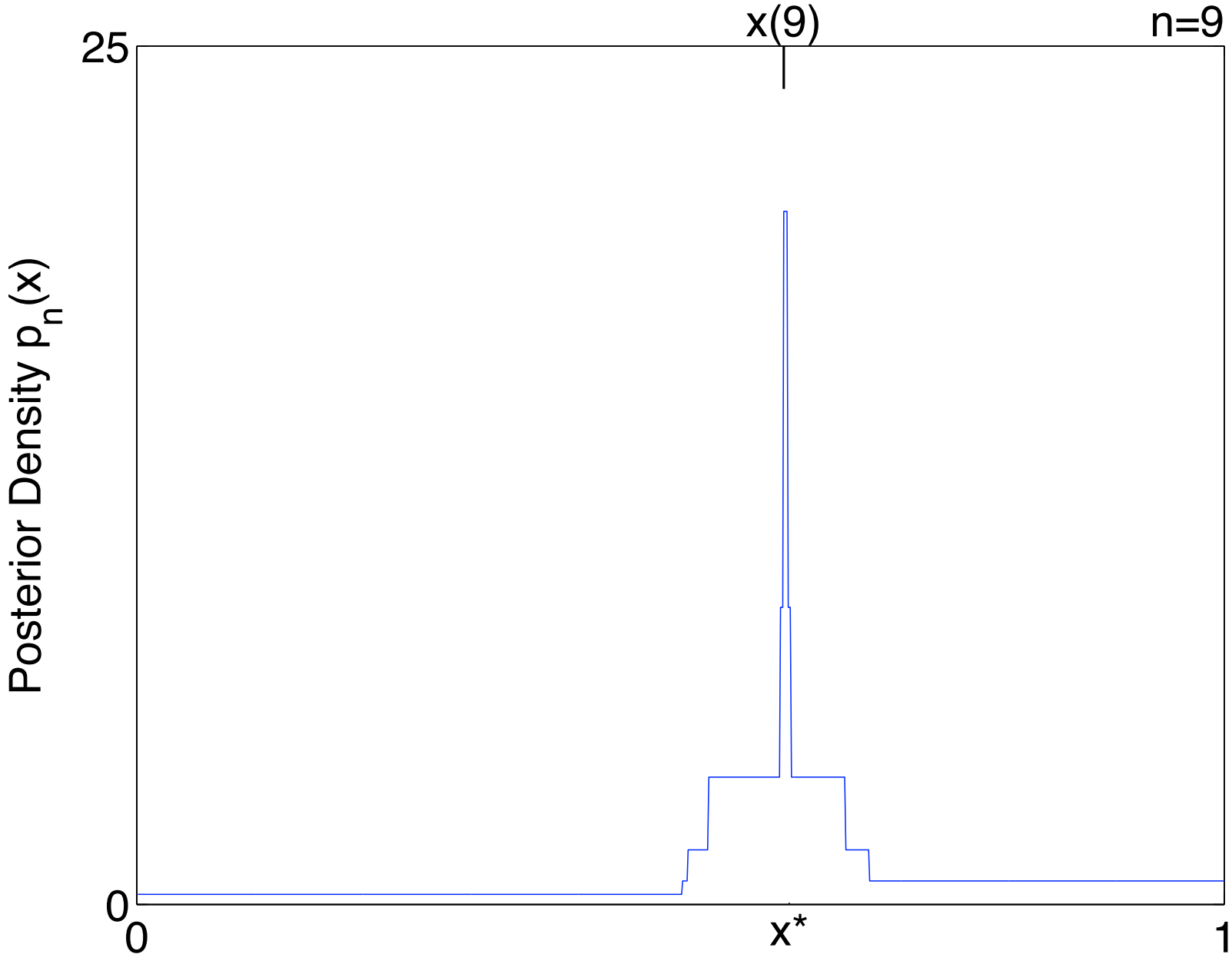

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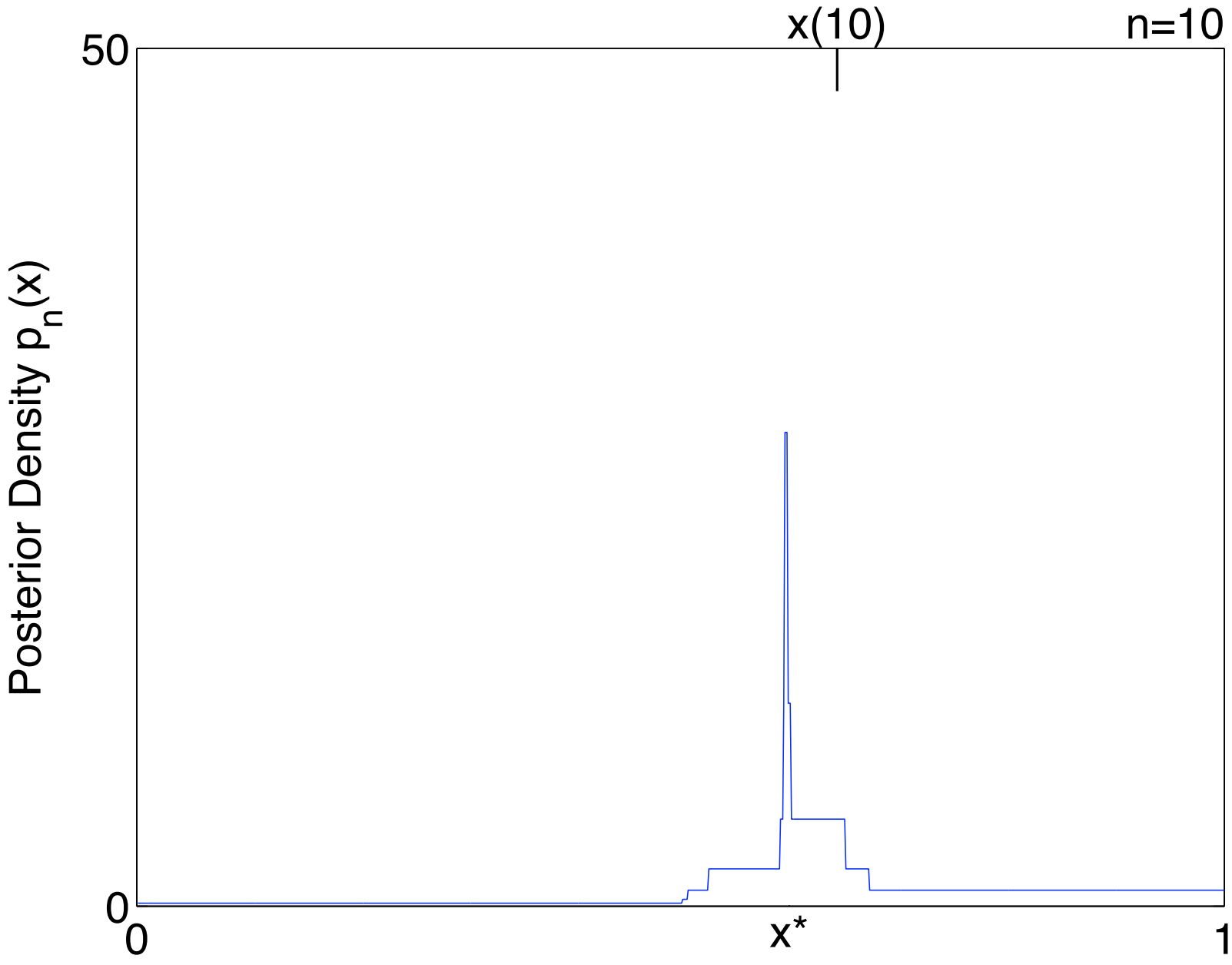

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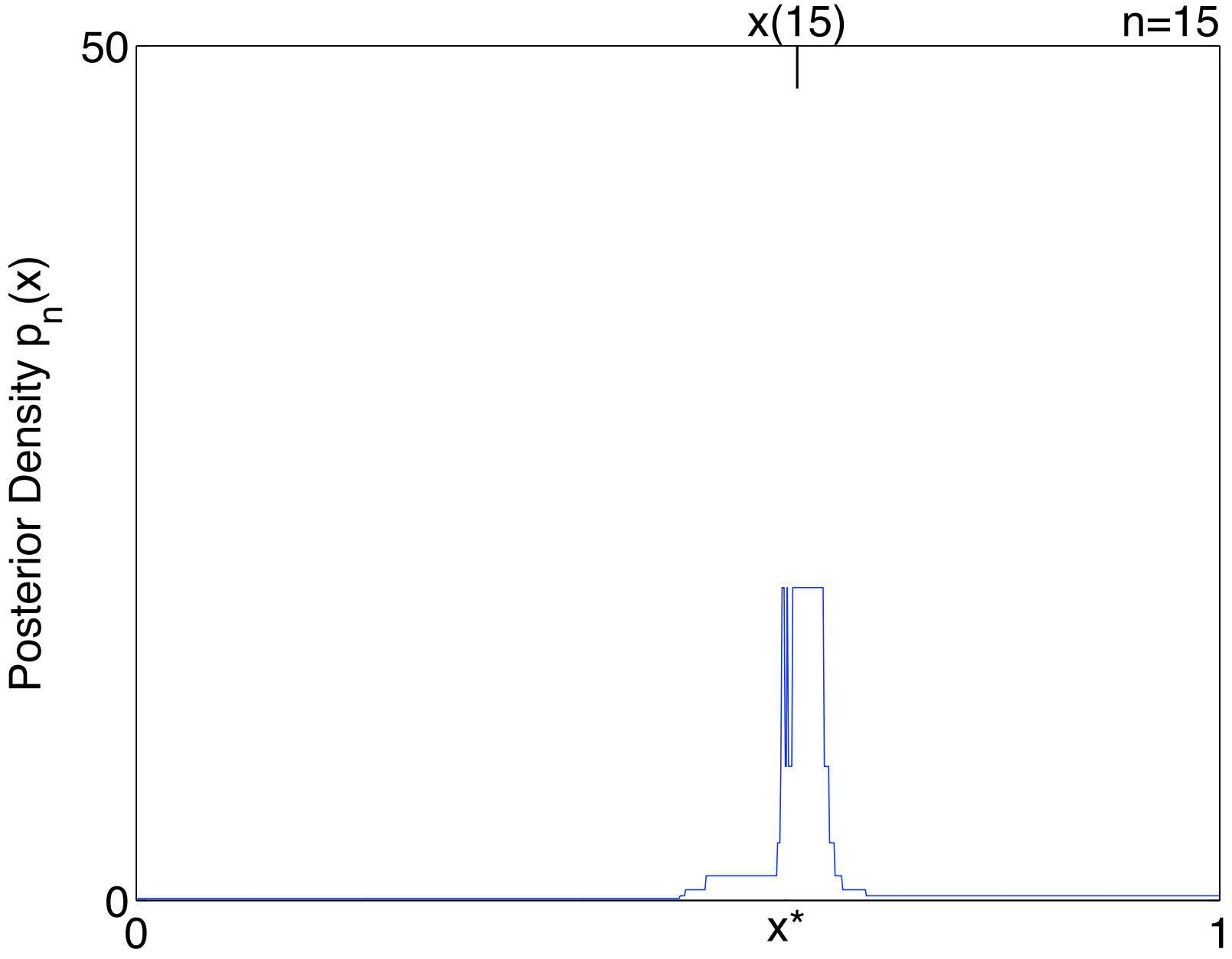

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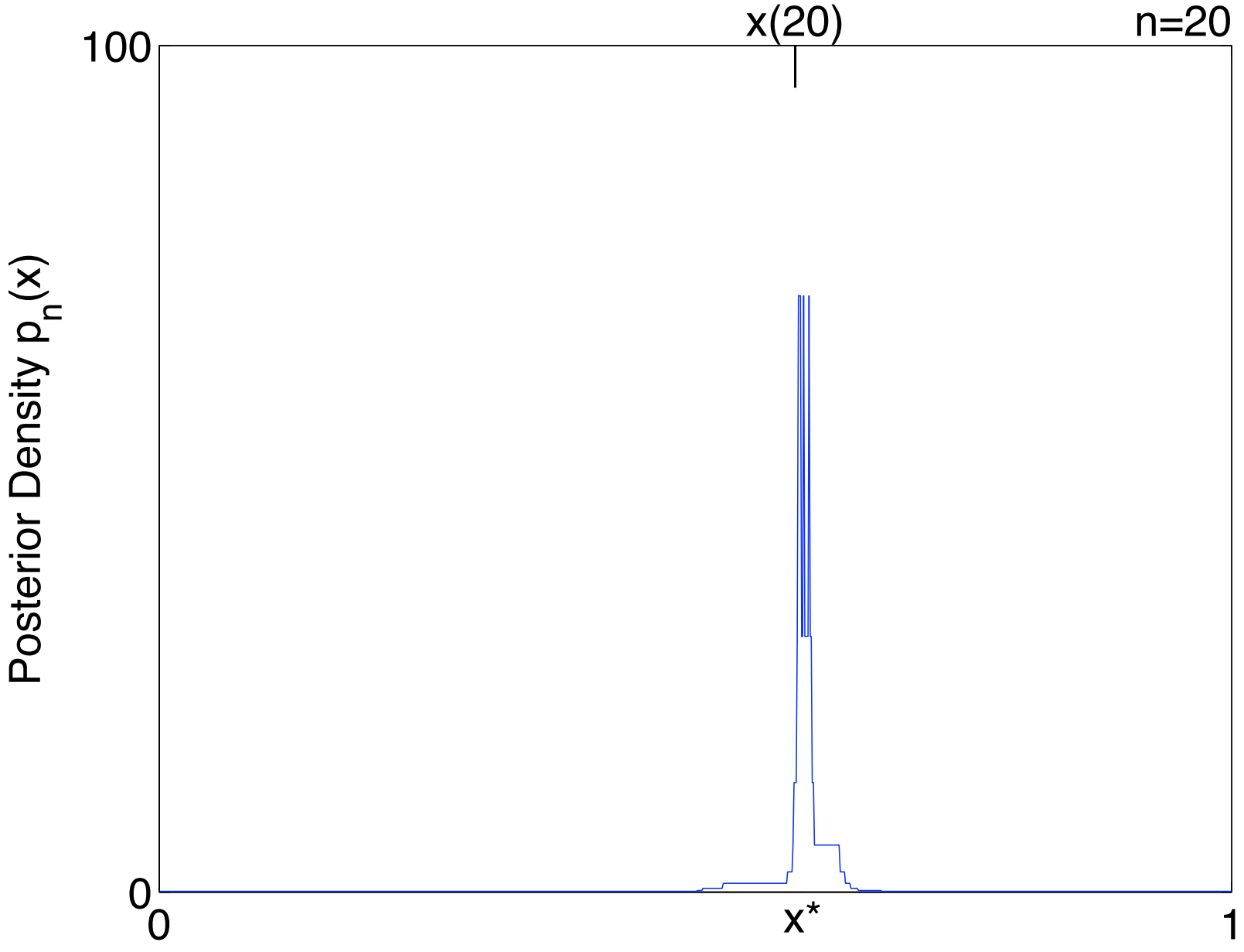

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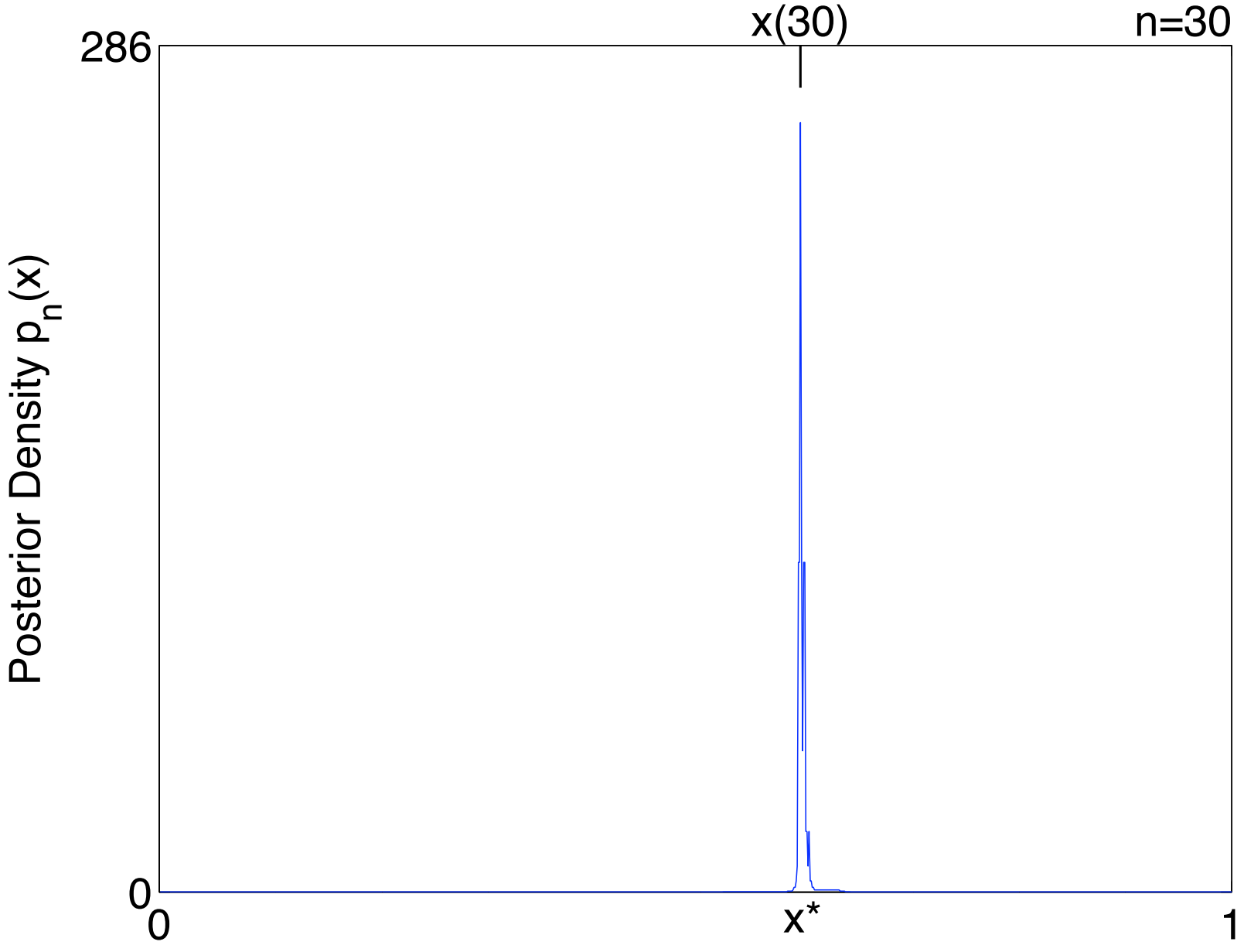


Consistency

- Allow $q(x)$ to vary with x.
- Continue to assume that updates are done with the correct $q(x)$.
- Then we have convergence to the root.

Theorem

$x_n \longrightarrow x_*$ almost surely as $n \longrightarrow \infty$.

[The following results are joint work with Shane Henderson]

Geometric Convergence

- q is fixed.
- Updates are done using q.
- Then x_n converges geometrically to the root x_*.

Theorem

Fix $\varepsilon > 0$ *and let* $A_\varepsilon = [x_* - \varepsilon, x_* + \varepsilon]$.
Let $\tau = \inf\{n : x_n \in A_\varepsilon\}$.
Let $c(q) = 1 + q\log_2(q) + (1-q)\log_2(1-q)$. *Then*

$$\mathbb{E}[\tau] \leq -\log(2\varepsilon)/c(q)$$

Unknown $q(x)$

- In practice, the probability of error $q(x)$ varies with x and is unknown.
- We can estimate $q(x_n)$ by performing multiple measurements at the same x_n, and then use this estimate in our update.
- Alternatively, we can sample sequentially to achieve an error probability $q(x_n)$ **bounded above by a constant**, call it $\widetilde{q}$.
  - Assume ε_n is normal with known variance.
  - We extend standard results from Siegmund 1985 for hypothesis testing of the mean of a normal random variable using curved boundaries.
  - Sampling the sign of $f(x_n)$ can be seen as deciding between three hypotheses: $f(x_n) > 0$; $f(x_n) < 0$; $f(x_n) = 0$.
  - $q(x_n)$ is the probability that the test chooses the wrong hypothesis.
  - Given any $0 < \widetilde{q} < \frac{1}{2}$, a test may be constructed whose $q(x_n) \leq \widetilde{q}$ whenever $P(y_n > 0) \neq \frac{1}{2}$.
  - When $P(y_n > 0)$ is close to $\frac{1}{2}$, the test takes more samples to decide. When $P(y_n > 0) = \frac{1}{2}$, the test may sample forever.

Convergence Rate

- Allow $q(x)$ to vary with x.
- Updates are done with $\widetilde{q}$, which is an upper bound on $q(x_n)$.

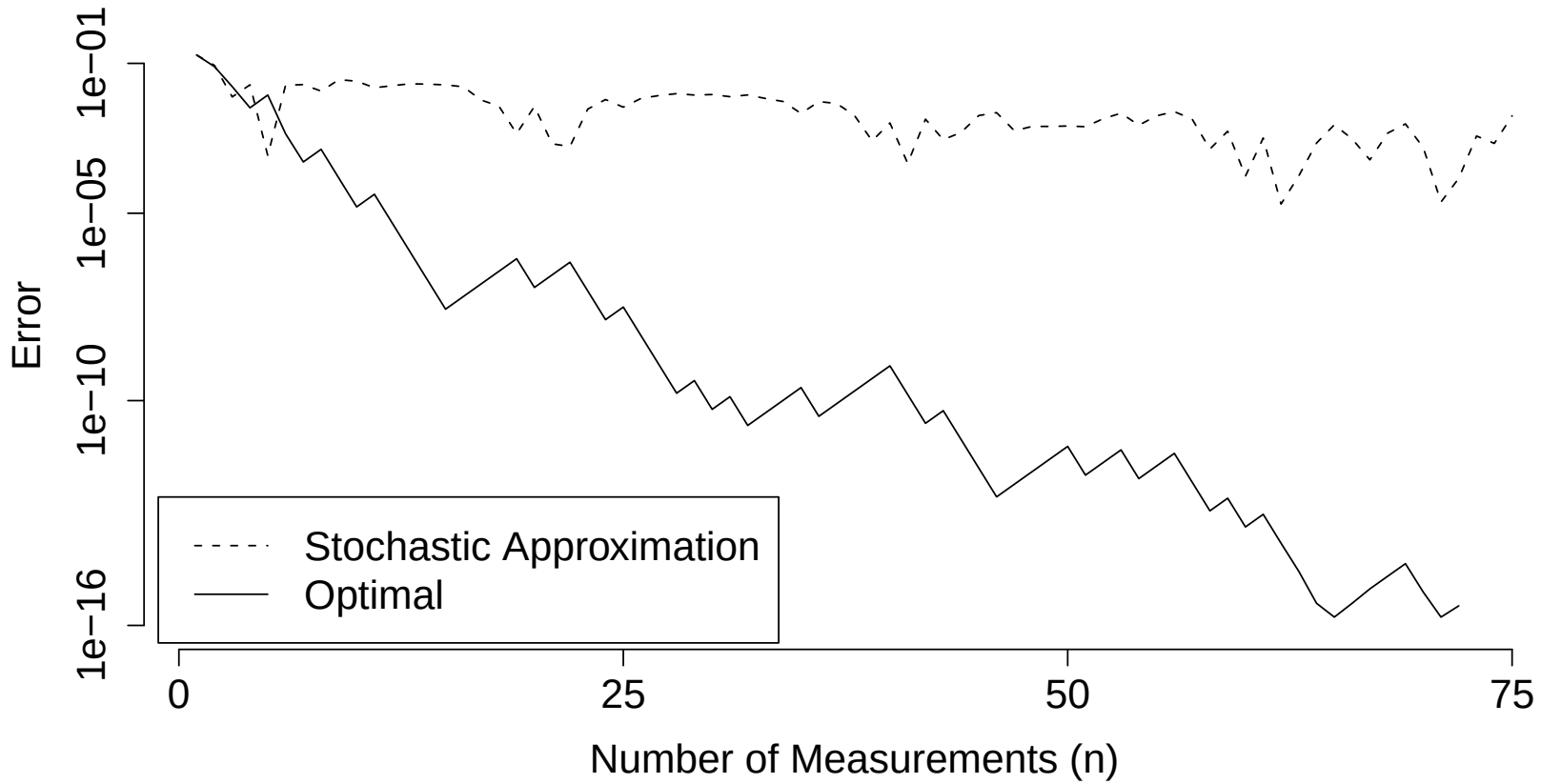
Theorem

Fix $\varepsilon > 0$ and let $A_\varepsilon = [x_* - \varepsilon, x_* + \varepsilon]$.
Let $\tau = \inf\{n : x_n \in A_\varepsilon\}$.
Let $c(\widetilde{q}) = 1 + \widetilde{q}\log_2(\widetilde{q}) + (1-\widetilde{q})\log_2(1-\widetilde{q})$. Then

$$\mathbb{E}[\tau] \leq -\log(2\varepsilon)/c(\widetilde{q})$$

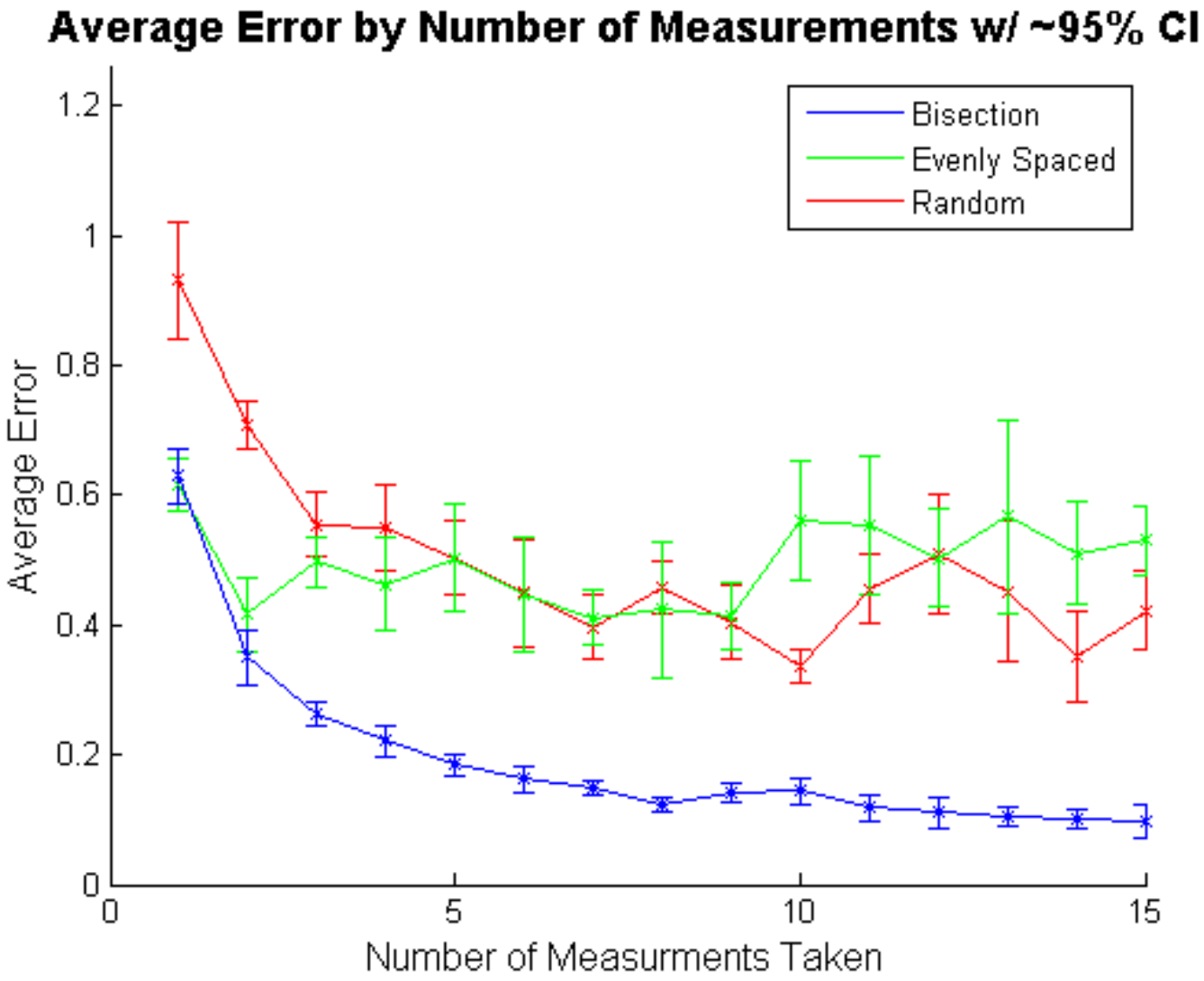
We still have geometric convergence in the number of different x_n sampled, but it may take more time to sample one x_n when x_n is closer to x_*.

Experimental Results (Simulation Problem)



Performance on a problem with $f(x) = \exp(x) - \exp(1/3)$ and domain $[0,1]$. Error is $|x_n - x_*|$ on one sample path. Stochastic approximation used stepsize $1/n$.

Experimental Results (Laboratory Problem)

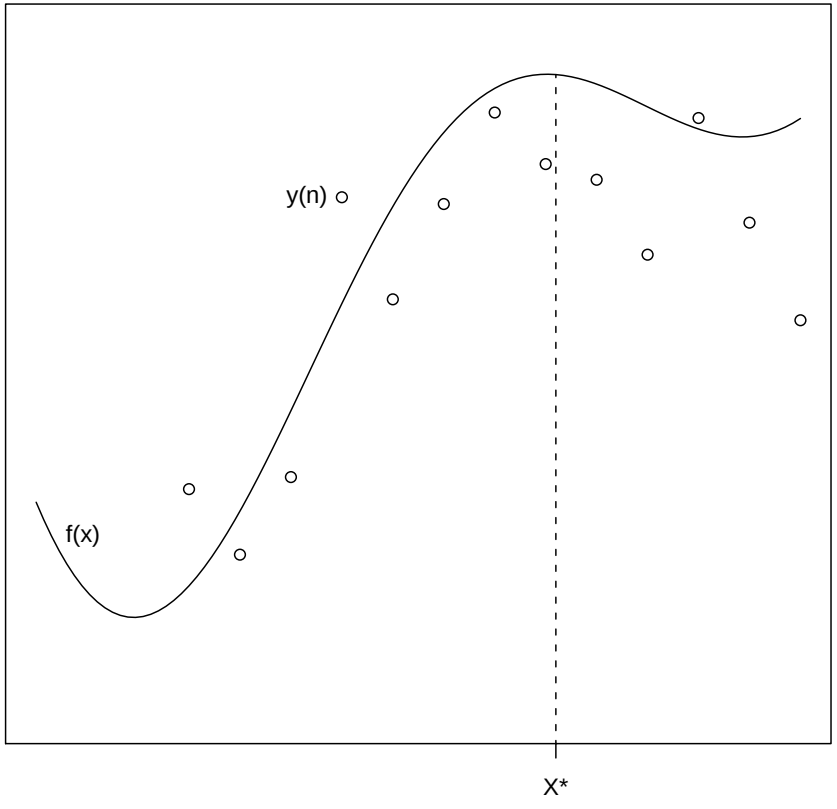


Joint work with Zach Owen, Thorsten Joachims, and Rodrigo Bicalho.

Outline

Global Optimization with Noise

We now consider a different problem:
Given a fixed budget of function evaluations, locate the global maximum of a continuous function.



[Joint work with Warren Powell & Savas Dayanik]

Global Optimization with Noise

- $f : [0,1]^d \mapsto \mathbb{R}$, not necessarily monotone or concave.
- $y_n = f(x_n) + \varepsilon_n$ where $\varepsilon_n \sim \mathcal{N}(0, \sigma^2(x_n))$ is independent noise.
- Our goal is to choose $\widehat{x_*}$ to make $f(\widehat{x_*})$ as large as possible.
- Central Question: Given a budget of N measurements, $x_1, \ldots, x_N$, how should we place them to choose x_* as well as possible?

Global Optimization with Noise

- For any fixed function f, and any fixed policy π, the expected performance is

$$\mathbb{E}^{\pi}\left[f(\widehat{x}_*) \mid f\right].$$

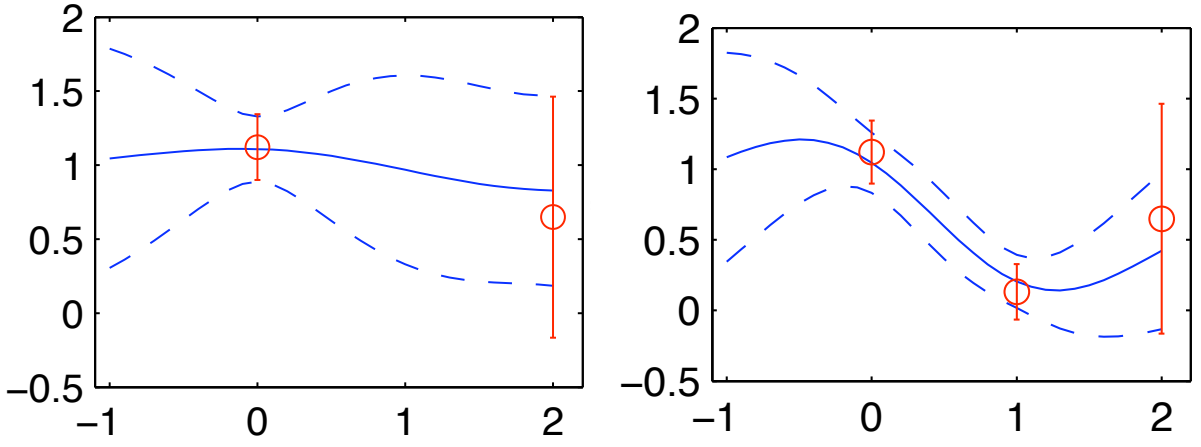
- Our goal is to solve

$$\sup_{\pi} \mathbb{E}\left[f(\widehat{x}_*)\right],$$

where the expectation over f is taken with respect to the prior $\mathbb{P}_0$.

Gaussian Process Prior

- Our prior $\mathbb{P}_0$ on f is a **Gaussian Process Prior (GPP)**.
- GPPs are commonly used in Bayesian spatial statistics to model continuous functions.
- GPPs are analytically convenient:
  they can be updated in closed-form.



Dynamic Programming

- The optimal policy is described by the dynamic programming equations.

$$V_N(\mathbb{P}_N) = \sup_{x \in [0,1]^d} \mathbb{E}_N [f(x)],$$
$$V_n(\mathbb{P}_n) = \sup_{x \in [0,1]^d} \mathbb{E}_n [V_{n+1}(\mathbb{P}_{n+1})].$$

- These DP equations are **extremely difficult to solve numerically** because the state space is so large.
  - The state space is the space of all possible posterior probability distributions on f.
  - It has $2N$ continuous dimensions.

Knowledge-Gradient Policy

- We construct a one-step approximation to the optimal policy.
- Recall $V_N(P)$ is the expected value of the best $\widehat{x}_*$ we can choose based on a posterior P.
- For each x, we define the **Knowledge-Gradient (KG) Factor**

$$KG_n(x) = \mathbb{E}_n \left[V_N(\mathbb{P}_{n+1}) - V_N(P_n) \mid x_n = x \right].$$

- $KG_n(x)$ is the expected difference in value between our knowledge $\mathbb{P}_n$ at time n, and our knowledge $\mathbb{P}_{n+1}$ at time $n+1$.
- $KG_n(x)$ is the (myopic) value of what we learn from sampling x.

Knowledge-Gradient Policy

- Recall the KG factor is defined as

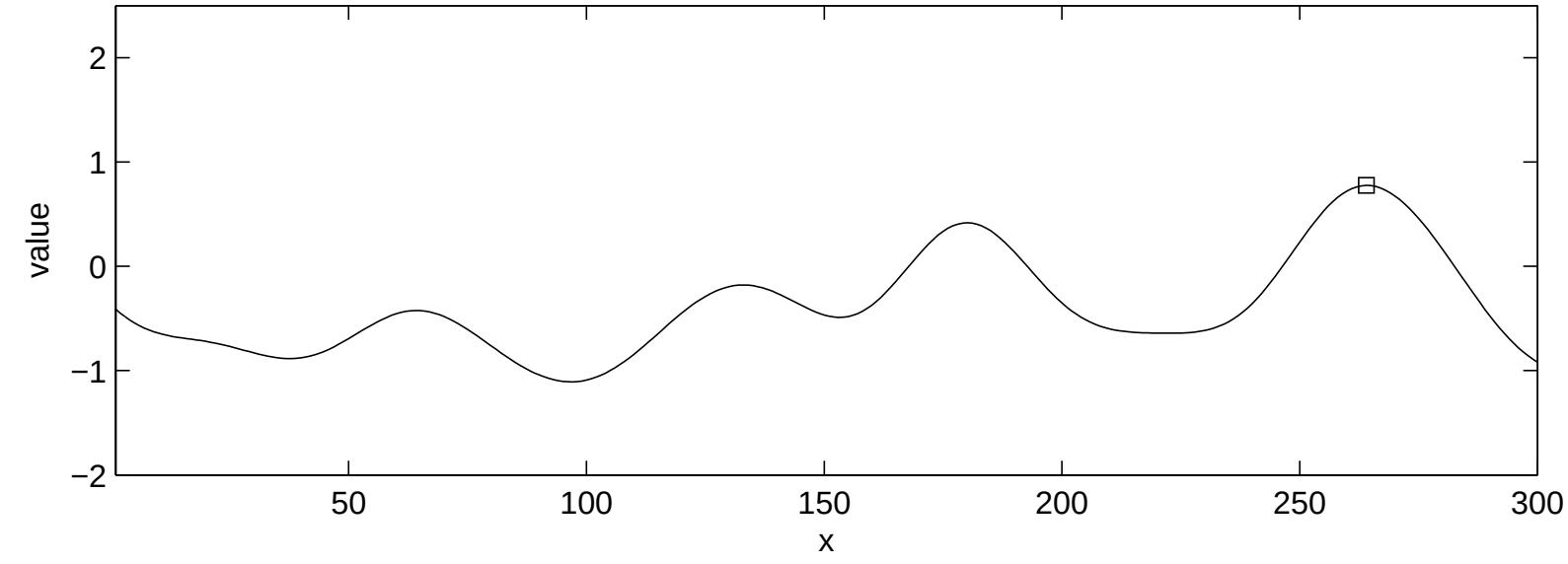
$$KG_n(x) = \mathbb{E}_n \left[V_N(\mathbb{P}_{n+1}) - V_N(P_n) \mid x_n = x \right].$$

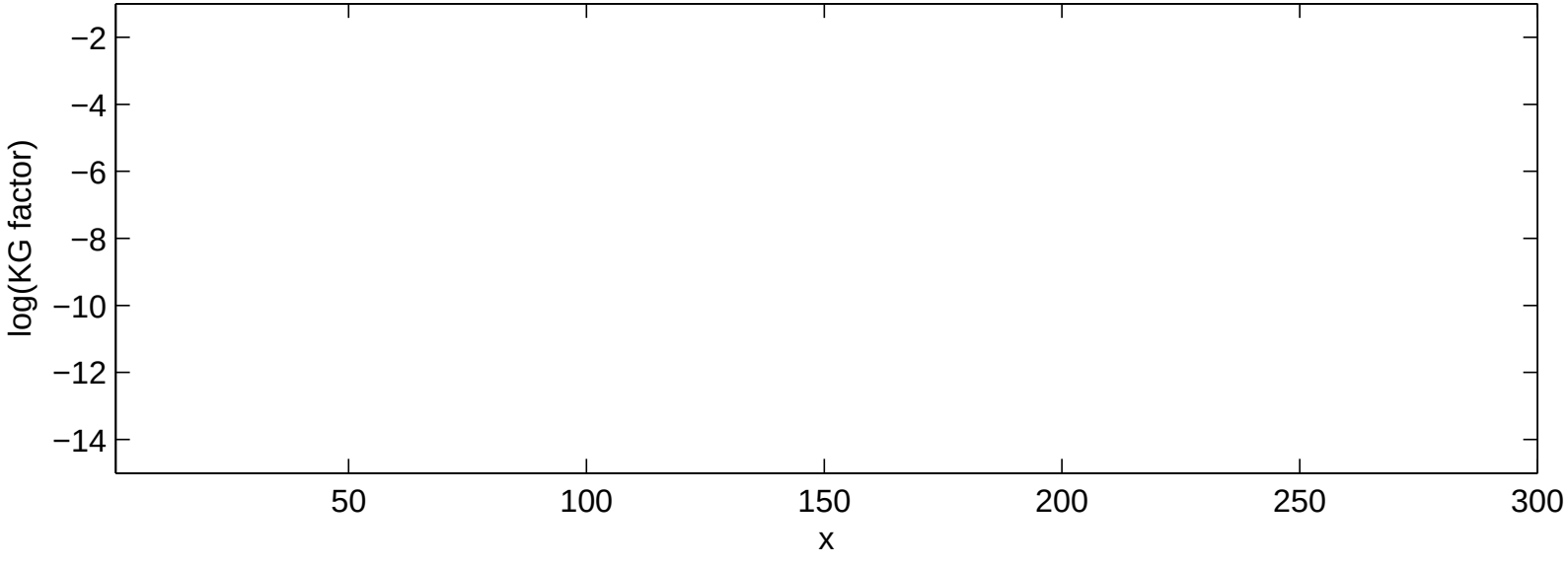
- The **knowledge-gradient (KG) policy** is

$$x_n \in \arg\max_x KG_n(x).$$

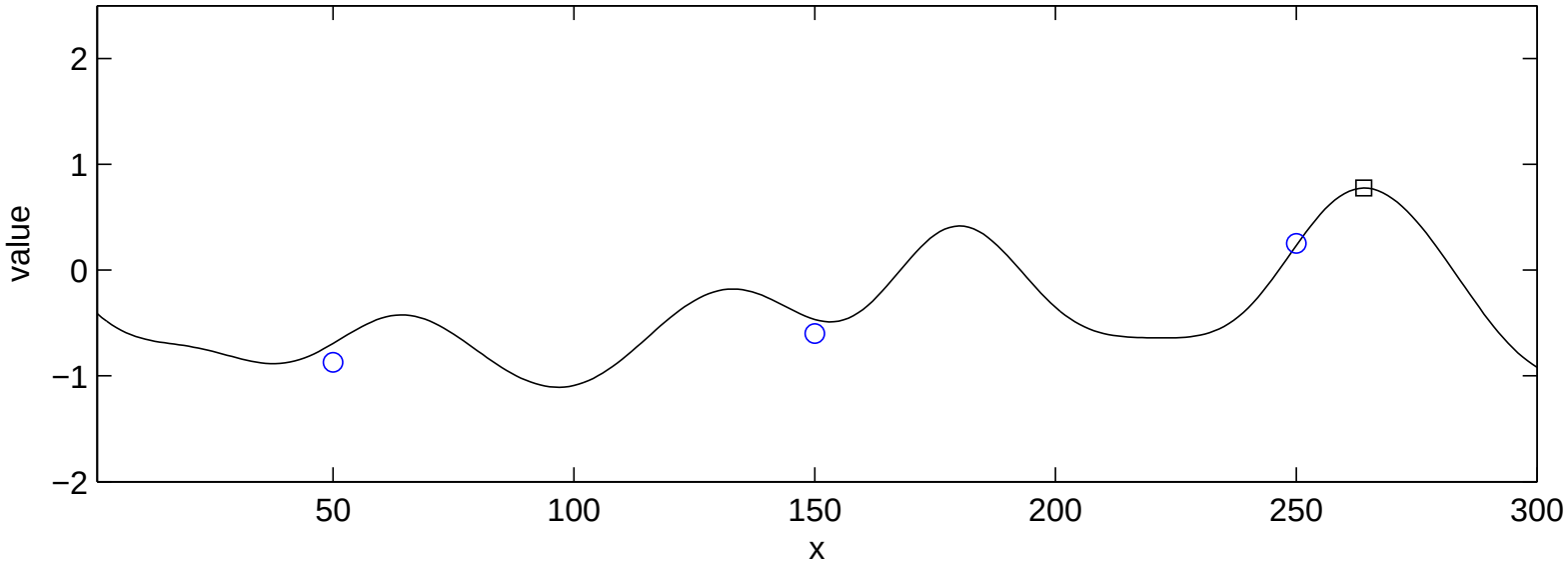
- The KG policy is optimal when $n = N - 1$, and so is a one-step lookahead policy.

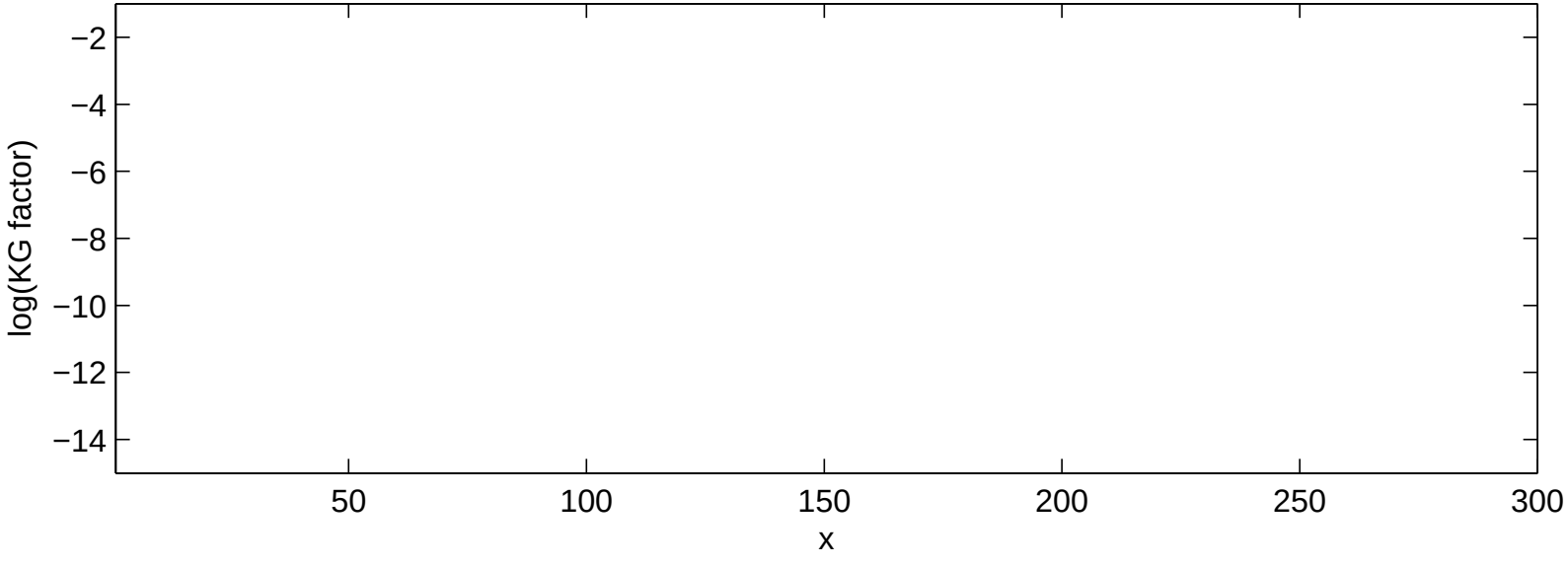
Global Optimization Example





Global Optimization Example





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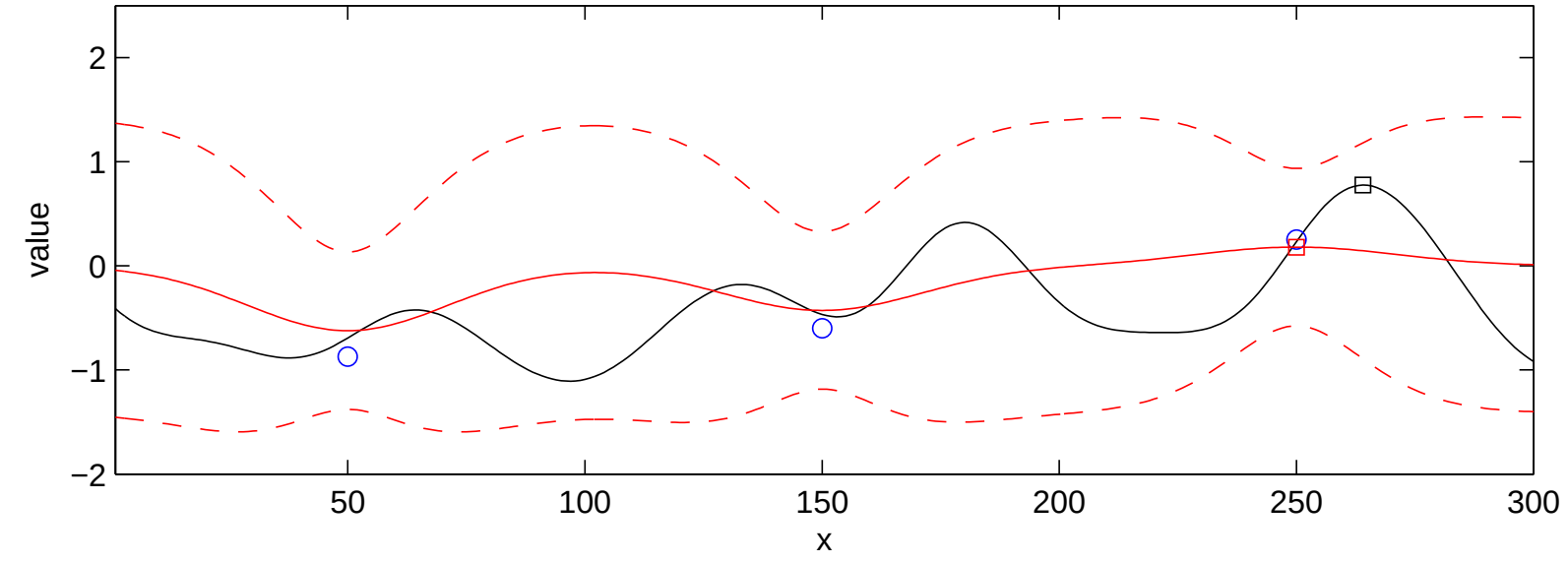

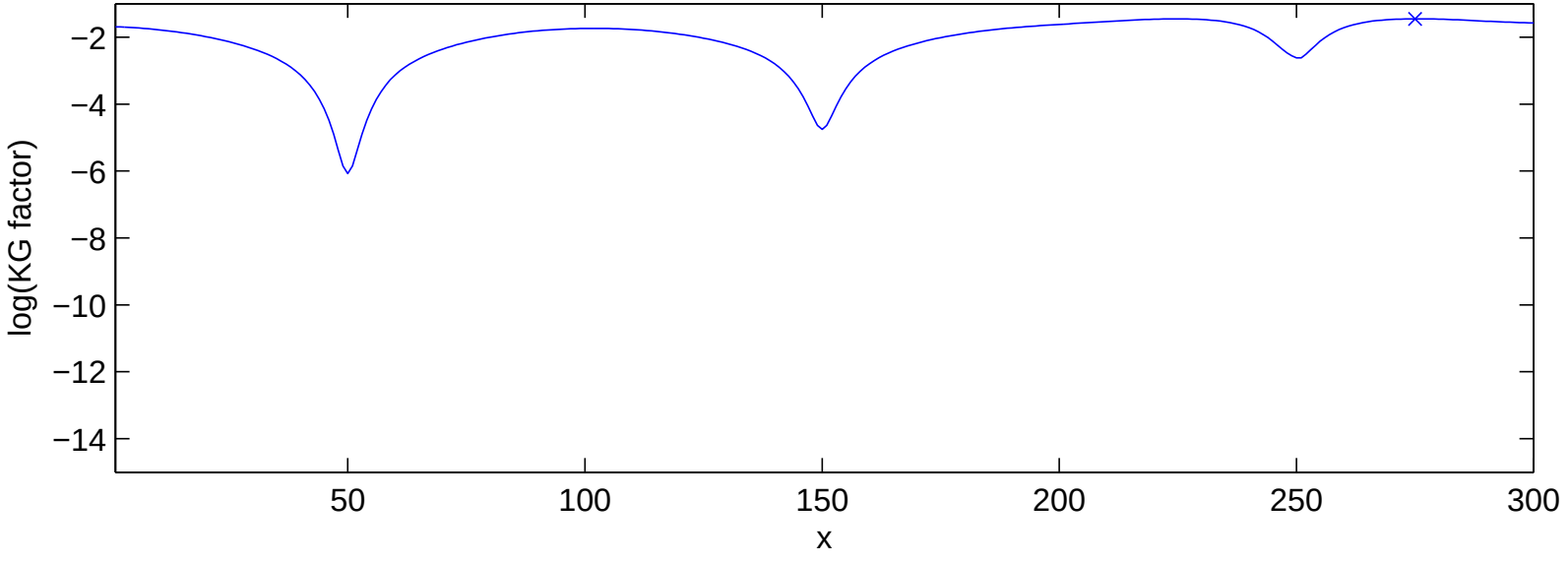

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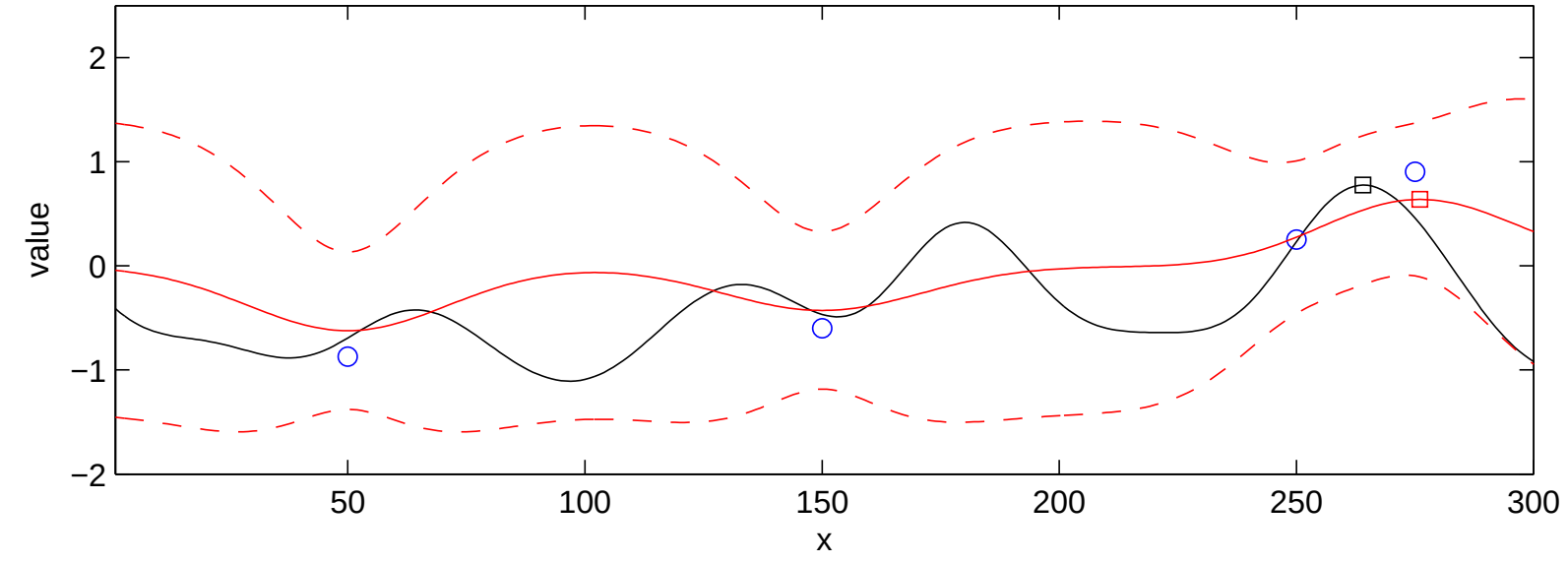
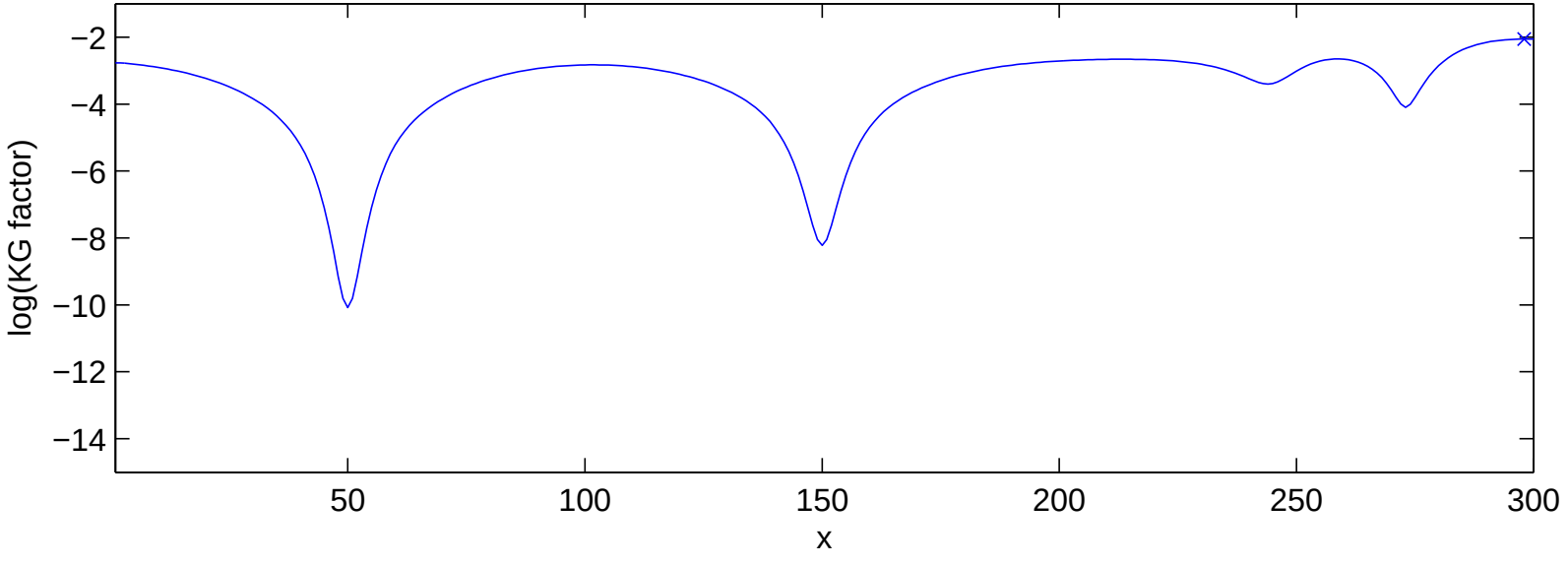
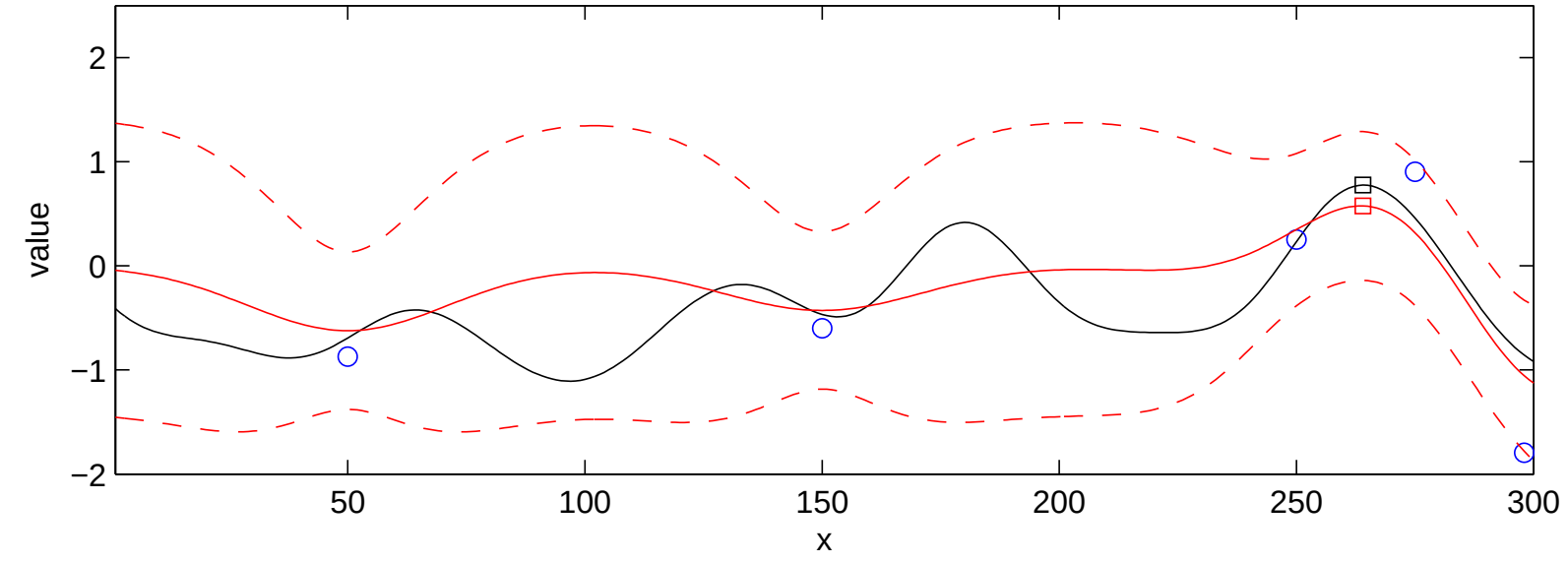
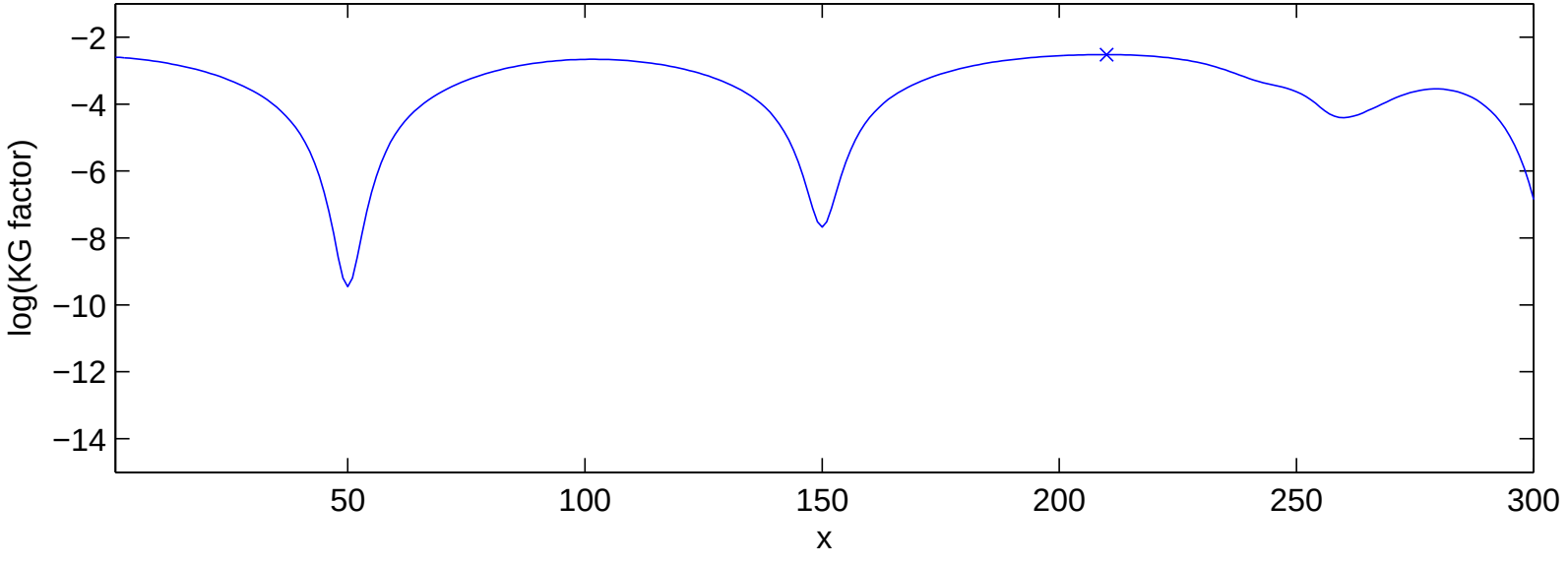


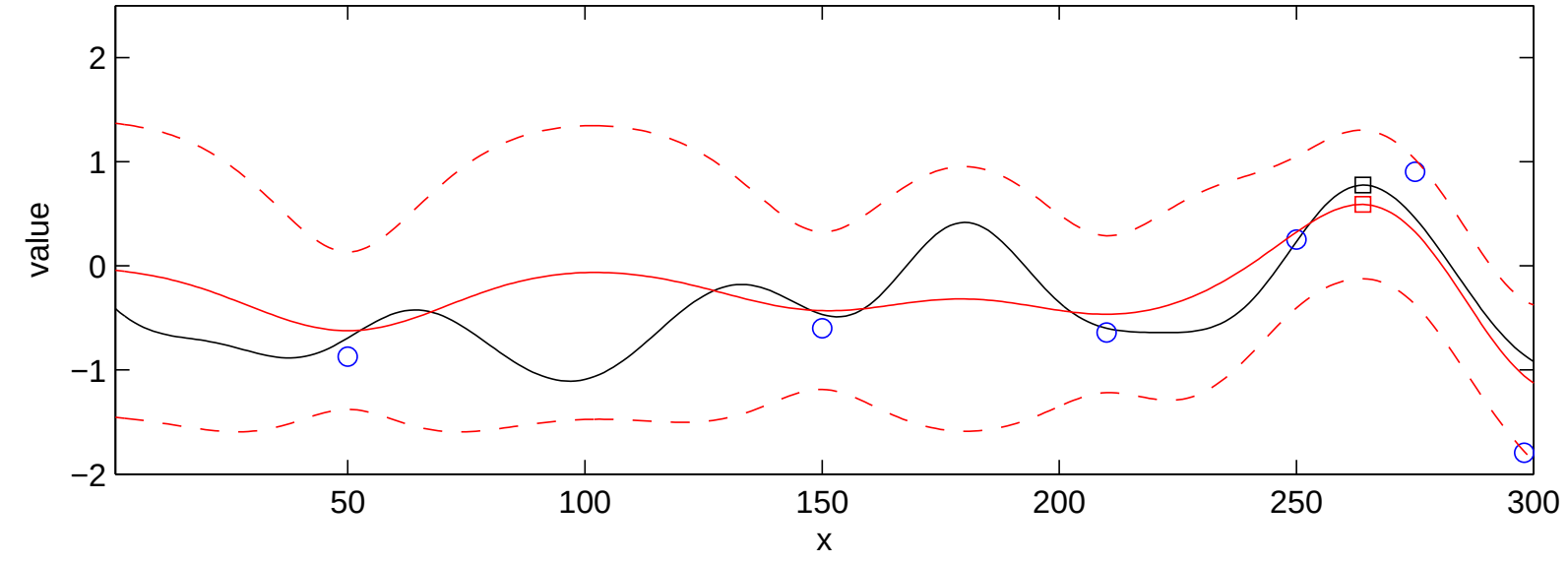


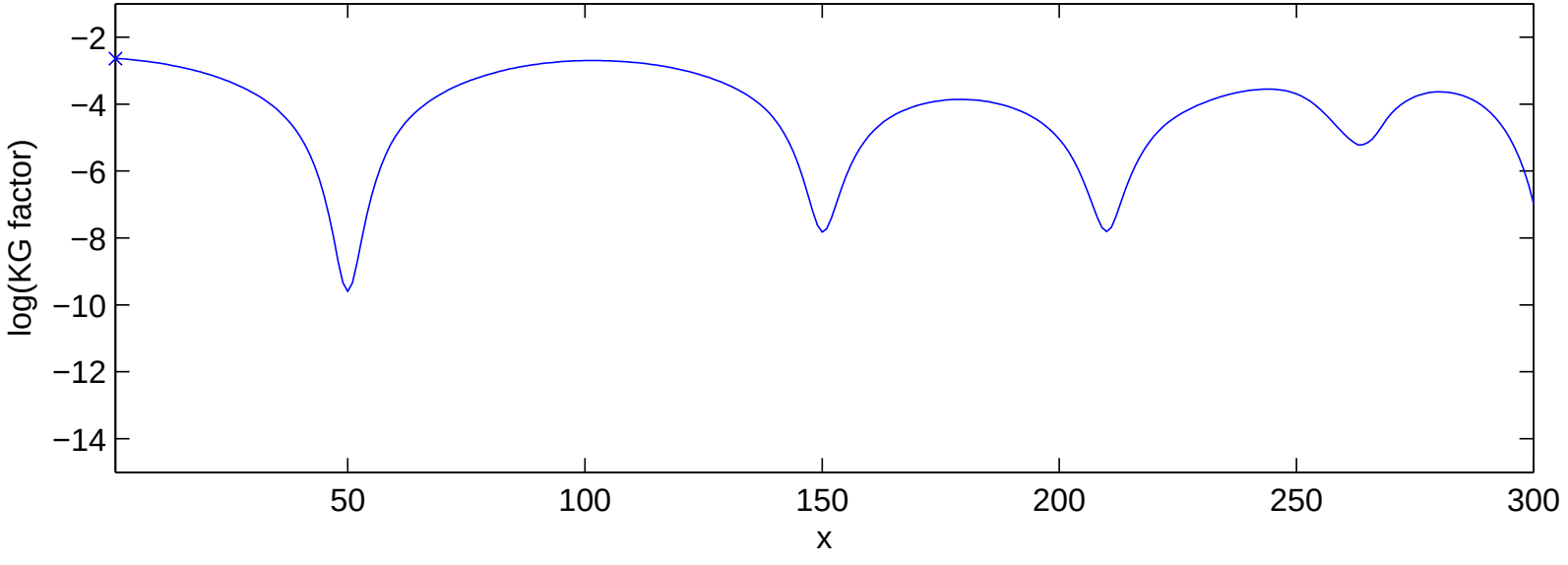
Global Optimization Example





Global Optimization Example





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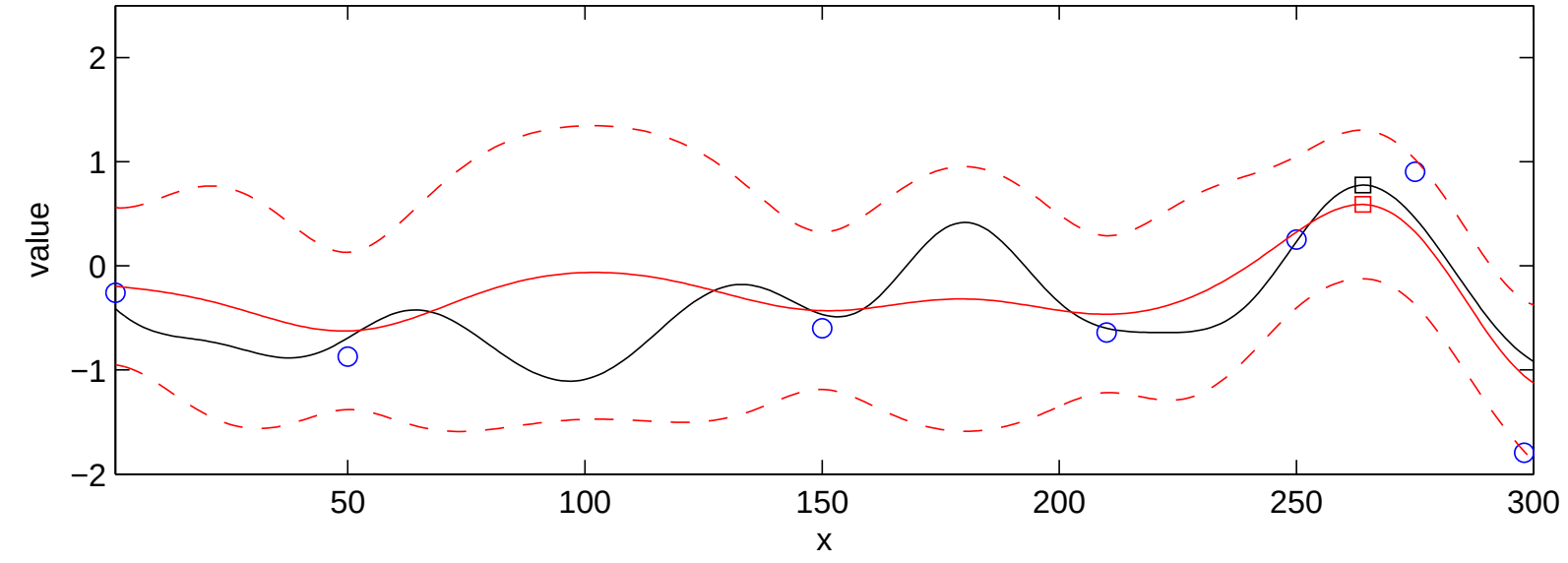

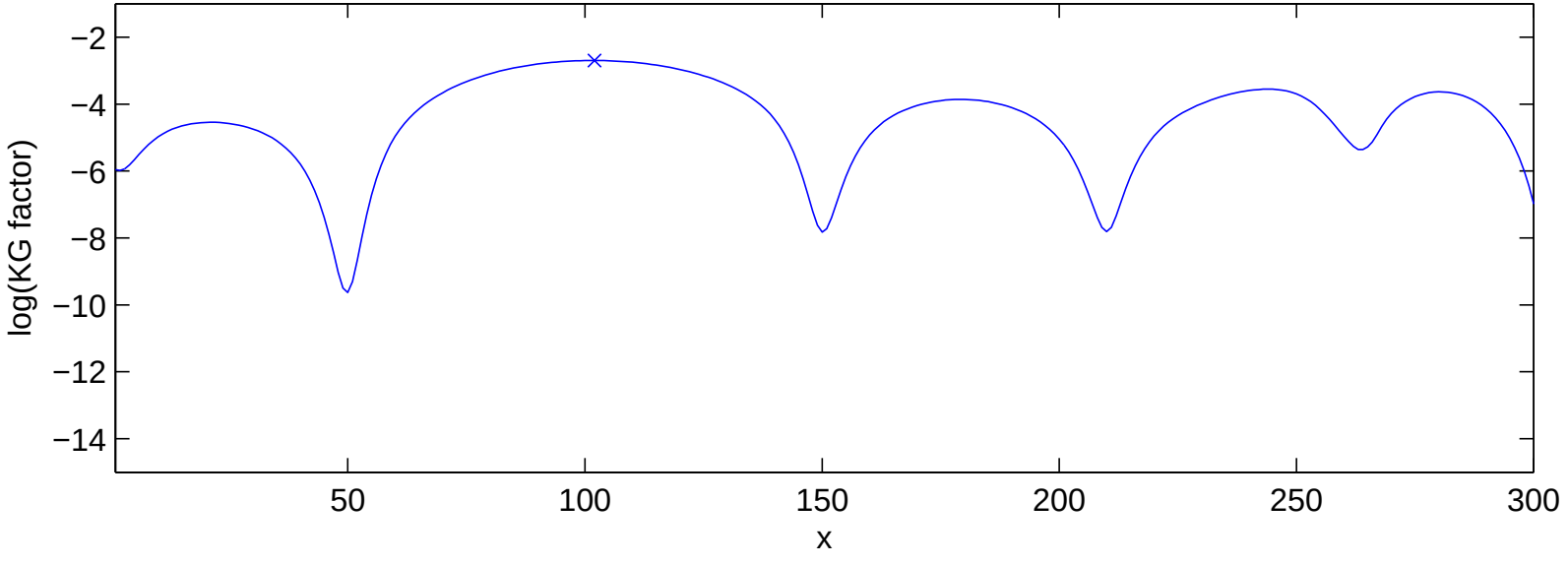

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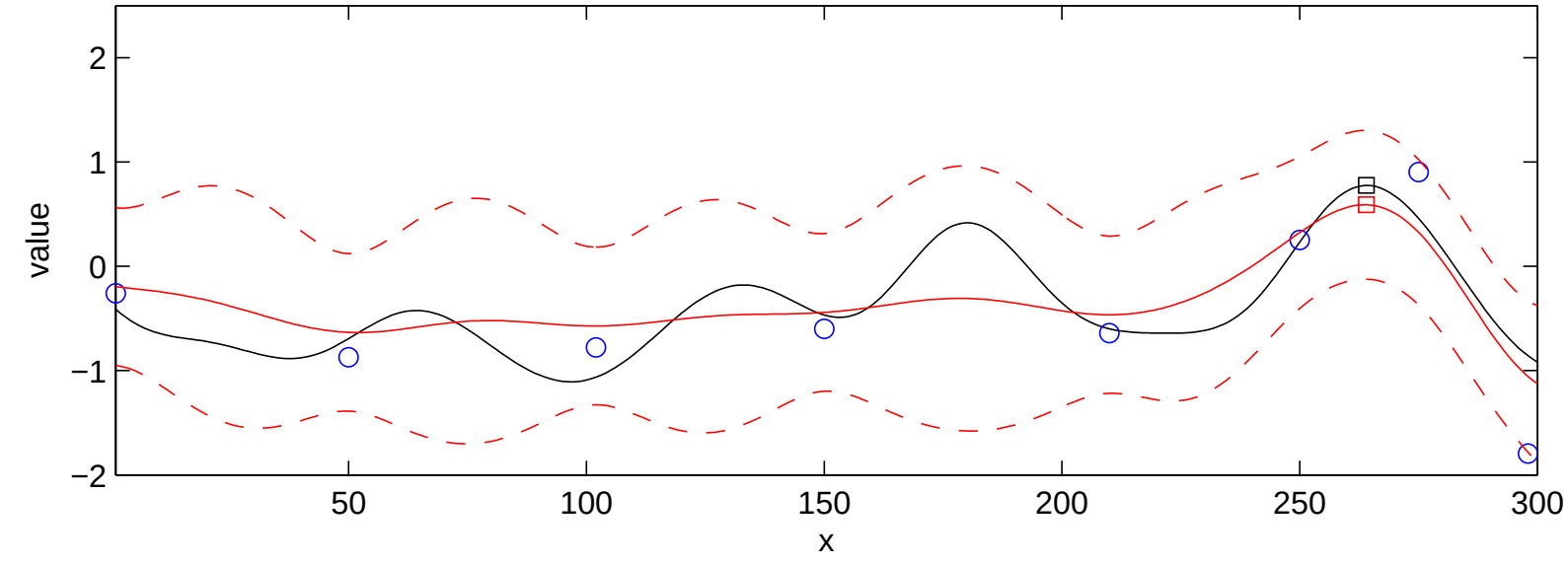

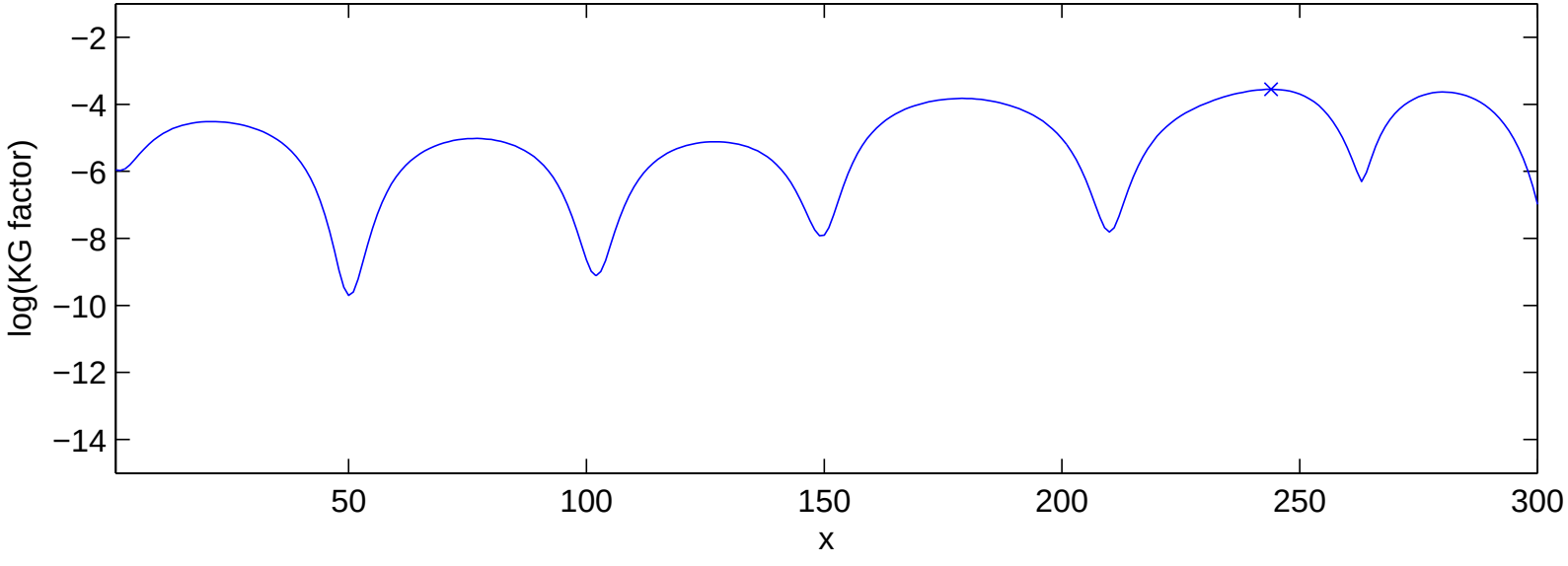

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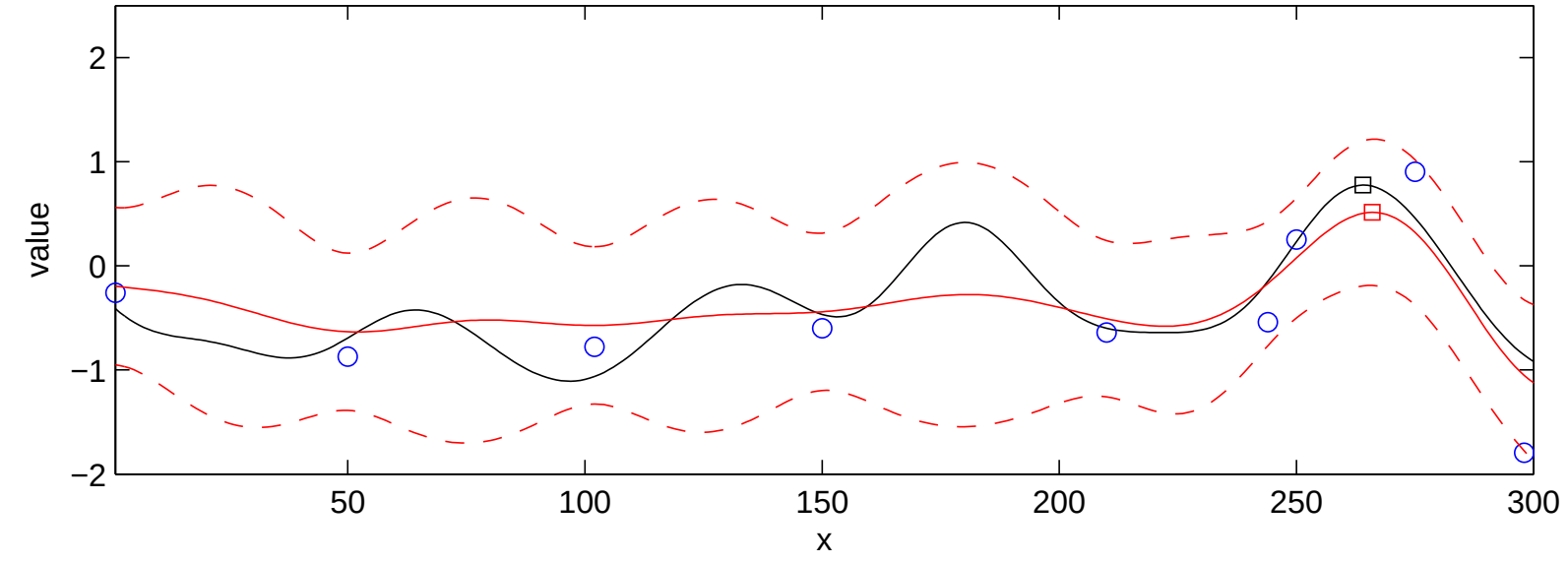

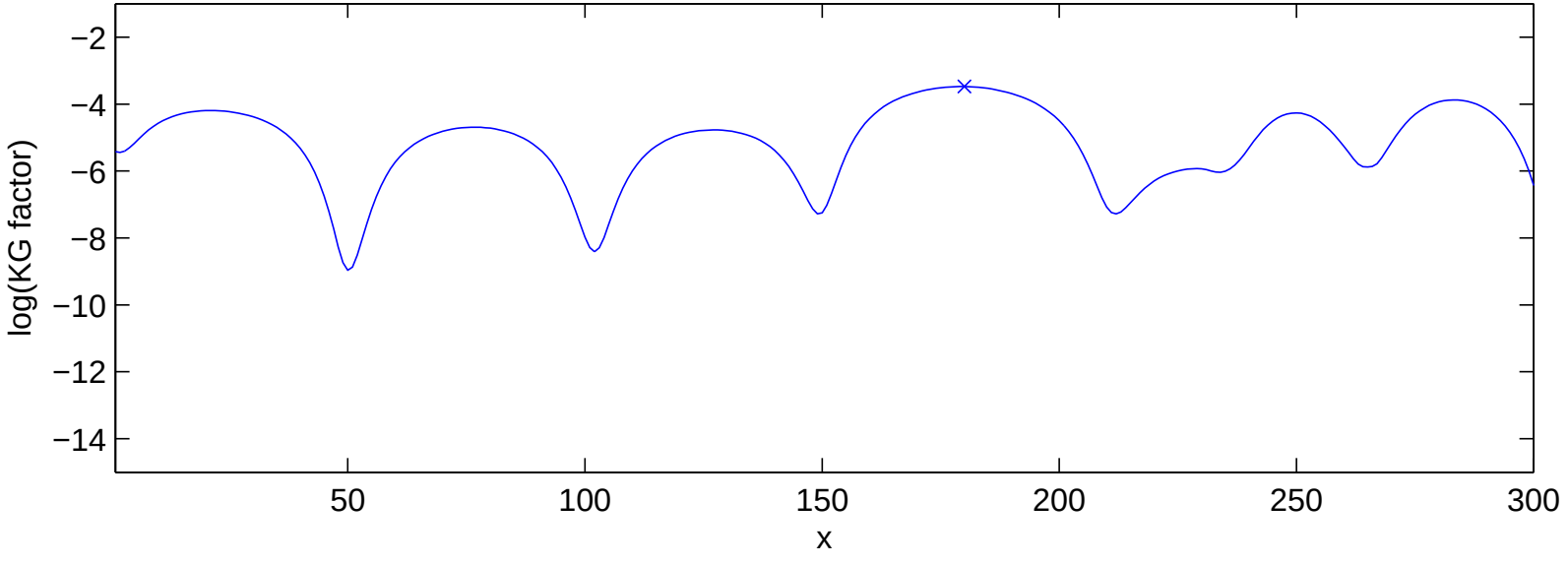

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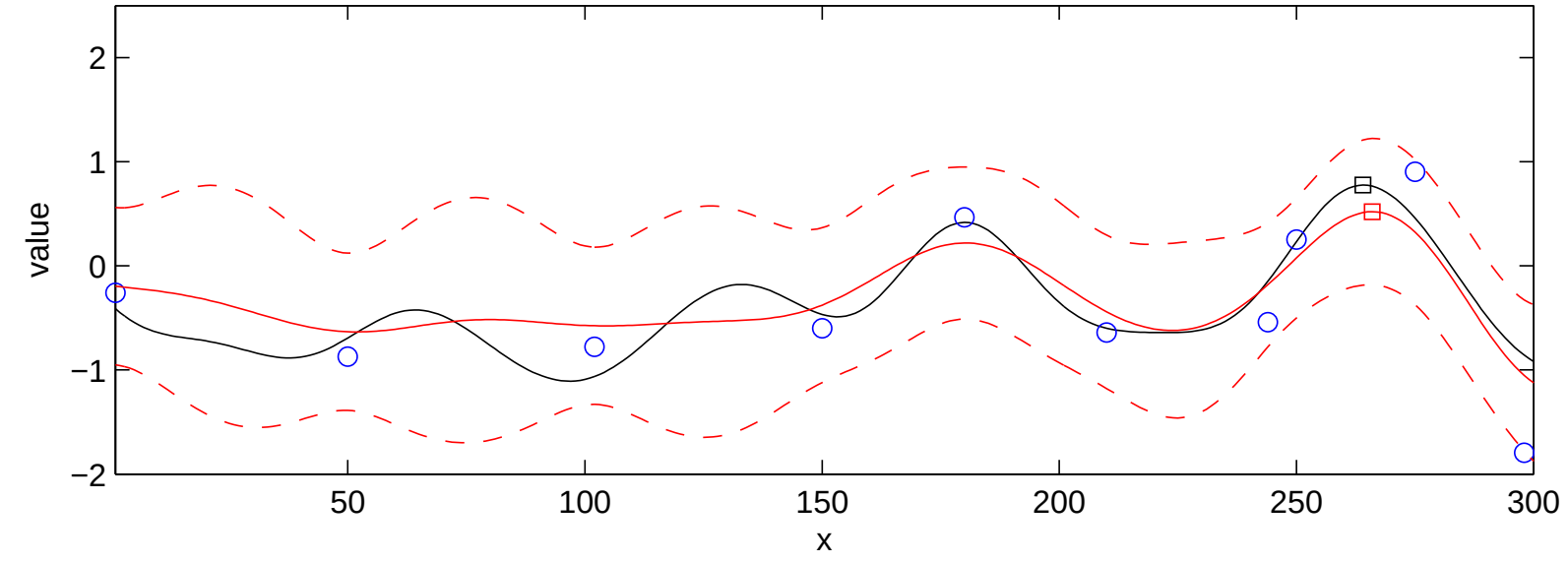

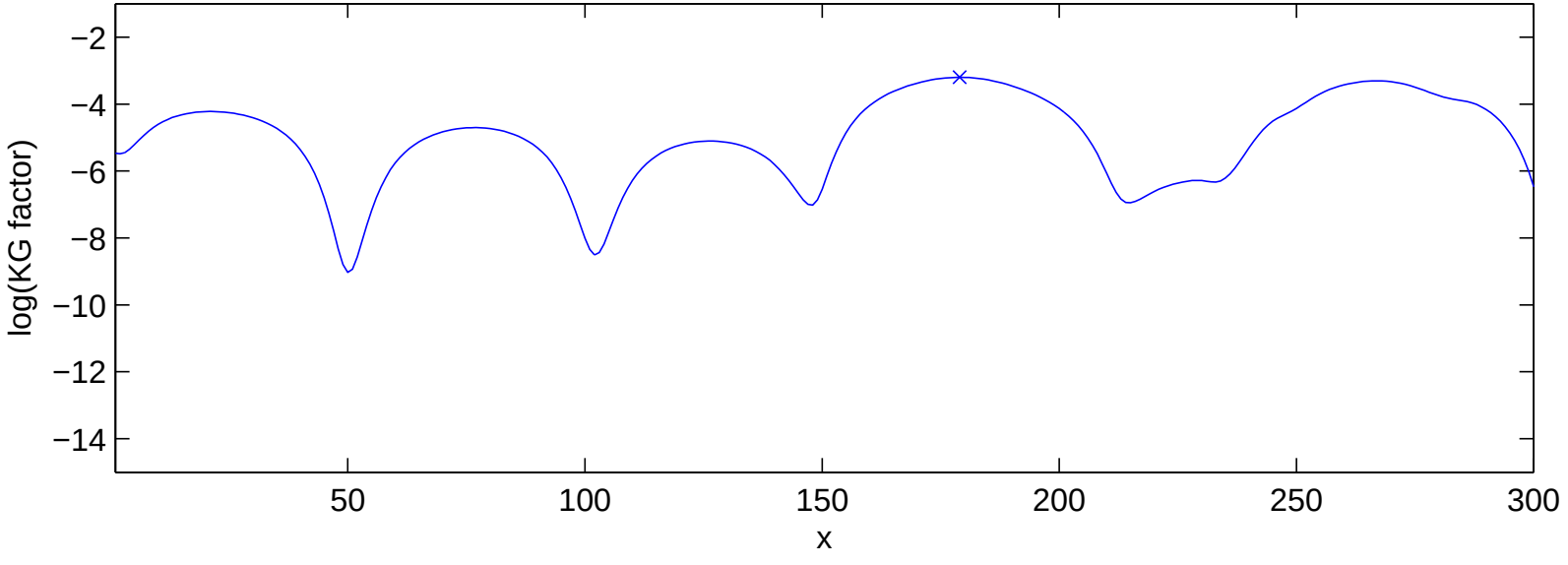

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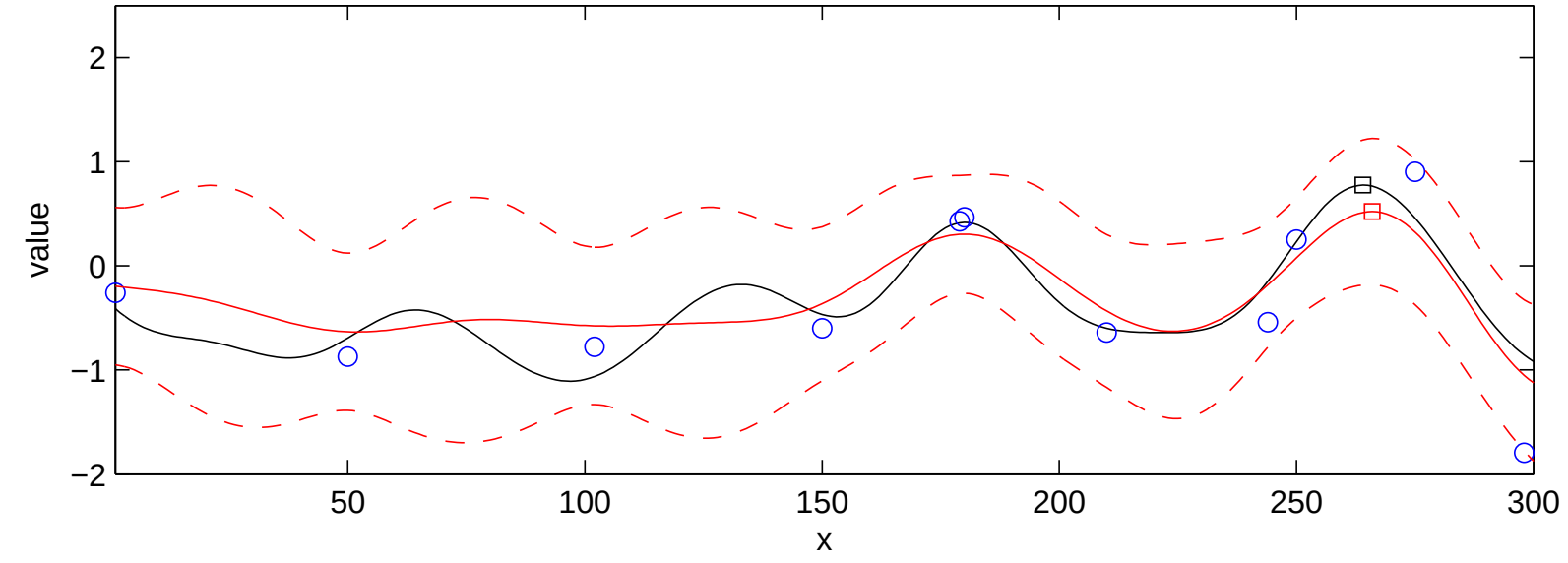

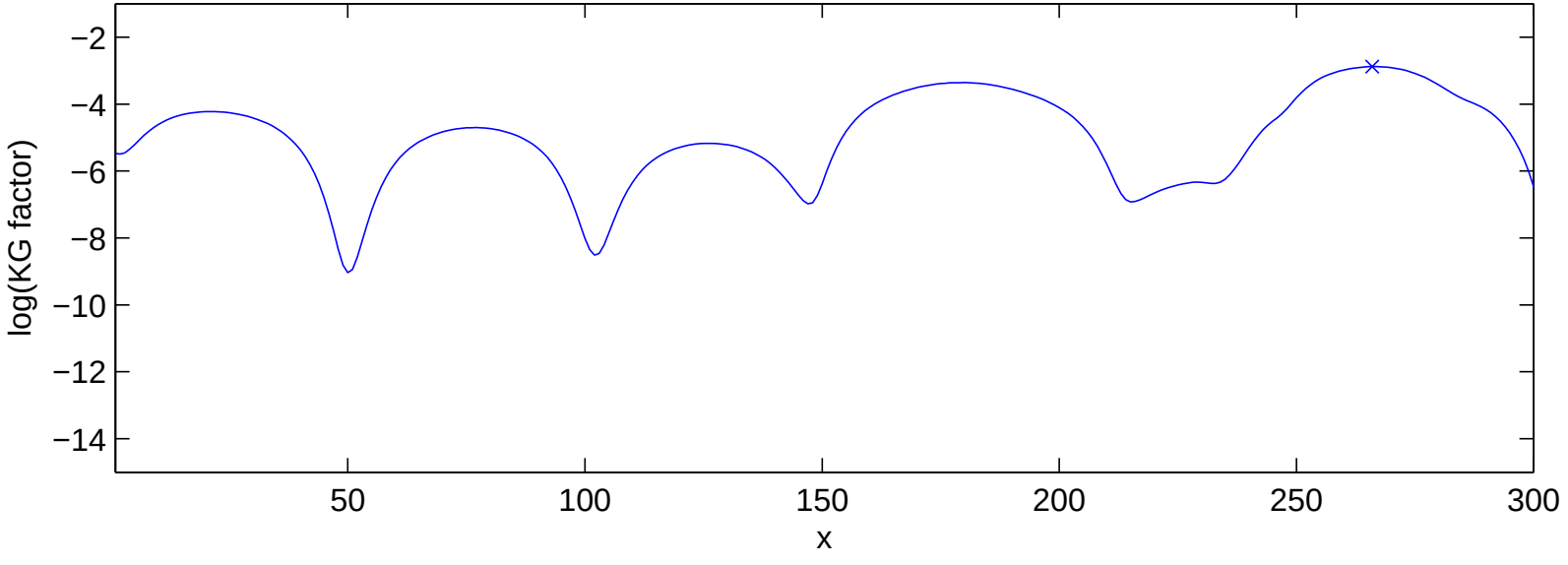

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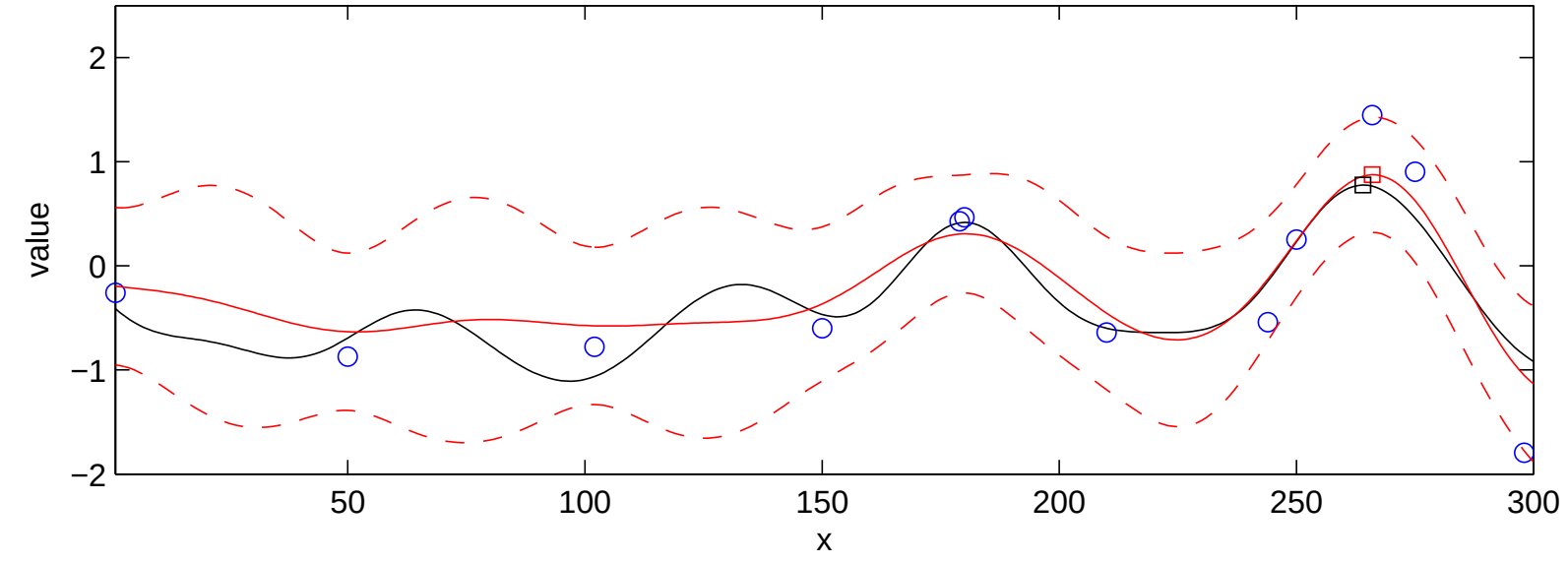
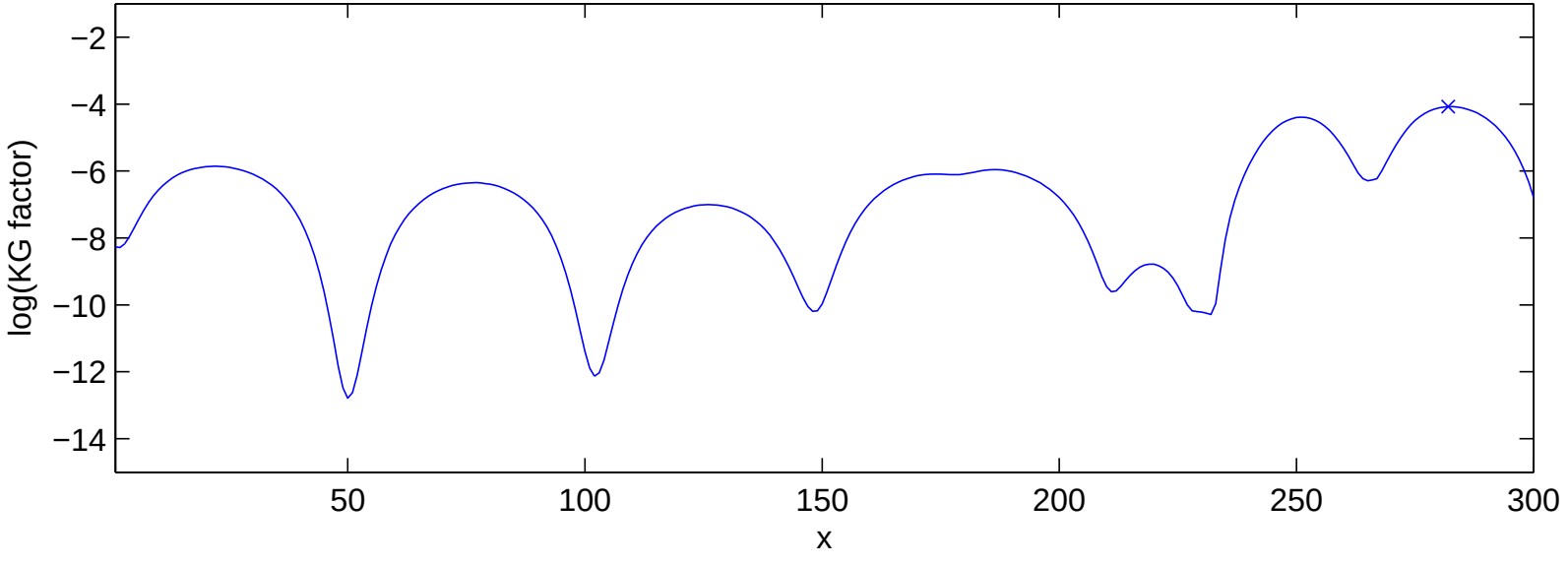
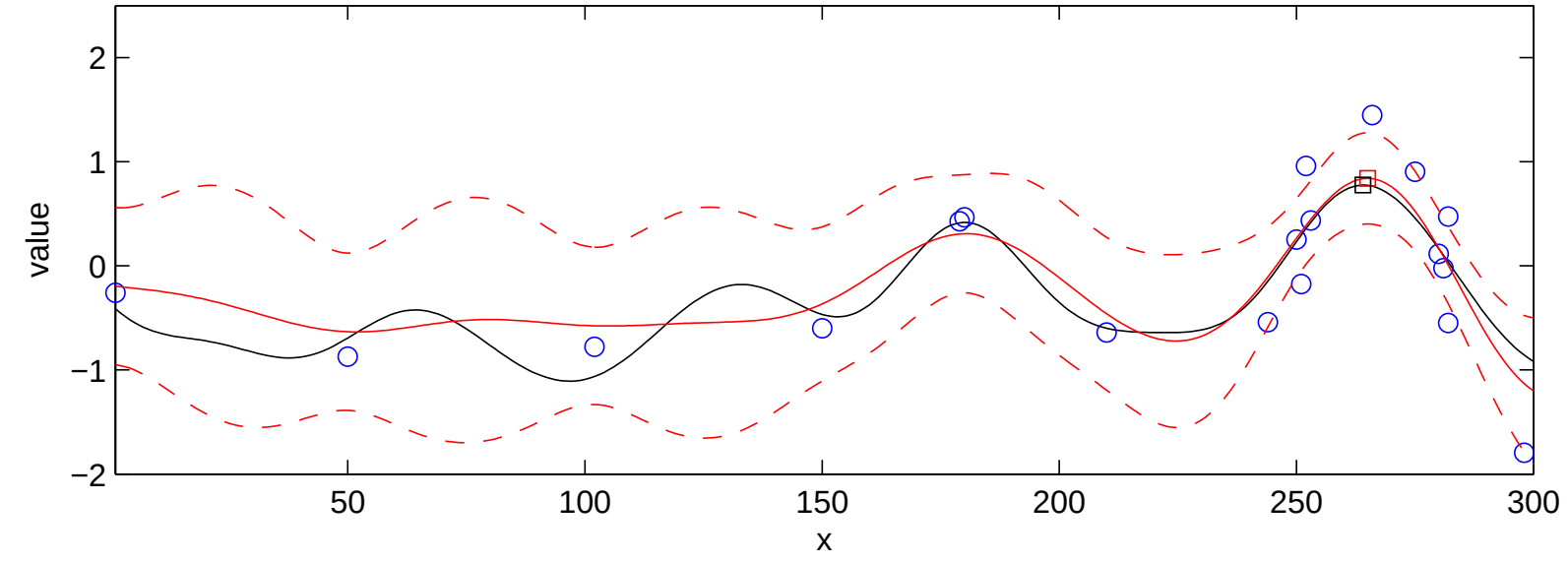
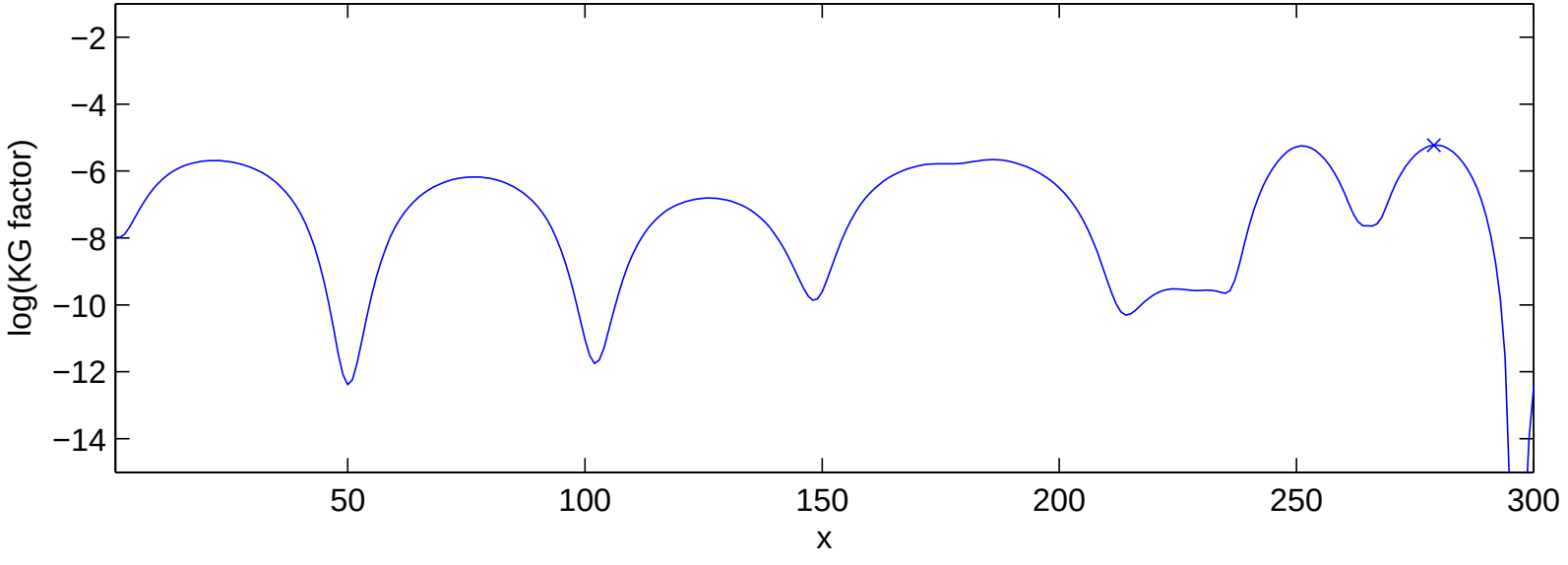




Global Optimization Example





Computing KG Factors

- To compute the KG factor, we must (approximately) compute

$$\mathbb{E}_n \left[\sup_{x \in [0,1]^d} \mu_{n+1}(x) \mid x_n = x \right].$$

- We choose a finite set $A \subset [0,1]^d$ and approximate this as

$$\mathbb{E}_n \left[\max_{x \in A} \mu_{n+1}(x) \mid x_n = x \right].$$

- We can evaluate this expectation because $\mu_{n+1}(x) = \mu_N(x) + s_n(x)Z$, where Z is a **univariate** standard normal random variable, and the function s_n depends on x_n.
- As A gets bigger, the approximation becomes more accurate.

Computing KG Factors

In general, to compute the approximate KG factor for a candidate measurement:

- Let $A' = (x^1, \ldots, x^m) \subseteq A$ contain those points that are best under the time-$n+1$ posterior with nonzero probability.
- Sort A' in order of decreasing $s_n(x^i)$.
- The approximate KG factor is

$$\sum_{i=1}^{m-1} (s_n(x^{i+1}) - s_n(x^i)) g\left(\frac{-|\mu_n(x^{i+1}) - \mu_n(x^i)|}{s_n(x^{i+1}) - s_n(x^i)}\right),$$

where $g(z) = \varphi(z) + z\Phi(z)$,
φ is the normal pdf and Φ is the normal cdf.

Consistency

Consider a discretized problem in which x_n and $\widehat{x}_*$ are restricted to a finite set $\mathscr{X} \subset [0,1]^d$. Then:

Theorem

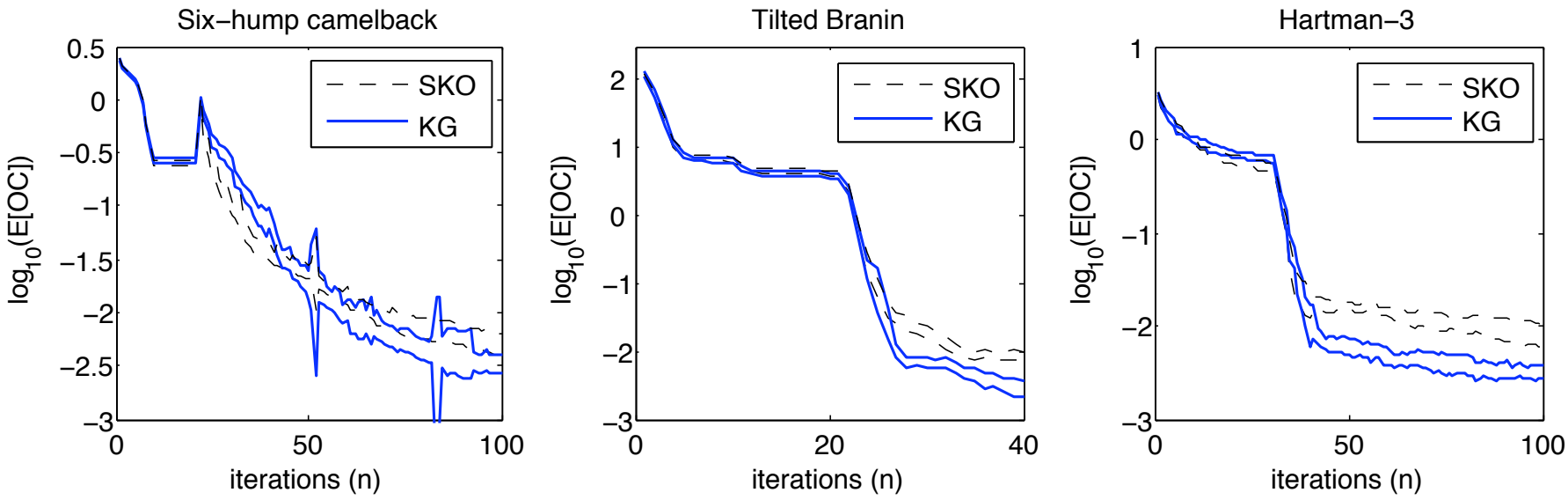
$$\lim_{N\to\infty} \arg\max_{x\in\mathscr{X}} \mu_N(x) = \arg\max_{x\in\mathscr{X}} f(x)$$

almost surely under $\mathbb{P}_0$.

This states that the global optimum is eventually discovered.
The proof uses a martingale convergence argument to show that every $x \in \mathscr{X}$ is evaluated infinitely often.

Global Optimization: Numerical Results

Sequential Kriging Optimization (SKO) is a recent method that uses Bayesian methods and spends a great deal of computational effort deciding where to sample next in order to minimize the number of function evaluations required.



Other Approaches to Continuous Global Optimization

- Many other derivative-free noise-tolerant global optimization methods exist, e.g.,
  - pattern search, e.g., Nelder-Mead
  - stochastic approximation, e.g., SPSA [Spall 1992].
  - evolutionary algorithms, simulated annealing, tabu search
- The KG method is a Bayesian global optimization (BGO) method because it places a Bayesian prior distribution on the underlying but unknown function. (See [Jones et al. 1998]).
- The posterior may understood as a surrogate model for the unknown function, and in this way BGO methods are similar to radial basis function methods [Gutmann 2001, Regis & Shoemaker 2007] and response surface methods [Myers & Montgomery 2002].
- Surrogate-based methods require more computation to decide where to evaluate next, but often require fewer evaluations to find global extrema.

Conclusion

- **We solved the dynamic program** for an idealized version of the stochastic root-finding problem. Other problems where preliminary results suggest that the DP can be solved:
  - Finding level sets of 1-dimensional continuous functions.
  - Multiple comparisons with a standard / finding level sets.
  - A search problem arising in computer vision.
- We used dynamic programming to find a **good heuristic policy** for stochastic global optimization. This technique is general and seems reasonably likely to work well in many problems.
- Dynamic programming is a **useful theoretical tools** for developing algorithms for simulation optimization and other applications requiring heavy computation.

Thank You

Any questions?