Probabilistic Numerics

II – Filtering and Quadrature

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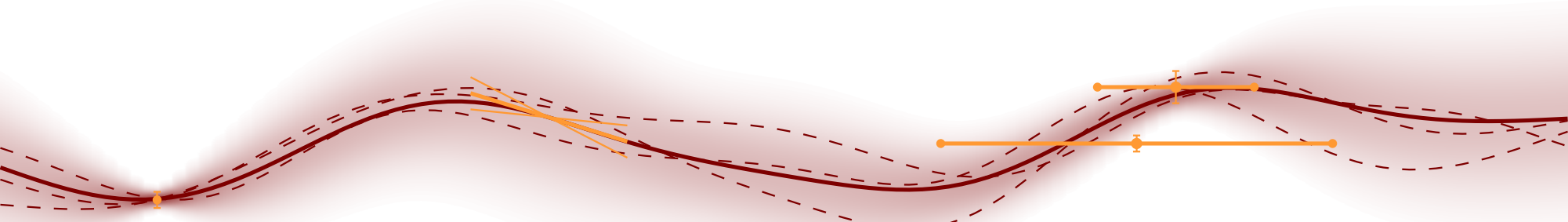


Quick recap:

- **probabilistic inference** is **the** framework to consistently handle (epistemic and aleatory) uncertainty
- **Gaussian measures** turn inference into linear algebra
- **Gaussian processes** allow inference on **functions**

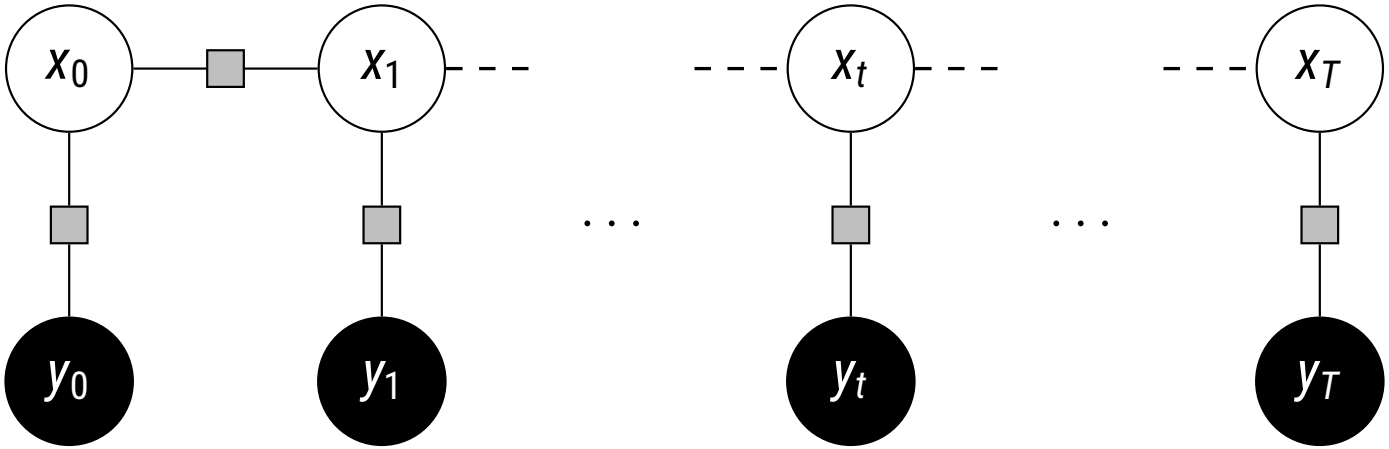
now:

- **filtering**: fast (linear time) inference for univariate GPs
- **quadrature**: a first probabilistic algorithm
- solving **ordinary differential equations**: a first “nonlinear” problem

A Markov Chain

local structure in ordered spaces

$$p(x_t \mid X_{0:t-1}) = p(x_t \mid x_{t-1}) \qquad \text{and} \qquad p(y_t \mid X) = p(y_t \mid x_t)$$



$$p(x_t \mid Y_{0:t-1}) = \frac{\int_{j \neq t} p(X)p(Y_{0:t-1} \mid X)\, dx_j}{\int p(X)p(Y_{0:t-1} \mid X)\, dX}$$

$$= \frac{\int_{j \neq t} p(Y_{0:t-1} \mid X_{0:t-1})p(x_0) \left(\prod_{0<j<t} p(x_j \mid x_{j-1})\, dx_j\right) p(x_t \mid x_{t-1}) \left(\prod_{j>t} p(x_j \mid x_{j-1})\, dx_j\right)}{\int p(Y_{0:t-1} \mid X_{0:t-1})p(x_0) \left(\prod_{0<j<t} p(x_j \mid x_{j-1})\right) p(x_t \mid x_{t-1}) \left(\prod_{j>t} p(x_j \mid x_{j-1})\right) dX}$$

$$= \frac{\int_{j<t} p(x_t \mid x_{t-1})p(Y_{0:t-1} \mid X_{0:t-1})p(x_0) \left(\prod_{0<j<t} p(x_j \mid x_{j-1})\, dx_j\right)}{\int_{j<t} p(Y_{0:t-1} \mid X_{0:t-1})p(x_0) \left(\prod_{0<j<t} p(x_j \mid x_{j-1})\, dx_j\right)} = \int p(x_t \mid x_{t-1})p(x_{t-1} \mid Y_{0:t-1})\, dx_{t-1}$$

$$p(x_t \mid Y_{0:t}) = \frac{p(y_t \mid x_t)p(x_t \mid Y_{0:t-1})}{\int p(y_t \mid x_t)p(x_t \mid Y_{0:t-1})\, dx_t}$$

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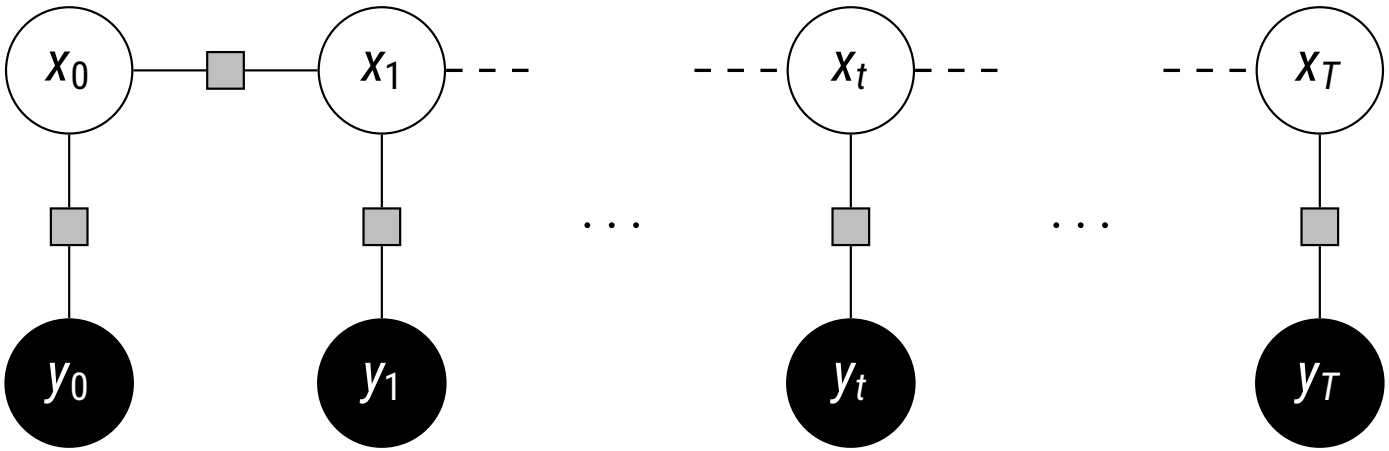

$$p(x_t \mid Y) = \int p(x_t, x_{t+1} \mid Y)\, dx_{t+1} = \int p(x_t \mid x_{t+1}, Y) p(x_{t+1} \mid Y)\, dx_{t+1} = \int p(x_t \mid x_{t+1}, Y_{0:t}) p(x_{k+1} \mid Y)\, dx_{t+1}$$

$$p(x_t \mid x_{t+1}, Y_{0:t}) = \frac{p(x_t, x_{t+1} \mid Y_{0:t})}{p(x_{t+1} \mid Y_{0:t})} = \frac{p(x_{t+1} \mid x_t, Y_{0:t}) p(x_t \mid Y_{0:t})}{p(x_{t+1} \mid Y_{0:t})} = \frac{p(x_{t+1} \mid x_t) p(x_t \mid Y_{0:t})}{p(x_{t+1} \mid Y_{0:t})}$$

$$p(x_t \mid Y) = p(x_t \mid Y_{0:t}) \int p(x_{t+1} \mid x_t) \frac{p(x_{t+1} \mid Y)}{p(x_{t+1} \mid Y_{1:t})}\, dx_{t+1}$$

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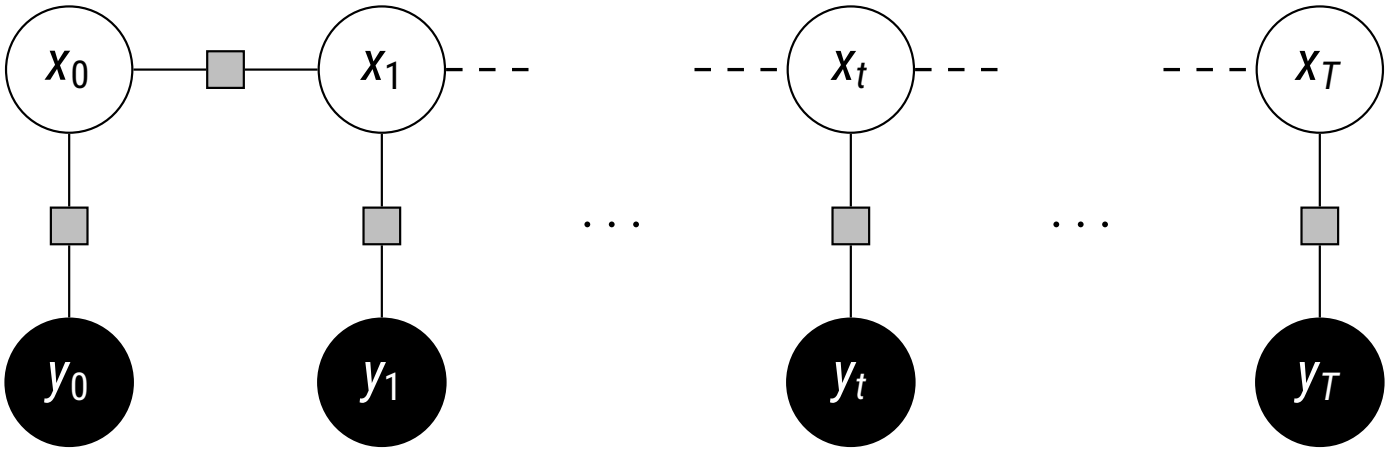


Filtering: $\mathcal{O}(T)$

predict: $$p(x_t \mid Y_{0:t-1}) = \int p(x_t \mid x_{t-1}) p(x_{t-1} \mid Y_{0:t-1})\, dx_{t-1}$$

update: $$p(x_t \mid Y_{0:t}) = \frac{p(y_t \mid x_t) p(x_t \mid Y_{0:t-1})}{p(y_t)}$$

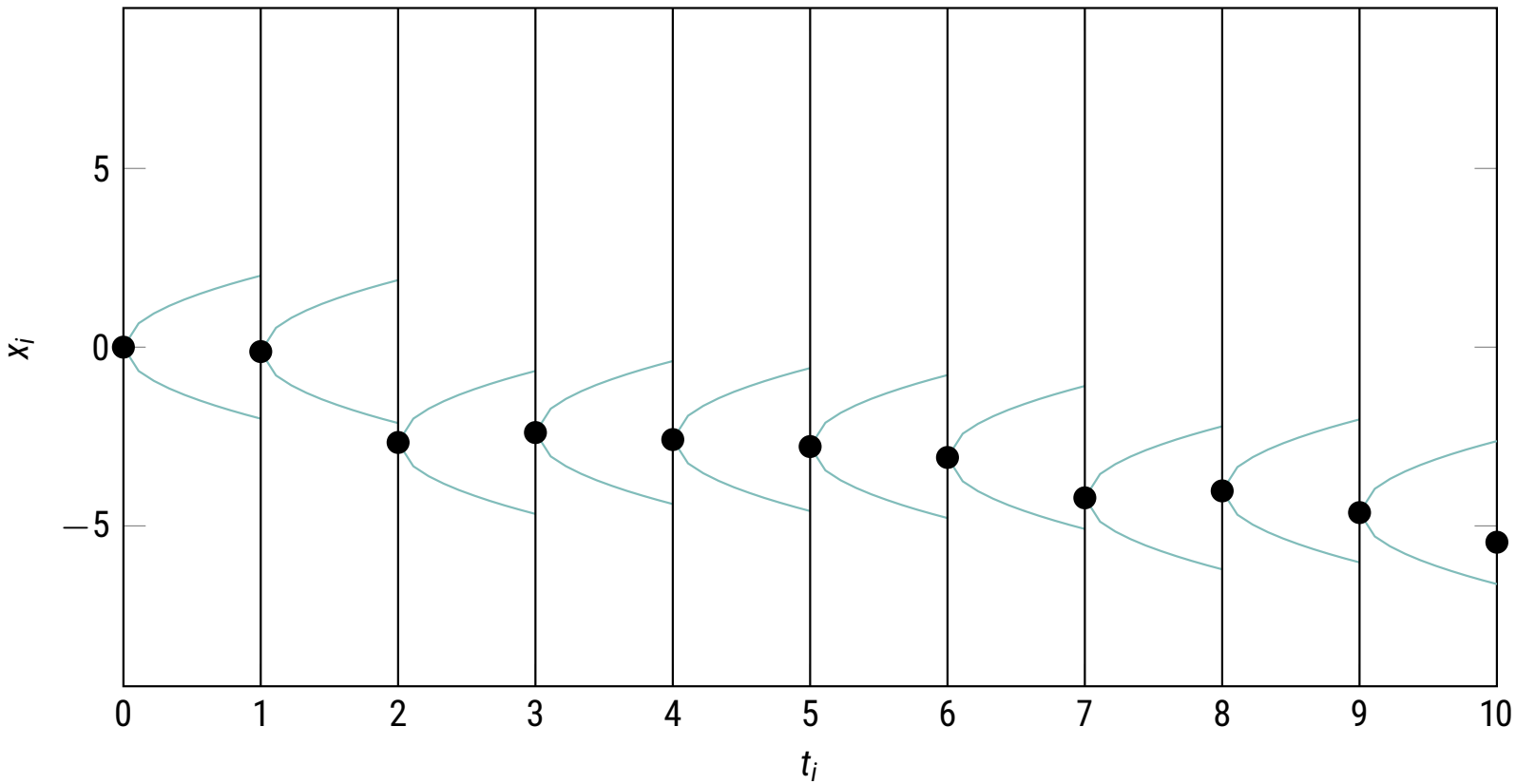
Smoothing: $\mathcal{O}(T)$

smooth: $$p(x_t \mid Y) = p(x_t \mid Y_{0:t}) \int p(x_{t+1} \mid x_t) \frac{p(x_{t+1} \mid Y)}{p(x_{t+1} \mid Y_{1:t})}\, dx_{t+1}$$

Gauss-Markov Models

Local structure for univariate Gaussian models

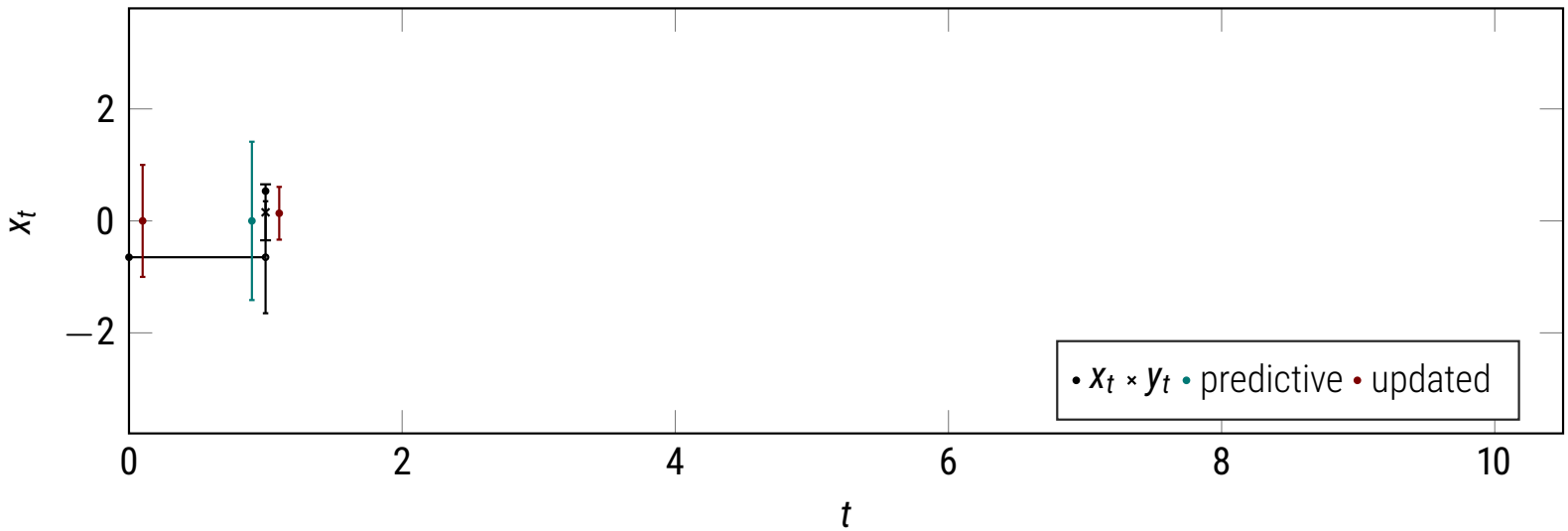
$$p(x(t_{i+1}) \mid x(t_i)) = \mathcal{N}(x_{i+1}; Ax_i, Q) \qquad \text{(figure: } x_0 = 0, A = Q = 1\text{)}$$



Kalman Filtering and Rauch-Tung-Striebel Smoothing

linear-time inference on Gaussian-Markov time series

$$p(x(t_i) \mid x(t_{i-1})) = \mathcal{N}(x_i; Ax_{i-1}, Q) \qquad p(y_t \mid x_t) = \mathcal{N}(y_t; Hx_t, R)$$



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$$G_t = P_tA^\mathsf{T} (P_t^-)^{-1},$$

smooth: $$p(x_t \mid Y) = p(x_t \mid Y_{0:t}) \int p(x_{t+1} \mid x_t) \frac{p(x_{t+1} \mid Y)}{p(x_{t+1} \mid Y_{1:t})}\, dx_{t+1} = \mathcal{N}(x_t, m_t^s, P_t^s)$$

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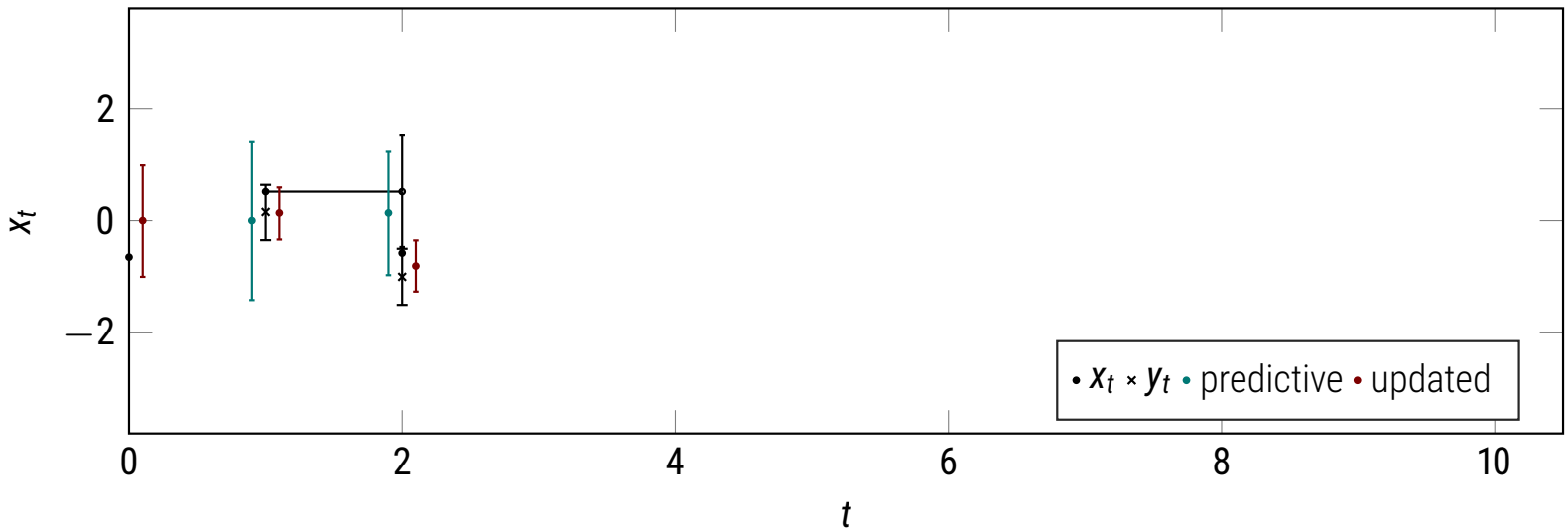

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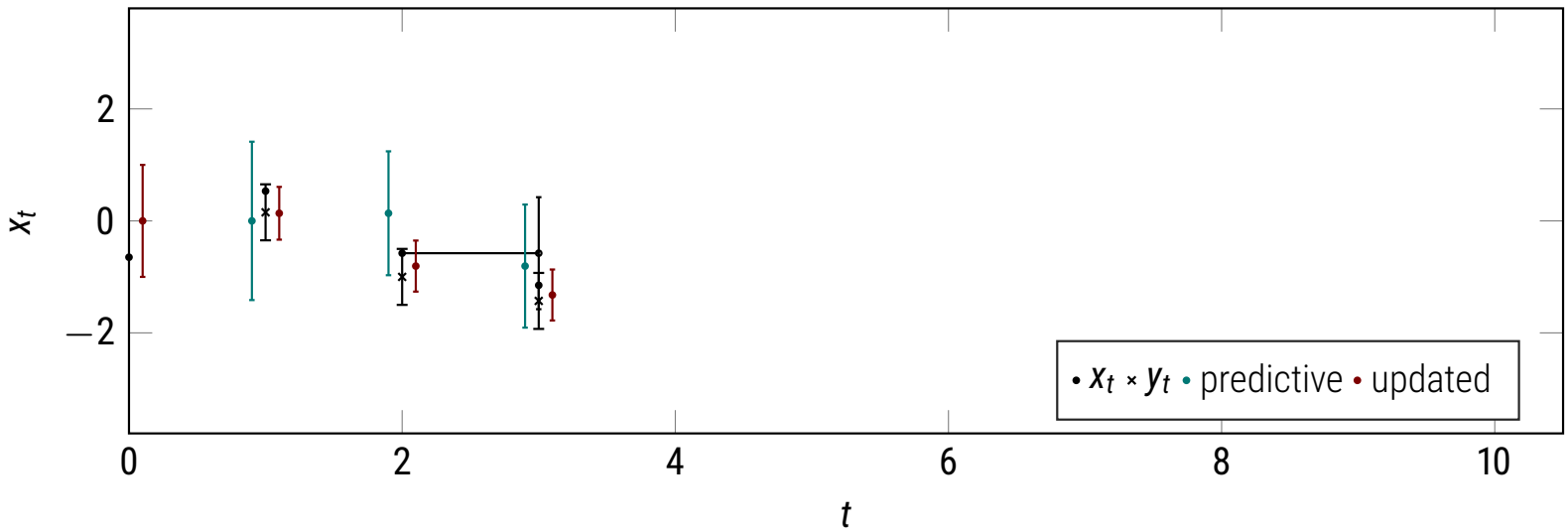

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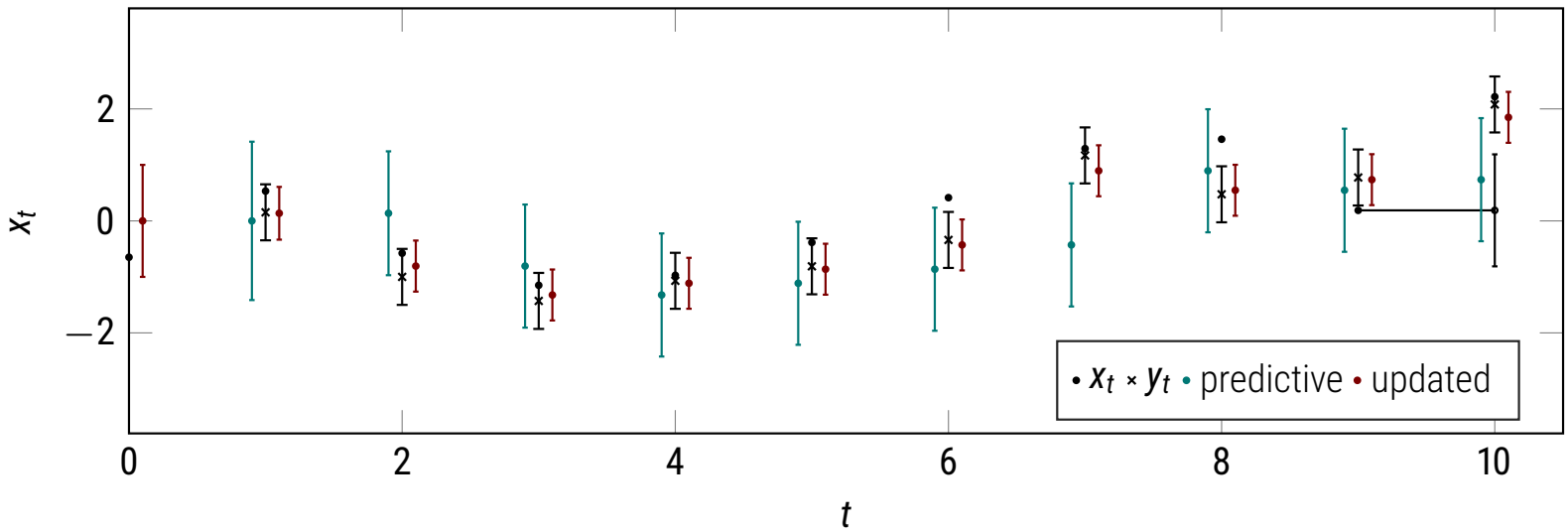

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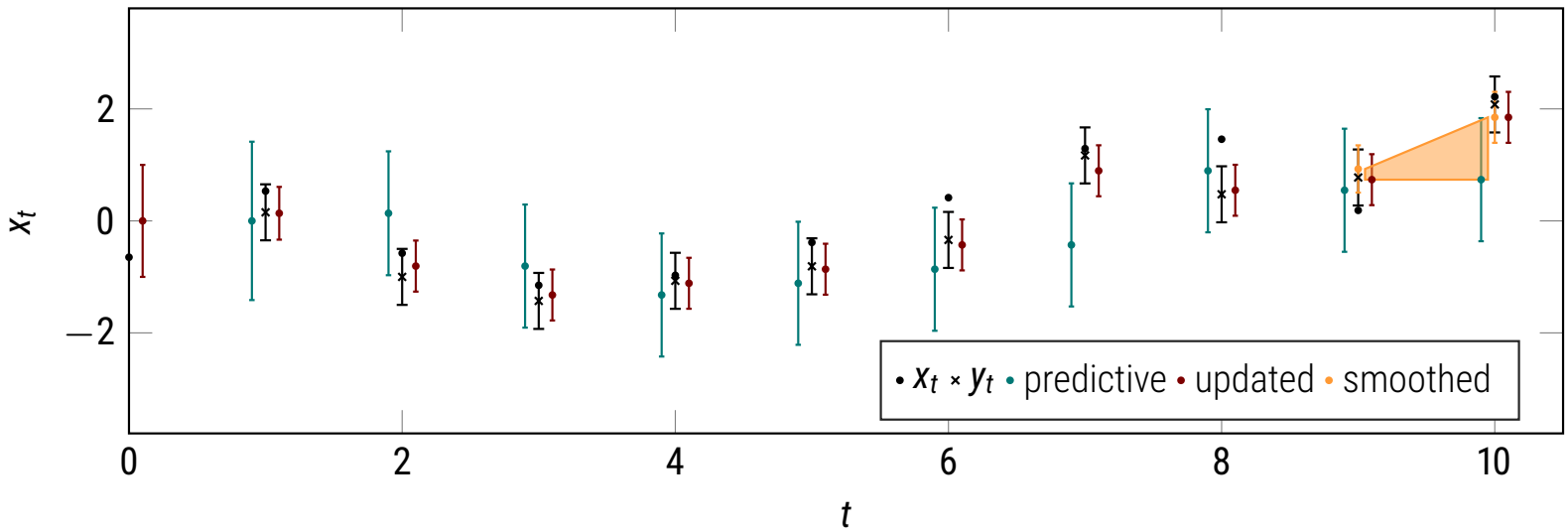

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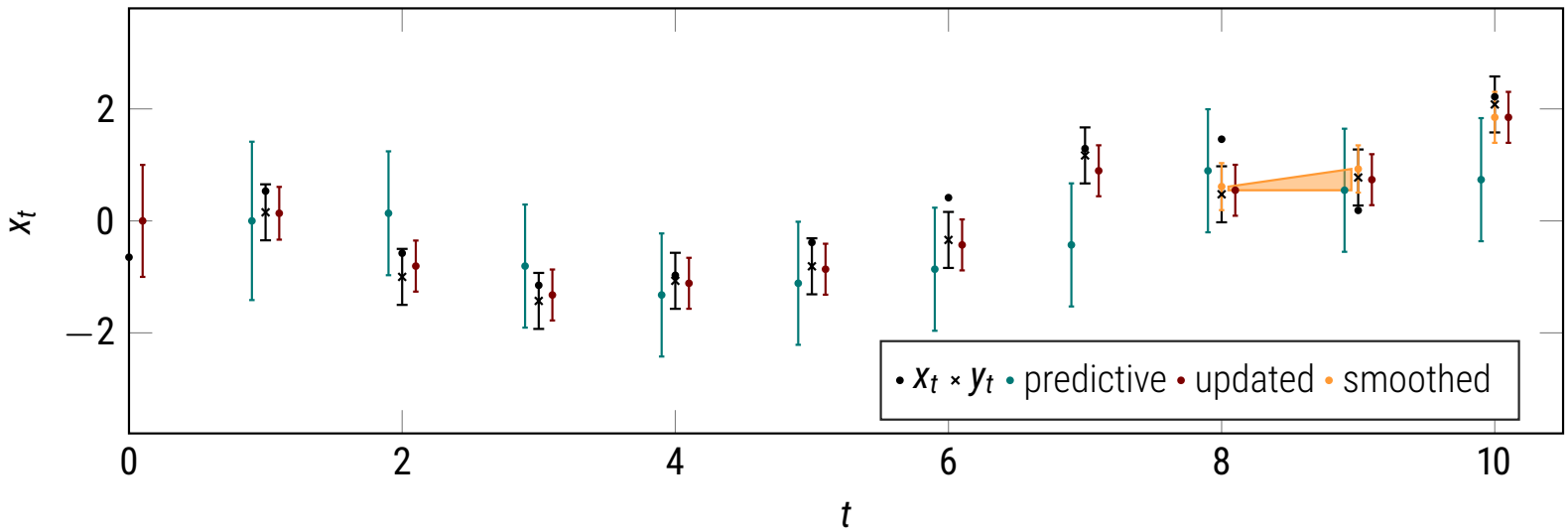

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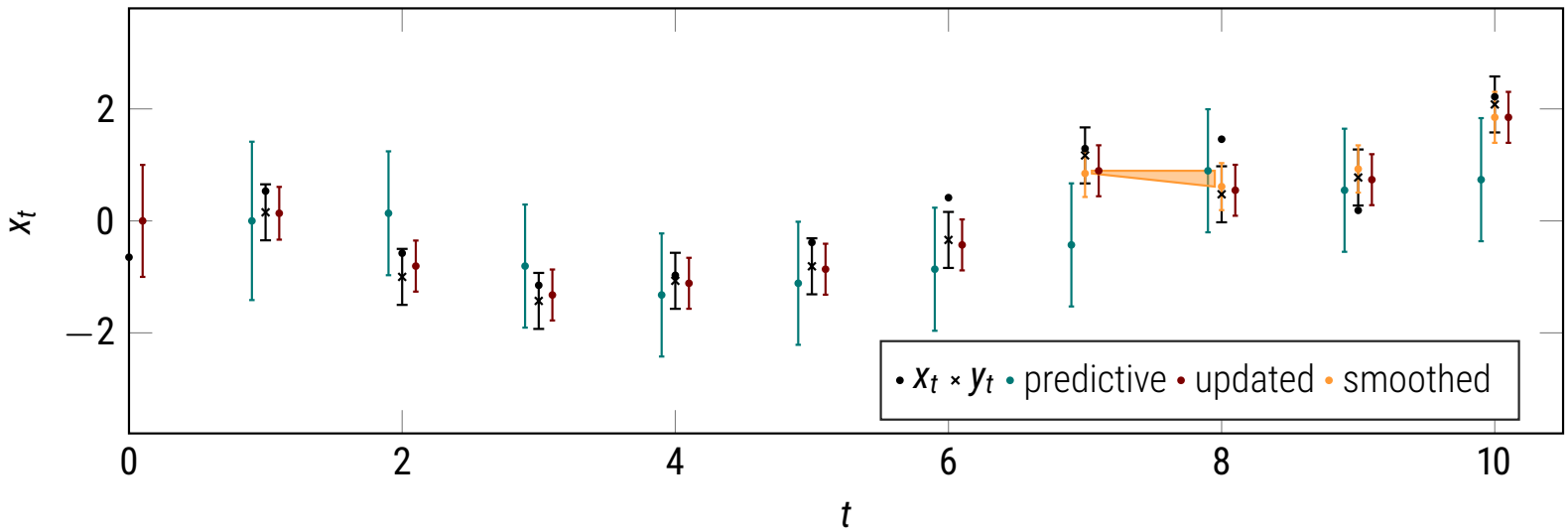

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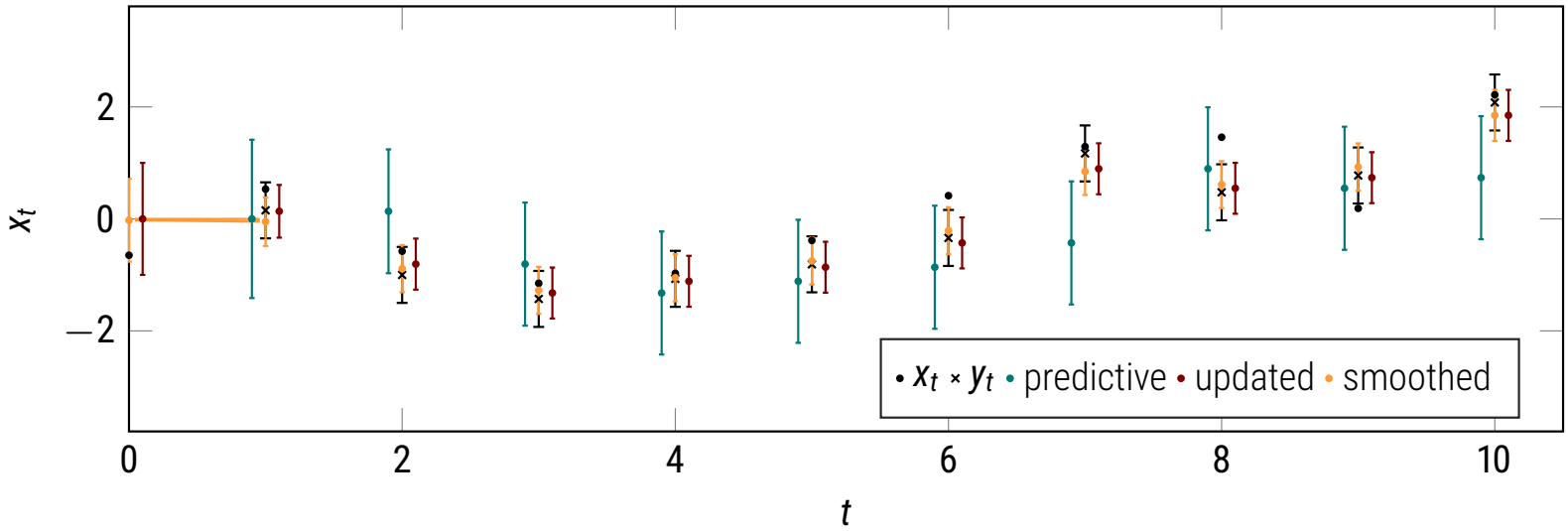


Filter:

$m_t^- = Am_{t-1}$ predictive mean

$P_t^- = AP_{t-1}A^\mathsf{T} + Q$ predictive covariance

$z_t = y - Hm_t^-$ innovation residual

$S_t = HP_t^- H^\mathsf{T} + R$ innovation covariance

$K_t = P_t^- H^\mathsf{T} S^{-1}$ Kalman gain

$m_t = m_t^- + Kz_t$ estimation mean

$P_t = (I - KH)P_t^-$ estimation covariance

Smoother:

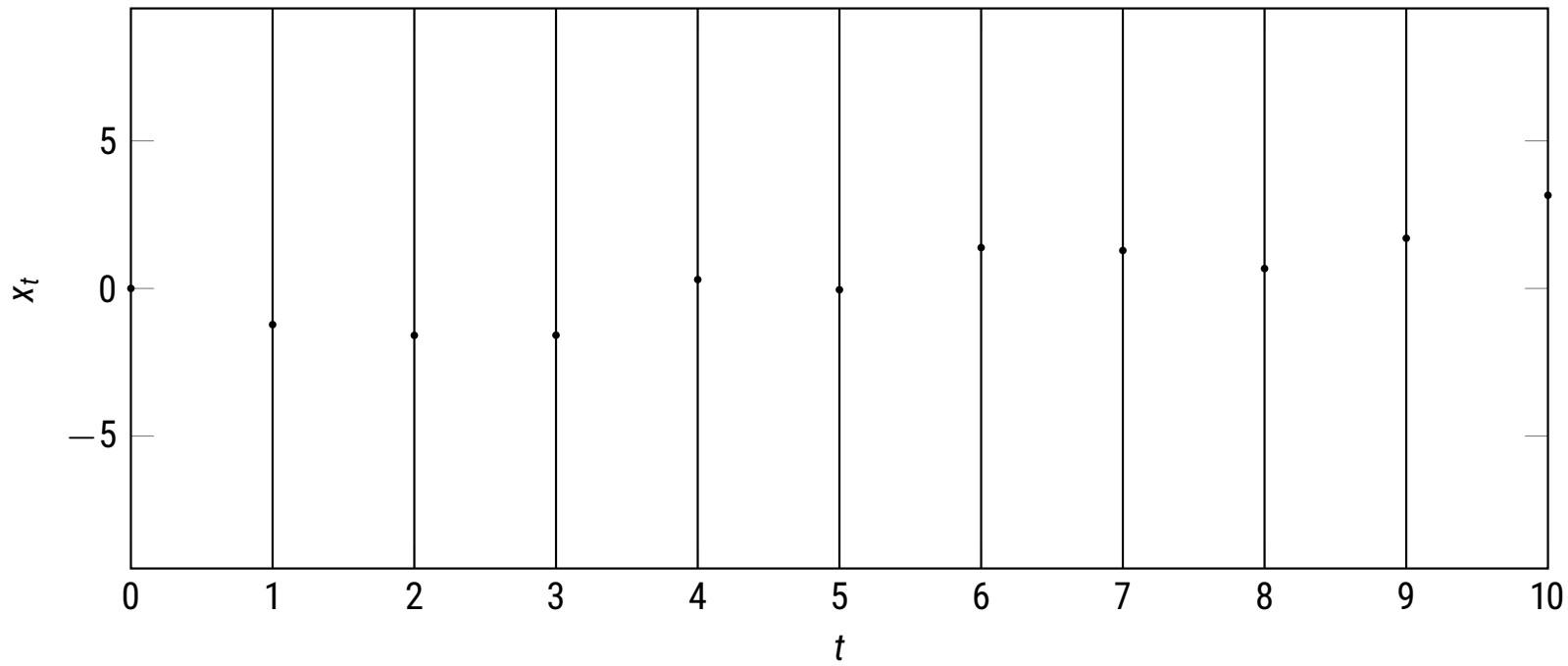
$G_t = P_t A^\mathsf{T} (P_{t+1}^-)^{-1}$ RTS gain

$m_t^s = m_t + G_t(m_{t+1}^s - m_{t+1}^-)$ smoothed mean

$P_t^s = P_t + G_t(P_{t+1}^s - P_{t+1}^-)G^\mathsf{T}$ smoothed covariance

Continuous Time

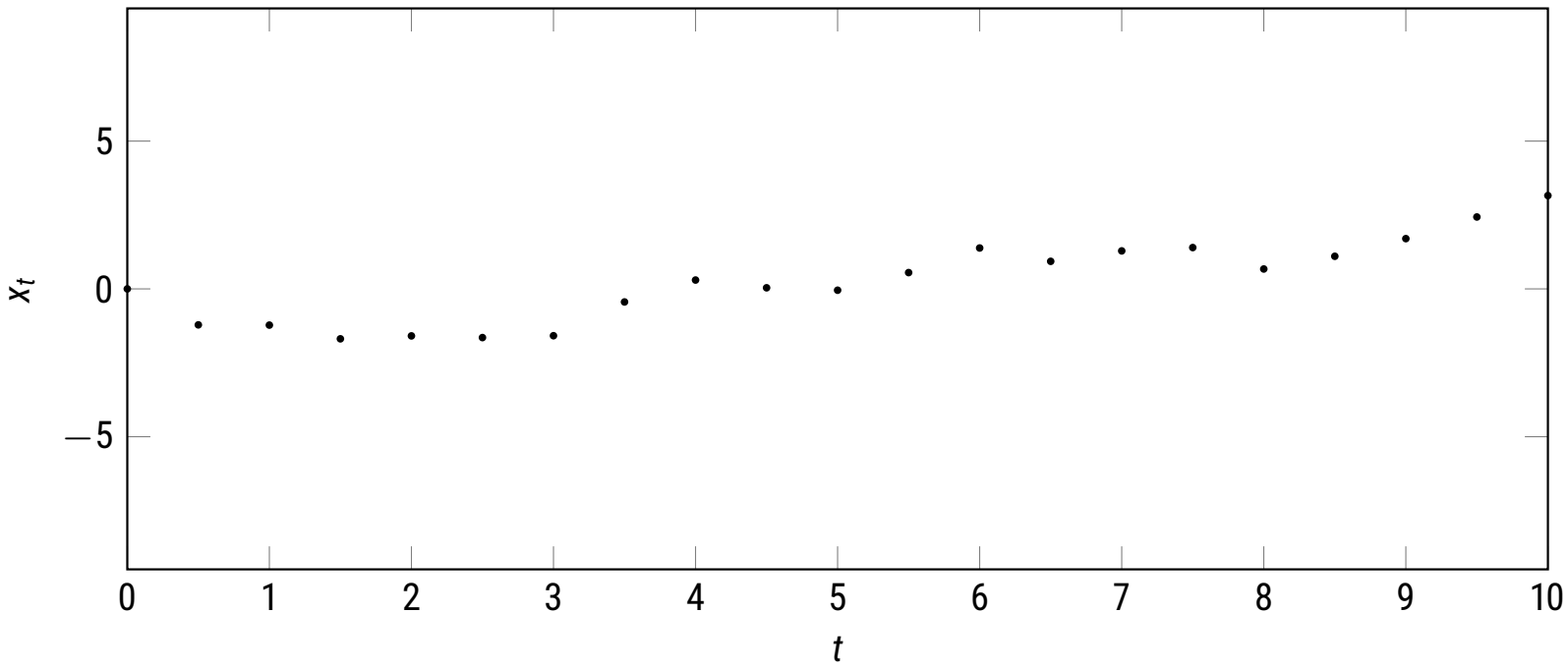
Differential equations defining non-differential curves



$\delta t = 1 \qquad Q = 1$

Continuous Time

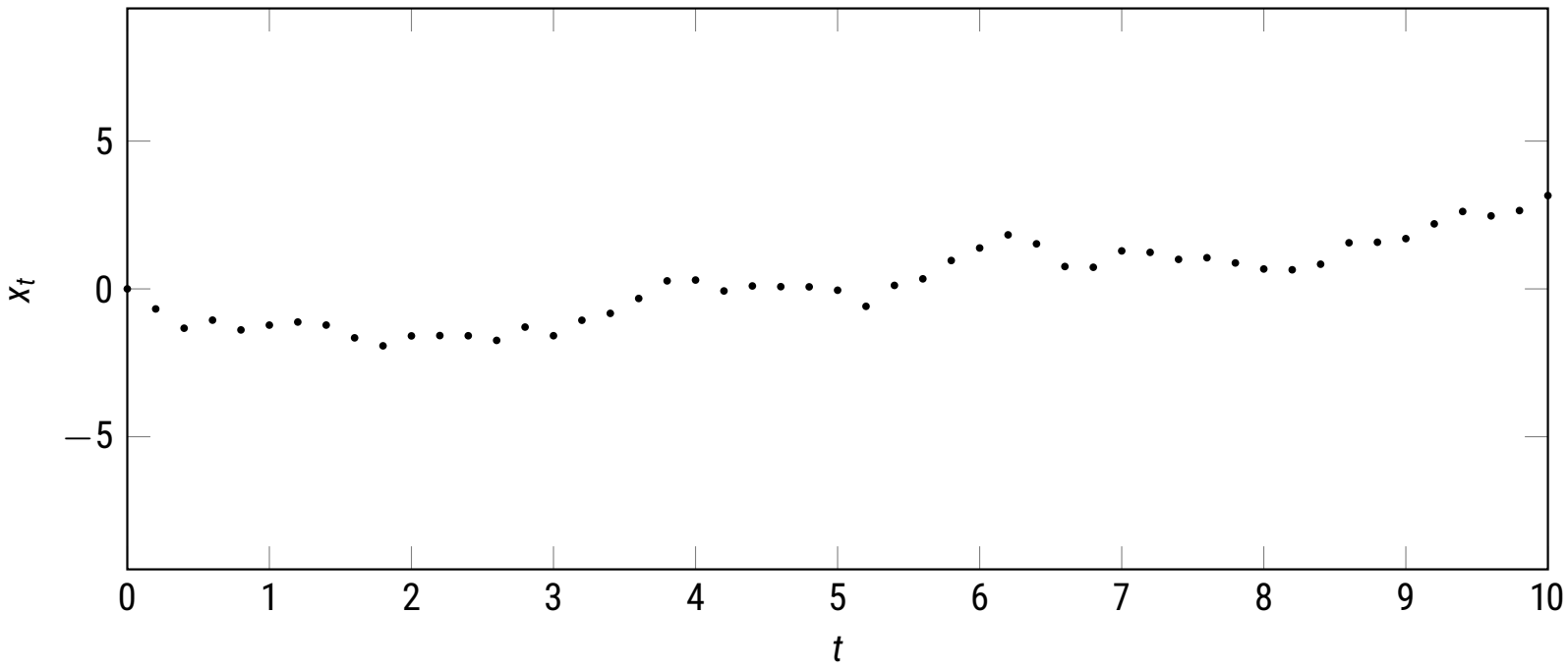
Differential equations defining non-differential curves



$\delta t = 1/2 \qquad Q = 1/2$

Continuous Time

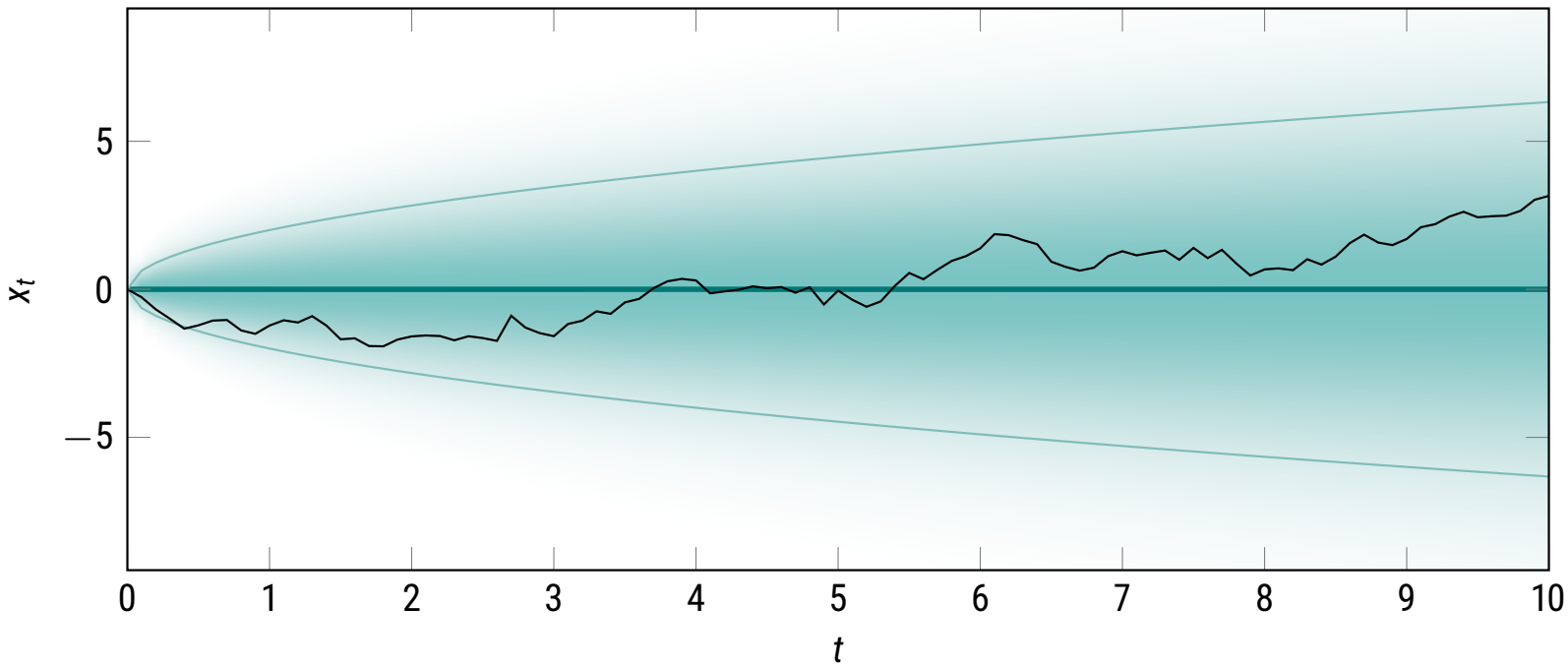
Differential equations defining non-differential curves



$\delta t = 1/4 \qquad Q = \delta t$

Continuous Time

Differential equations defining non-differential curves



$$\delta t \to 0 \qquad Q = ???$$

Stochastic Differential Equations

a pragmatic definition

For our purposes the (linear, time-invariant) **Stochastic Differential Equation**

$$dx(t) = Fx\,dt + L\,d\omega,$$

together with $x(t_0) = x_0$, describes the local behaviour of the (unique) Gaussian process with the following mean and covariance function

$$\mathrm{E}[x(t)] = e^{F(t-t_0)}x_0 \qquad k(t_a, t_b) = \int_{t_0}^{\min t_a, t_b} e^{F(t_a-\tau)}LL^\intercal e^{F^\intercal(t_b-\tau)}\,d\tau$$

This GP is known as the **complete solution** of the SDE. It gives rise to the discrete-time stochastic recurrence relation $p(x_{t_{i+1}} \mid x_{t_i}) = \mathcal{N}(x_{t_{i+1}}; A_{t_i}x_{t_i}, Q_{t+i})$ with

$$A_{t_i} = e^{F(t_{i+1}-t_i)} \quad \text{and} \quad Q_{t_i} = \int_0^{t_{i+1}-t_i} e^{F\tau}LL^\intercal e^{F\tau}\,d\tau.$$

$$e^X := \sum_{i=0}^{\infty}\frac{X^i}{i!}. \quad e^0 = I, \quad (e^X)^{-1} = e^{-X}, \quad \det e^X = e^{\mathrm{tr}\,X}, \quad X = VDV^{-1} \Rightarrow Ve^DV^{-1}, \quad e^{\mathrm{diag}_i\,d_i} = \mathrm{diag}_i\,e^{d_i}.$$

- **Markov** structure allows **linear time** inference on ordered spaces
- In **Gauss-Markov** models this involves only comparably simple linear algebra, the **Kalman filter**, and RTS smoother
- the conceptually tricky continuous time limit is known as a linear **stochastic differential equation**

For more on Filters and SDEs see

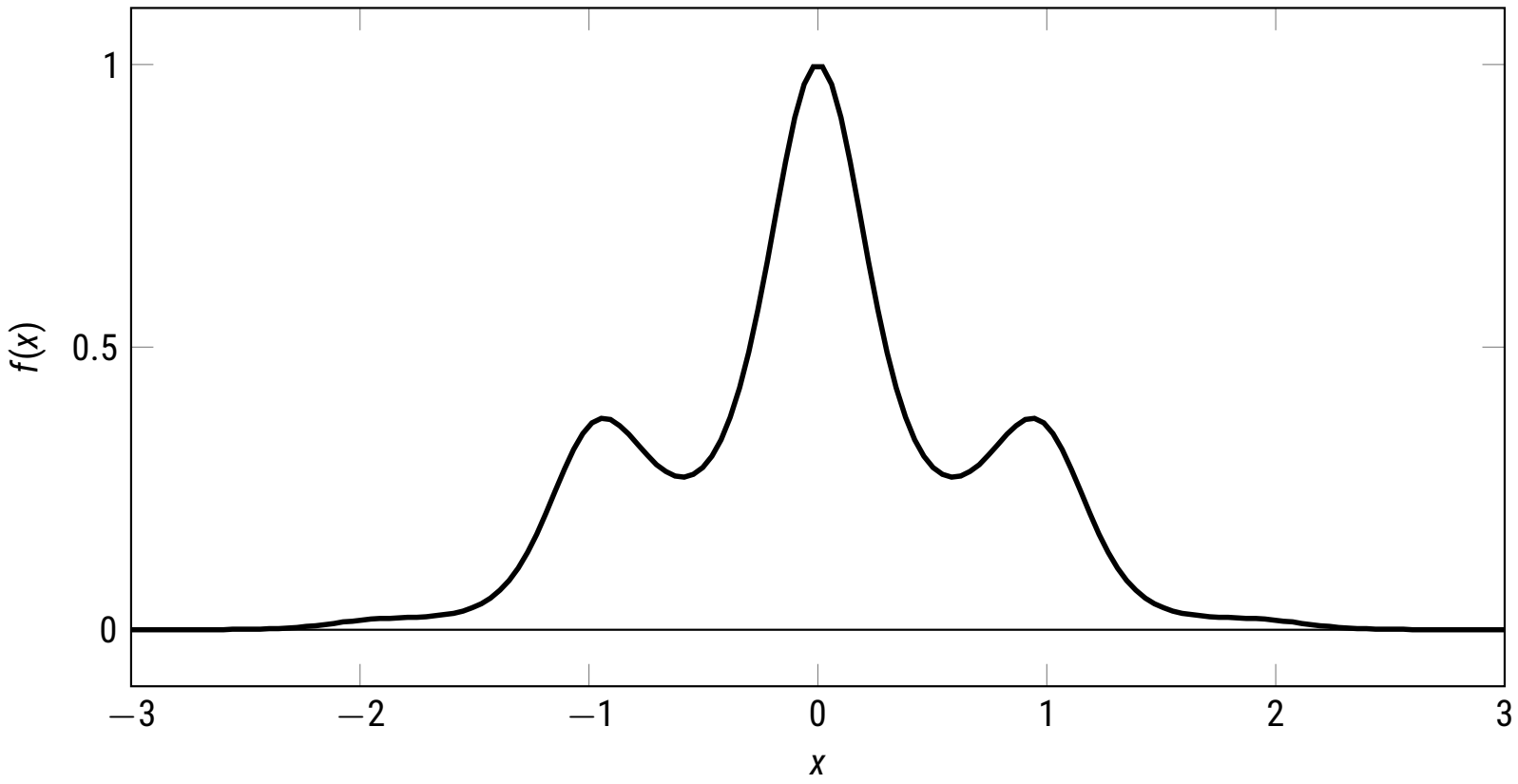
- Särkkä. **Bayesian Filtering and Smoothing**. Cambridge, 2013
- Rogers & Williams. **Diffusions, Markov Processes and Martingales** (Vols. I & II). Cambridge, 2000

coming up:

- our first **probabilistic numerical algorithm**

A Univariate Integration Problem

let's start slow



$$f(x) = \exp(-\sin(3x)^2 - x^2) \qquad G = \int_{-3}^{3} f(x)\,dx = ?$$

A Quadrature SDE

Phrasing Integration as Bayesian Inference

$$dz(x) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} z(x)\,dx + \begin{bmatrix} 0 \\ \theta \end{bmatrix} d\omega$$

- given initial value $z_2(x_0) = z_0, z_1(x_0) = 0$, this encodes $z_1(x) = \int_{x_0}^{x} z_2(\tilde{x})\,d\tilde{x}$
- thus can interpret

$$z(x) = \begin{bmatrix} \int_{x_0}^{x} \tilde{f}(\tilde{x})\,d\tilde{x} \\ \tilde{f}(x) \end{bmatrix}$$

- from Definition of SDE, with $\underline{x} := \min(x_a, x_b)$:

$$\begin{aligned} \operatorname{cov}(z(x_a), z(x_b)) &= \int_{x_0}^{\min(x_a,x_b)} \begin{bmatrix} 1 & (x_a - \tau) \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \theta \end{bmatrix} \begin{bmatrix} 0 & \theta \end{bmatrix} \begin{bmatrix} 1 & 0 \\ (x_b - \tau) & 1 \end{bmatrix} d\tau \\ &= \theta^2 \begin{bmatrix} x_a x_b(\underline{x} - x_0) - 1/2(x_a + x_b)(\underline{x}^2 - x_0^2) + 1/3(\underline{x}^3 - x_a^3) & \\ x_b(\underline{x} - x_0) - 1/2(\underline{x}^2 - x_0^2) & \underline{x} - x_0 \end{bmatrix} \end{aligned}$$

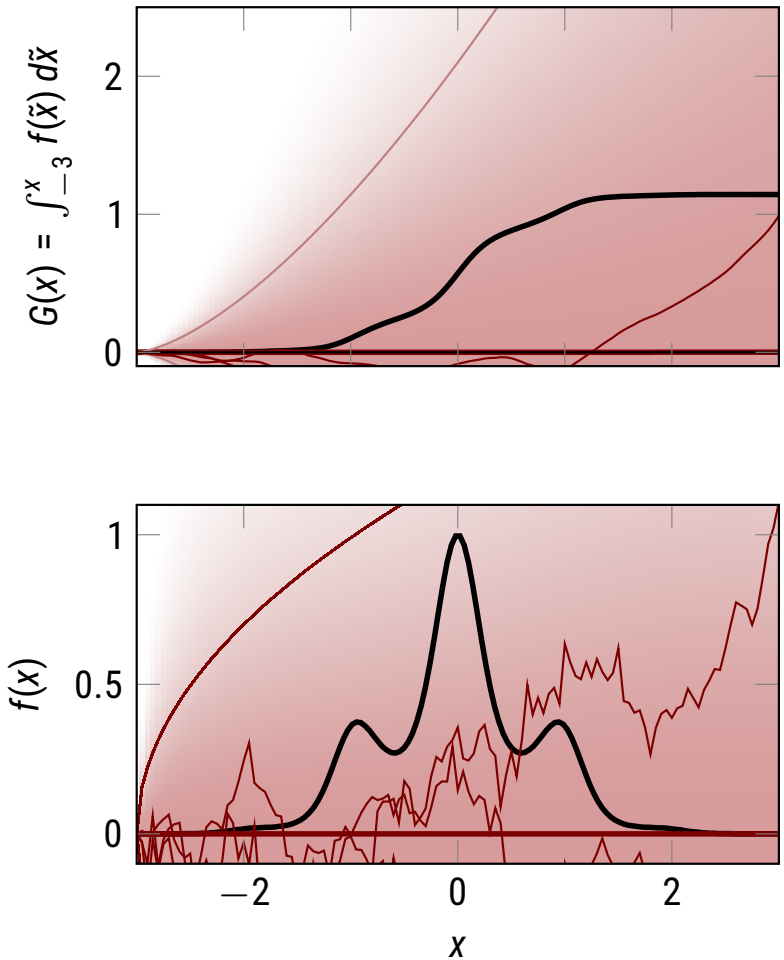
$\Rightarrow$ **Wiener process** prior $p(f) = \mathcal{GP}(0, \min(x_a, x_b))$

- filter parameters: $A(h) = \begin{bmatrix} 1 & h \\ 0 & 1 \end{bmatrix}$, $Q(h) = \begin{bmatrix} h^3/3 & h^2/2 \\ h^2/2 & h \end{bmatrix}$, $H = \begin{bmatrix} 0 & 1 \end{bmatrix}$, $R = 0$.

A Quadrature Filter

Bayesian inference need not be expensive

[cf. Diaconis, 1988]

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7          x ⇐ x + h  // move
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16     return m₁, P₁₁        // probabilistic estimate
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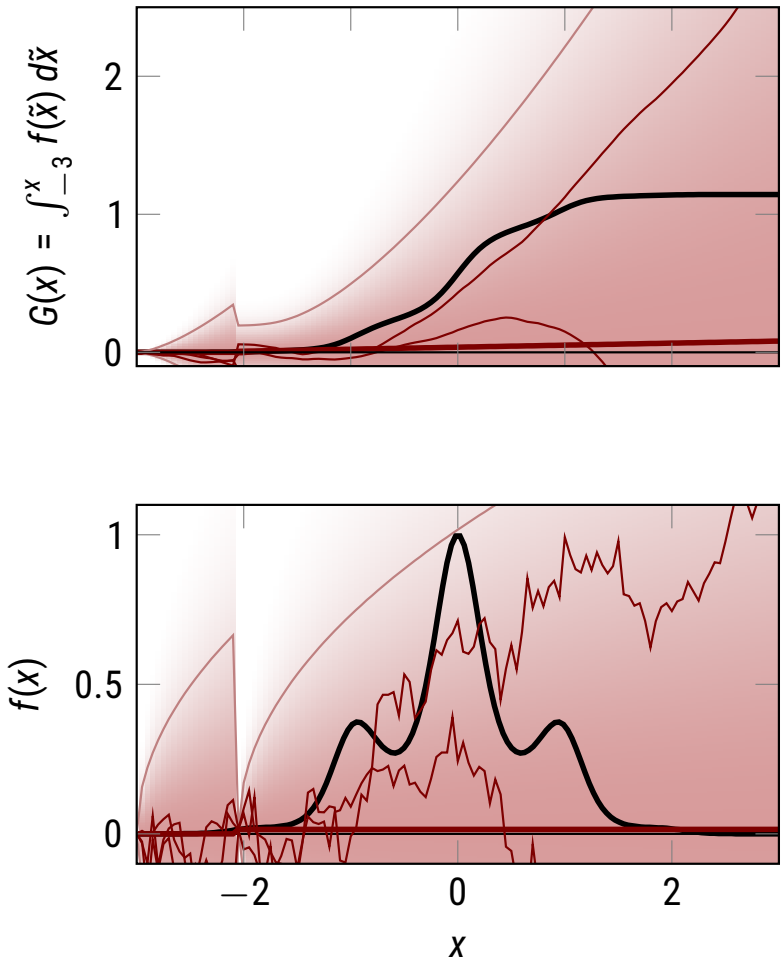


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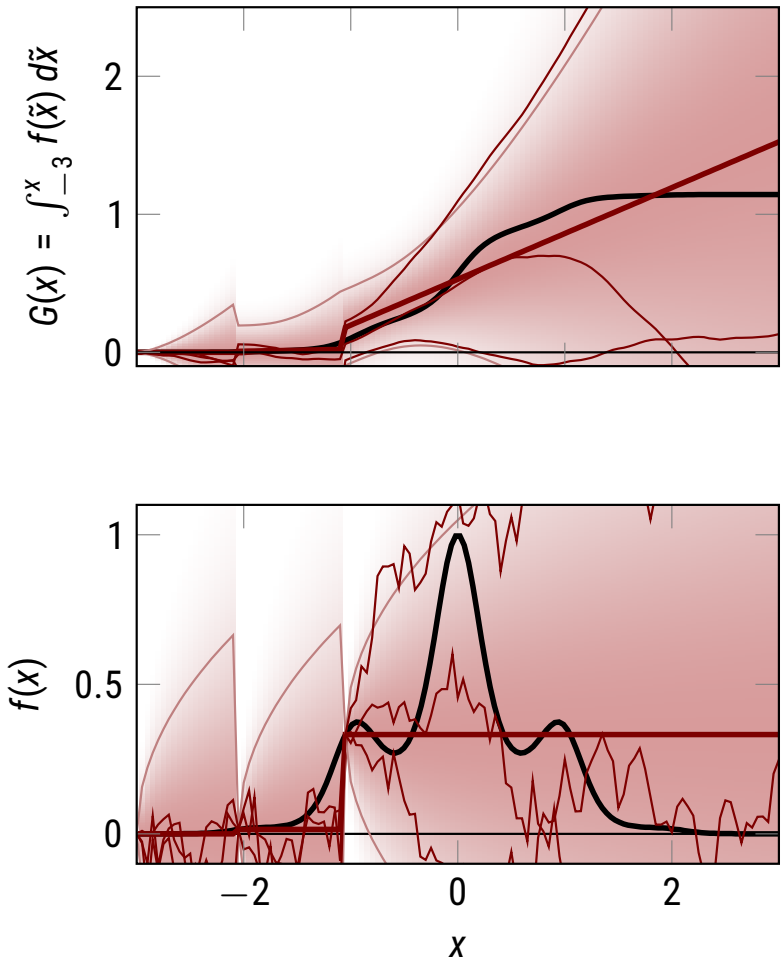


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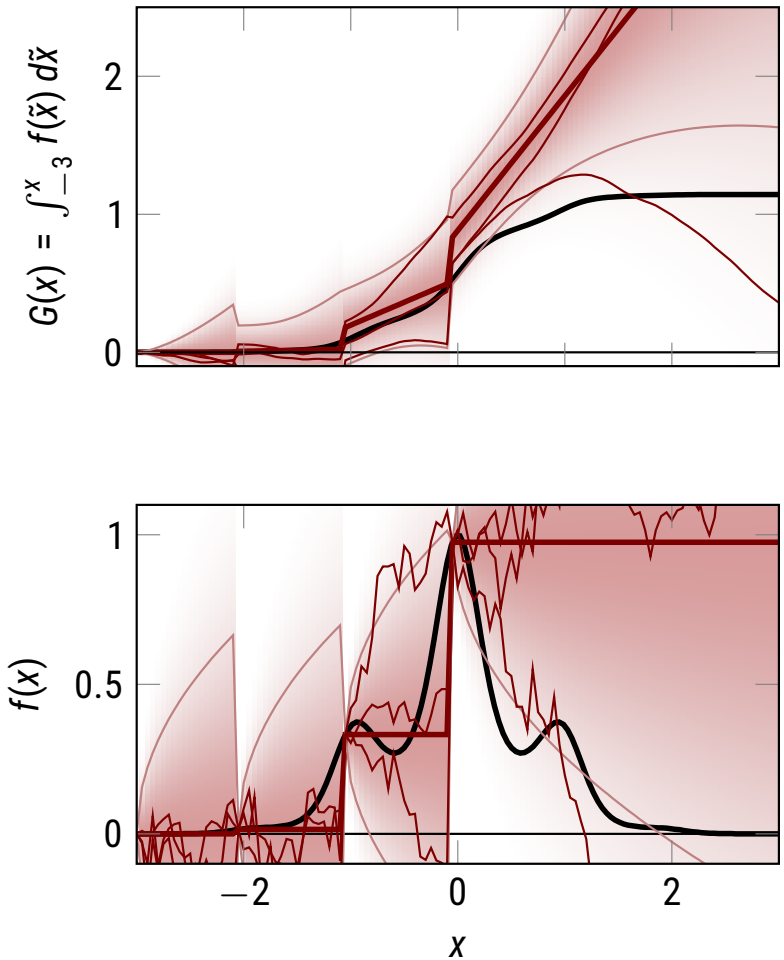


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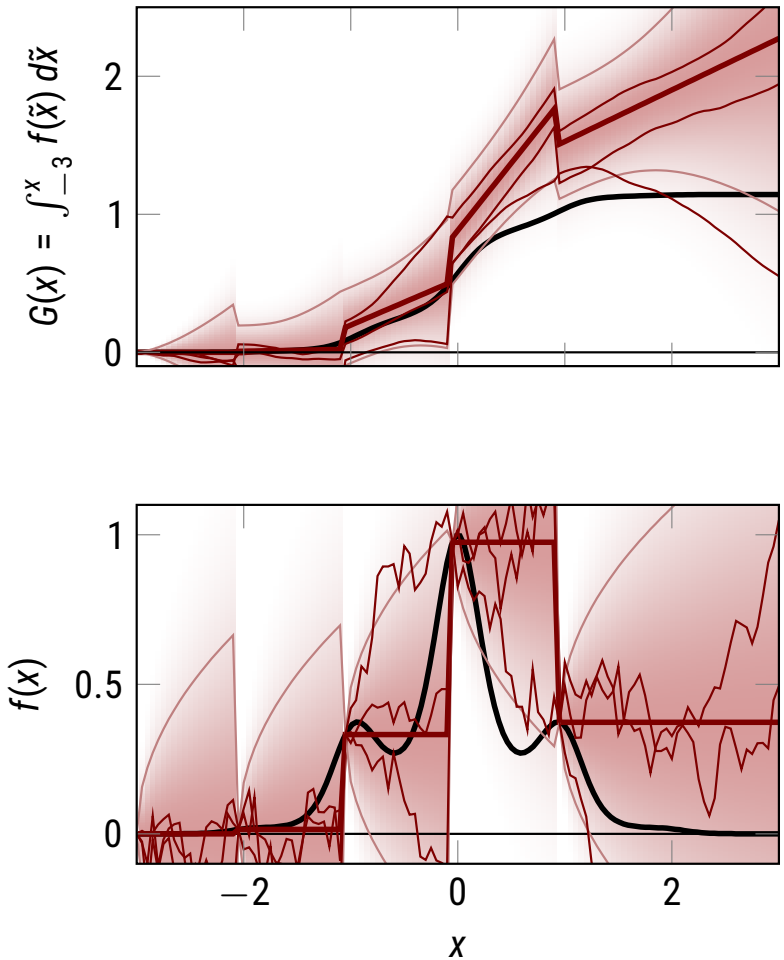


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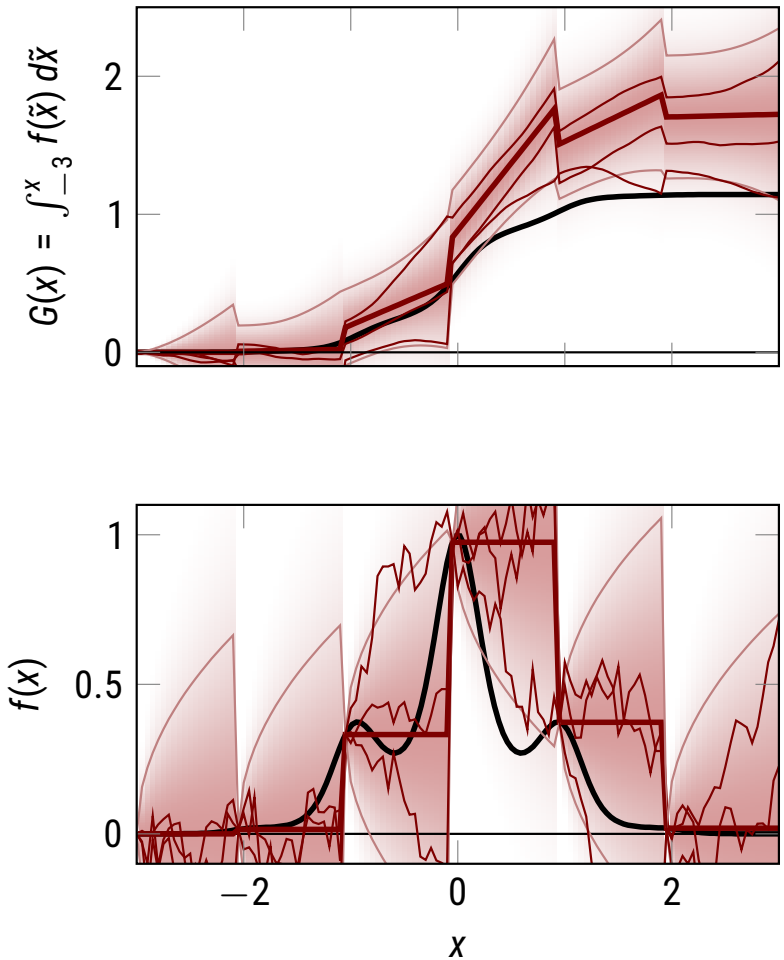


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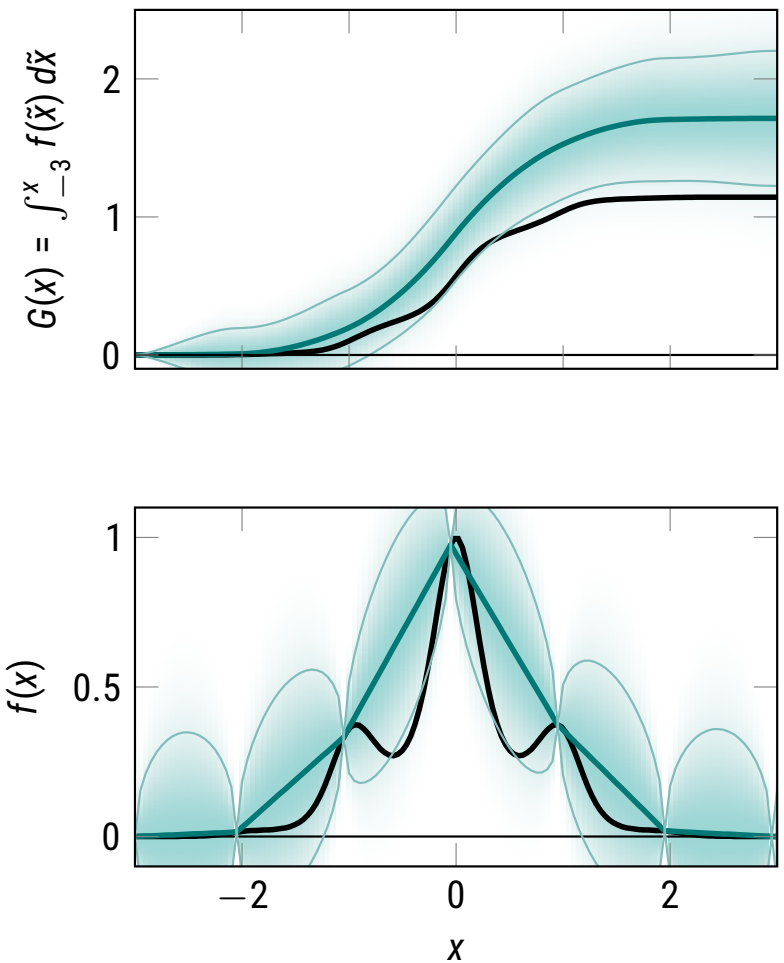


$$m_{i+1} = Am_i + \frac{(APA^\intercal + Q)H^\intercal}{H(APA^\intercal + Q)H^\intercal}(f(x_i) - HAm_i)$$

$$= \begin{bmatrix} [m_i]_1 + {}^{h}/_{2}(f(x_{i-1} + f(x_i)) \\ f(x_i) \end{bmatrix}$$

$$\Rightarrow \quad \mathbb{E}[G] = [m_N]_1 = \sum_{i=1}^{N-1} {}^{h_i}/_{2}(f(x_{i+1}) + f(x_i))$$

$$P_{i+1} = (I - KH)(APA^\intercal + Q)$$

$$= \begin{bmatrix} [P_i]_{11} + {}^{\theta^2}/_{12} \cdot h^3 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Rightarrow \quad \mathrm{var}[G] = [P_N]_{11} = \frac{\theta^2}{12} \sum_{i=1}^{N} h_i^3$$

$$\Rightarrow \quad h_i = \underset{\tilde{\mathbf{h}}, \sum_i \tilde{h}_i = (b-a)}{\arg\min} \mathrm{var}[G] = (b-a)/N$$

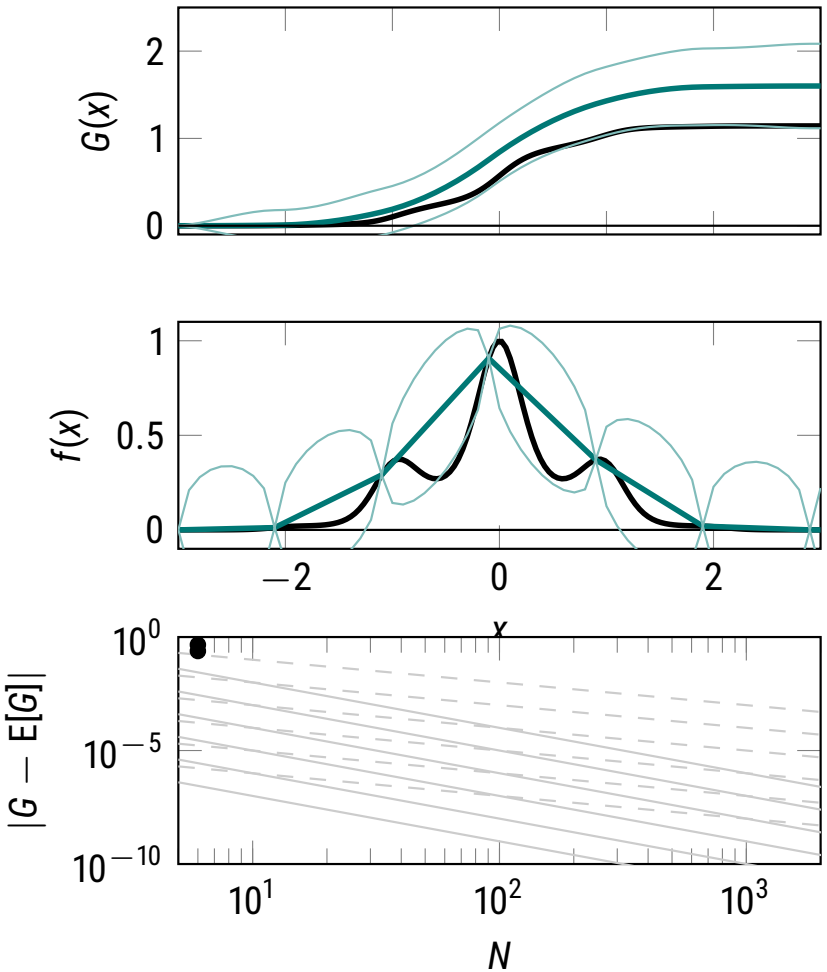
$$\Rightarrow \quad \mathrm{var}[G] = \frac{\theta^2}{12} \frac{x_N - x_0}{N^2}$$

Trapezoidal rule is **MAP** estimate arising under a **Wiener process** prior on f.
Regular grid arises as minimum entropy (most informative) choice.

Convergence

classic asymptotic analysis

[cf. Davis & Rabinowitz, 1984, pp. 52–54]



Let $w(\delta) = \max_{|x_1 - x_2| \leq \delta} |f(x_2) - f(x_1)|$, for $a < x_1, x_2 < b$, the **modulus of continuity**.

Theorem [Davis & Rabinowitz, p. 52]

Let $f(x)$ be continuous in $[a, b]$. Then

$$|G - \mathrm{E}[G]| \leq (b - a) w\left(\frac{b - a}{N}\right).$$

Theorem [Davis & Rabinowitz, p. 54]

Let $f(x) \in \mathcal{C}^2[a, b]$. Then $\exists \xi \in (a, b)$, so that

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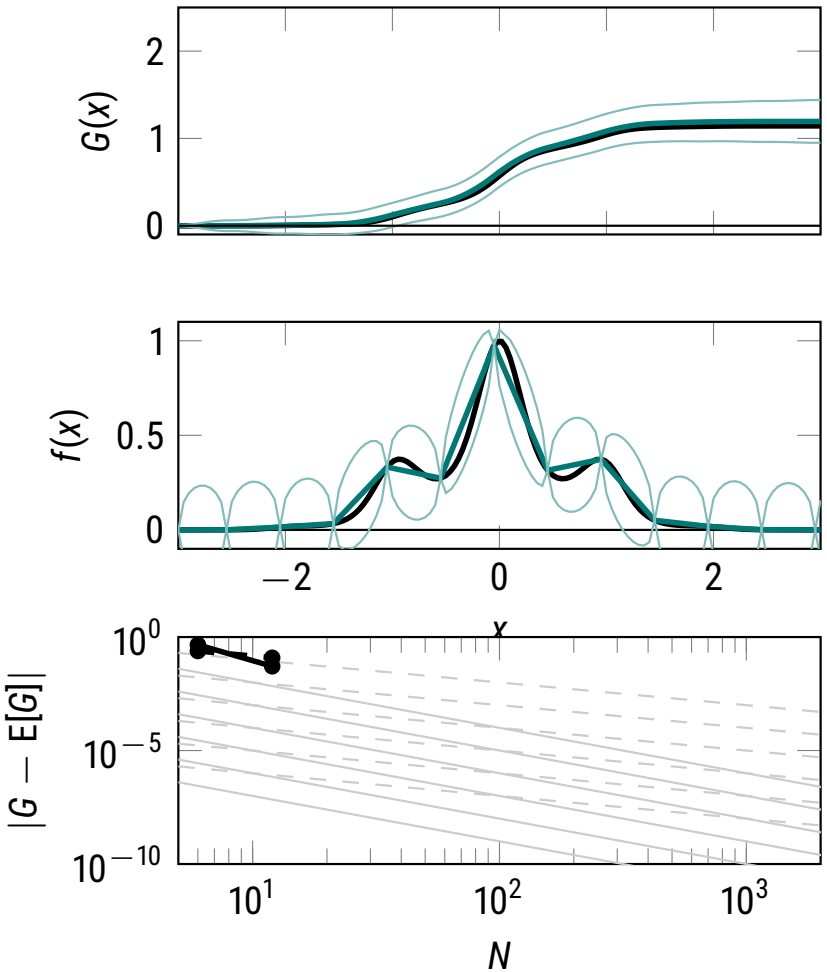

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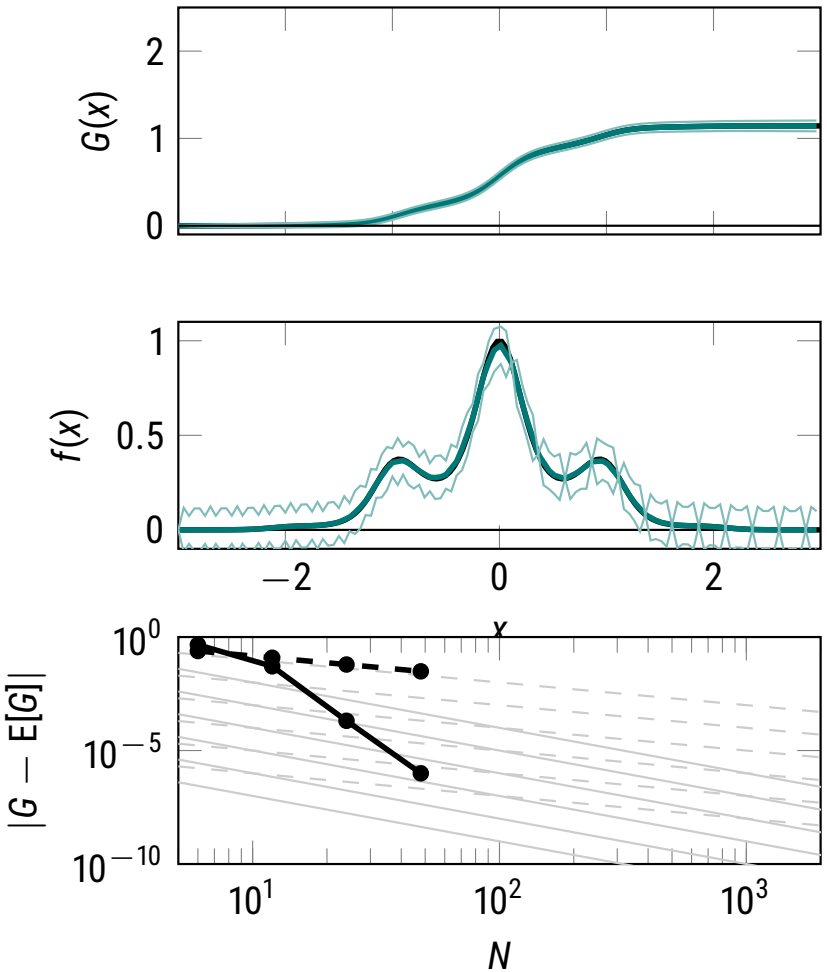

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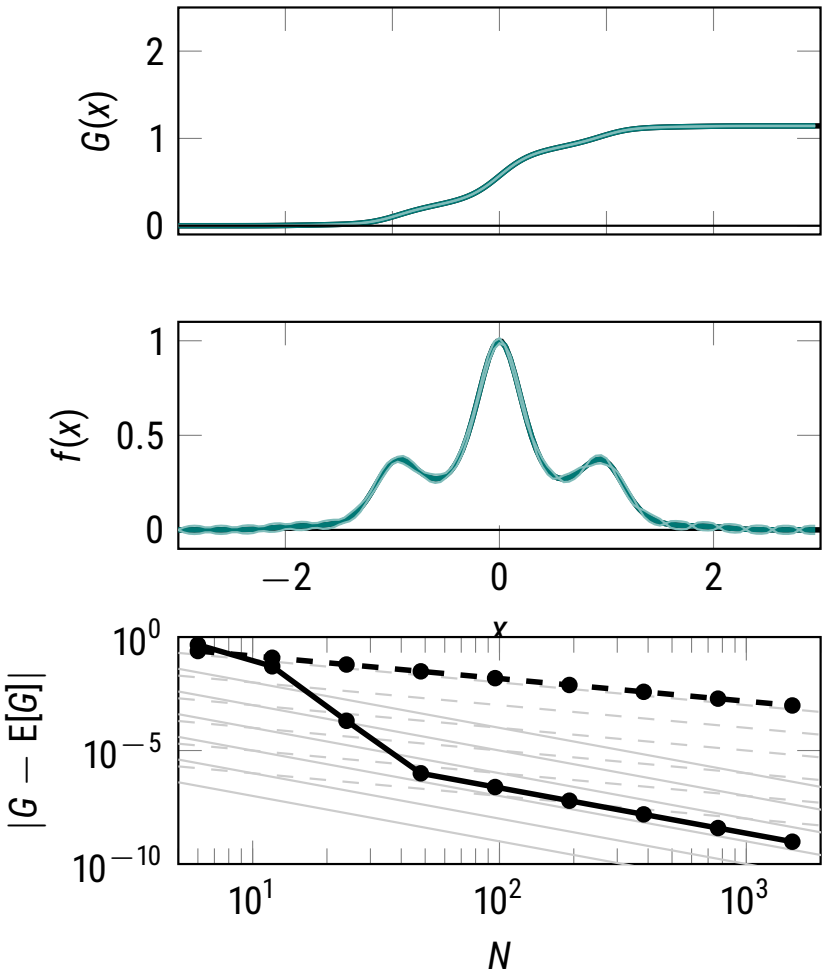

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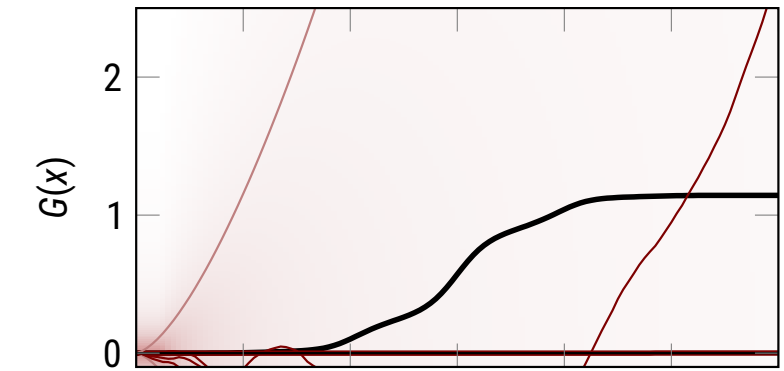
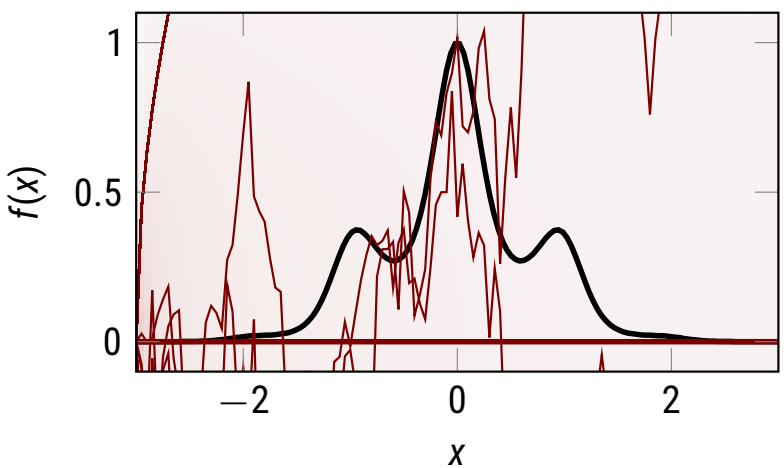
Error Estimation

a rare case of exact hyperparameter inference





- recall $p(y \mid \theta) = \int p(y, f \mid \theta)\, df = \mathcal{N}(y; m_X, k_{XX})$
- consider Gamma **conjugate prior**

$$p(\theta^{-2}) = \mathcal{G}(\theta^{-2}; \alpha_0, \beta_0) = \frac{\beta_0^{\alpha_0}}{\Gamma(\alpha_0)} (\theta^{-2})^{\alpha_0 - 1} e^{-\beta_0 \theta^{-2}}$$

$$\begin{aligned} p(\theta \mid y) &= p(y \mid \theta) p(\theta) \\ &= \mathcal{G}(\theta^{-2}, \alpha_N := \alpha_0 + N/2, \\ &\qquad \beta_N := \beta_0 + 1/2 (y - \mu_X)^\intercal k_{XX}^{-1} (y - \mu_X)) \end{aligned}$$

- **Student-*t*** marginal. var: $\beta_N / (\alpha_N - 1)$

$$\begin{aligned} p(f_x \mid y) &= \int p(f \mid y, \theta^{-2}) p(\theta^{-2} \mid y)\, d\theta^{-2} \\ &= \mathrm{St}(f; \mu_y, \alpha_N, \beta_N \mathbb{V}_y) \\ &=: \frac{\Gamma(\alpha_N + 1/2)}{\Gamma(\alpha_N)(2\pi\beta_N \mathbb{V}_y)^{1/2}} \left(1 + \frac{(f_x - \mu_y)^2}{2\beta_N \mathbb{V}_y}\right)^{-\alpha_N - 1/2} \end{aligned}$$

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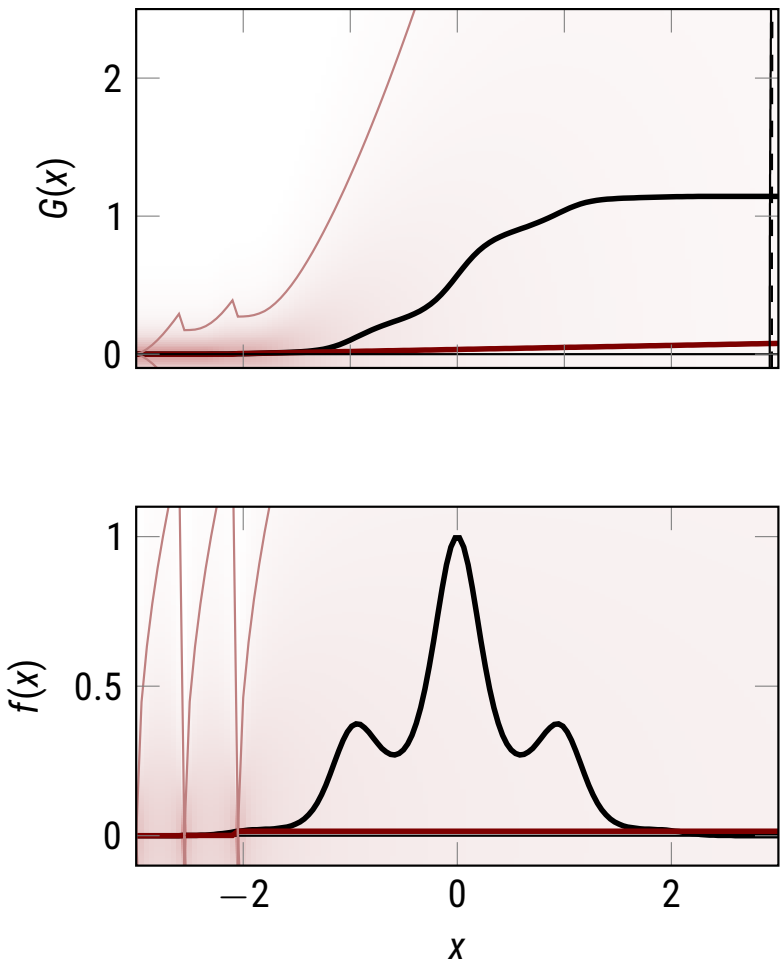

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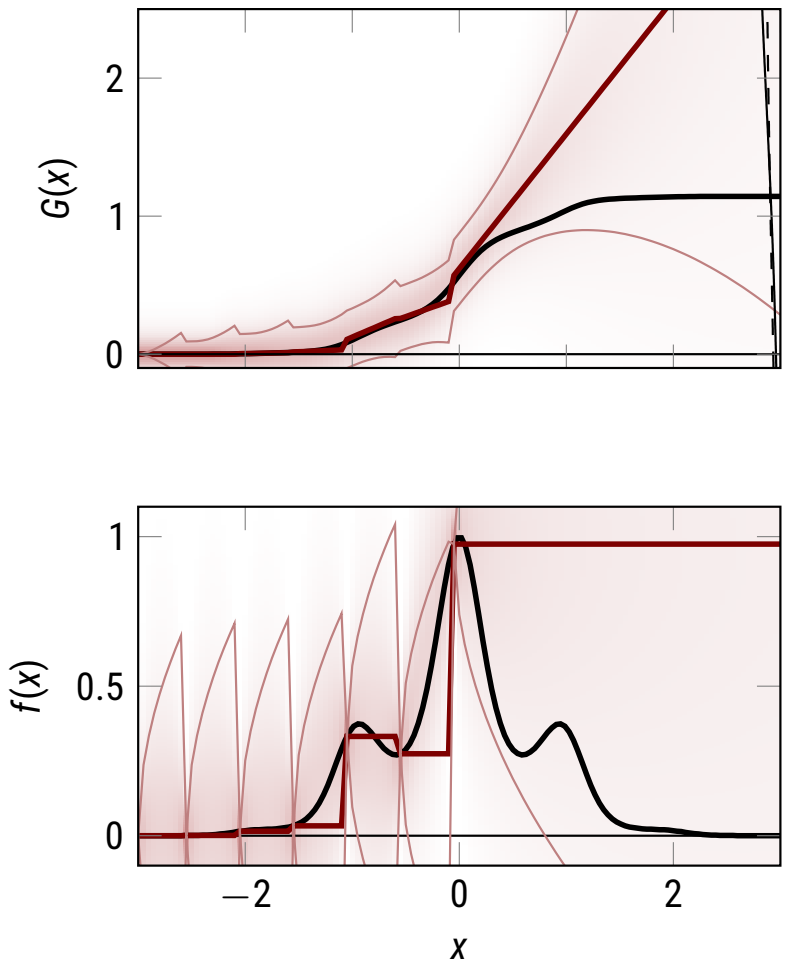

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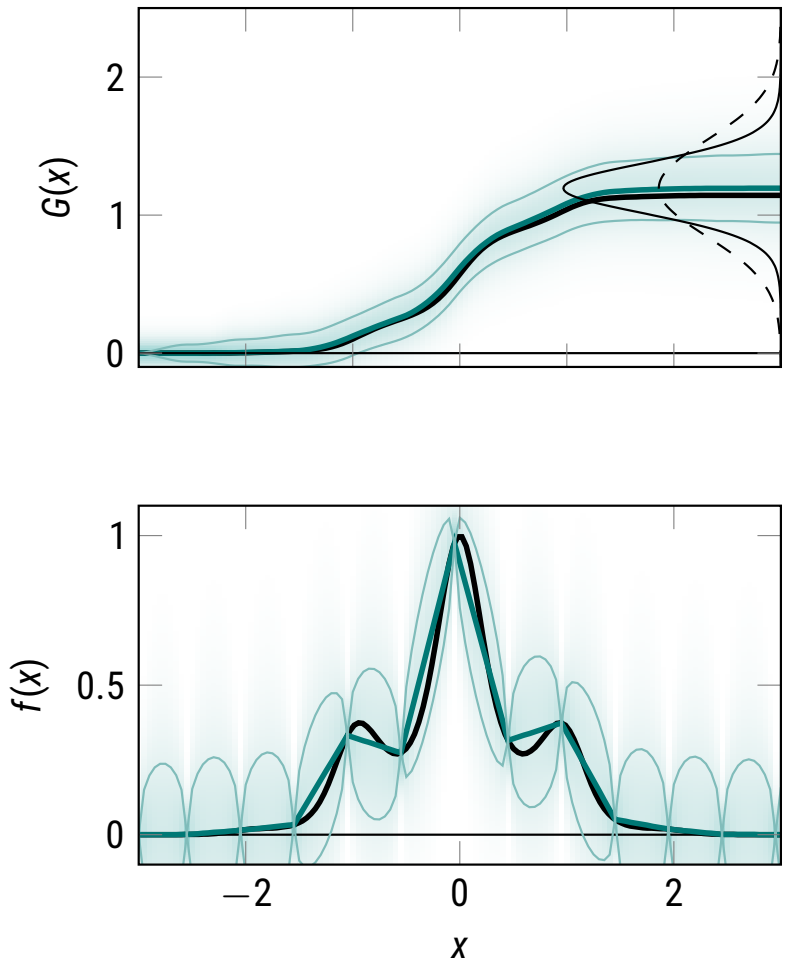
$$\begin{aligned} p(\theta \mid y) &= p(y \mid \theta) p(\theta) \\ &= \mathcal{G}(\theta^{-2}, \alpha_N := \alpha_0 + N/2, \\ &\qquad \beta_N := \beta_0 + 1/2 (y - \mu_X)^\intercal k_{XX}^{-1} (y - \mu_X)) \end{aligned}$$

- **Student-*t*** marginal. var: $\beta_N / (\alpha_N - 1)$

$$\begin{aligned} p(f_x \mid y) &= \int p(f \mid y, \theta^{-2}) p(\theta^{-2} \mid y)\, d\theta^{-2} \\ &= \mathrm{St}(f; \mu_y, \alpha_N, \beta_N \mathbb{V}_y) \\ &=: \frac{\Gamma(\alpha_N + 1/2)}{\Gamma(\alpha_N)(2\pi \beta_N \mathbb{V}_y)^{1/2}} \left(1 + \frac{(f_x - \mu_y)^2}{2\beta_N \mathbb{V}_y}\right)^{-\alpha_N - 1/2} \end{aligned}$$

Error Estimation

a rare case of exact hyperparameter inference



- for filter: use **prediction-error decomposition** ($\tilde{P} = P/\theta^2$)

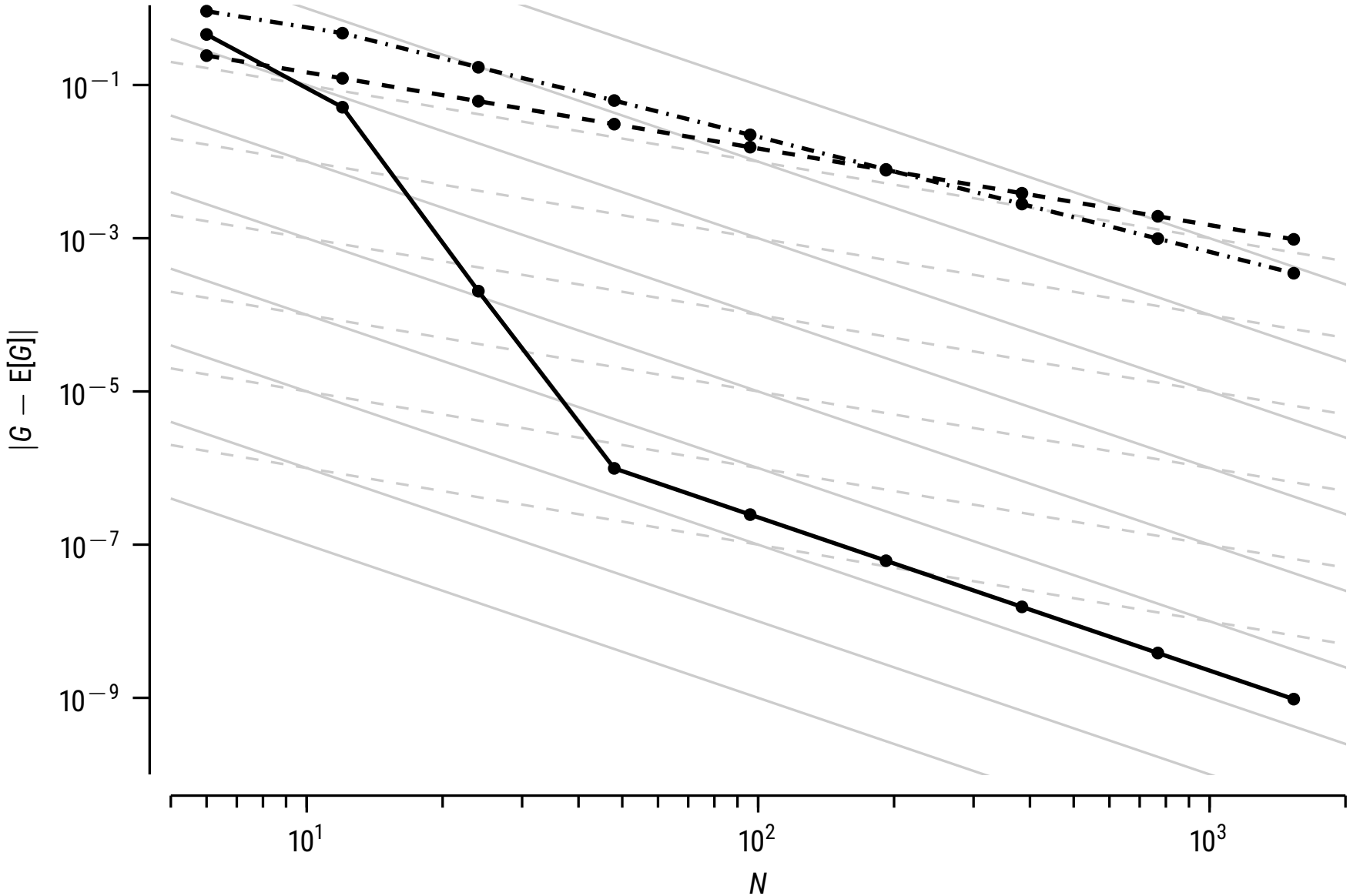
$$p(y \mid \theta) = \prod_{i=1}^{N} p(y_i \mid y_{1:i-1}, \theta)$$

$$= \prod_{i} \mathcal{N}(y_i; Hm_i^-, \theta^2 H\tilde{P}^- H)$$

```
1  procedure INTEGRATE(@f, a, b, N)
2      x ⇐ a, m ⇐ [0; f(a)], P ⇐ [0, 0; 0, 0]
3      β ⇐ 0
4      for i = 1, ..., N − 1 do
5          x ⇐ x + (b − a)/N
6          m⁻ = Am
7          P⁻ = APAᵀ + Q
8          y = f(x) − Hm⁻
9          S = HP⁻Hᵀ
10         β ⇐ β + y²/(2s)
11         K = P⁻Hᵀ/S
12         m ⇐ m⁻ + Ky
13         P ⇐ (I − KH)P⁻
14     end for
15     return m₁, β/(α−1) P₁₁        // calibrated estimate
16 end procedure
```

Error Estimation

it's tricky to fix a broken prior, though



Higher Order Filters

spline quadrature rules as MAP estimation

for more, see Schober et al. 2017; Kersting et al. 2017

$$dz(x) = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \vdots \\ \vdots & & \ddots & \ddots & 0 \\ \vdots & & & \ddots & 1 \\ 0 & \cdots & & 0 & 0 \end{bmatrix} z(x)\,dx + \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ \theta \end{bmatrix} d\omega \qquad z(x) = \begin{bmatrix} \int_{x_0}^{x} \tilde{f}(\tilde{x})\,d\tilde{x} \\ \tilde{f}(x) \\ \tilde{f}'(x) \\ \vdots \\ \tilde{f}^{q}(x) \end{bmatrix}$$

This gives q-th order **spline interpolants** as means, and

$$[A(h)]_{ij} = [\exp(Fh)]_{ij} = \mathbb{I}(j \geq i)\frac{h^{j-i}}{(j-i)!}$$

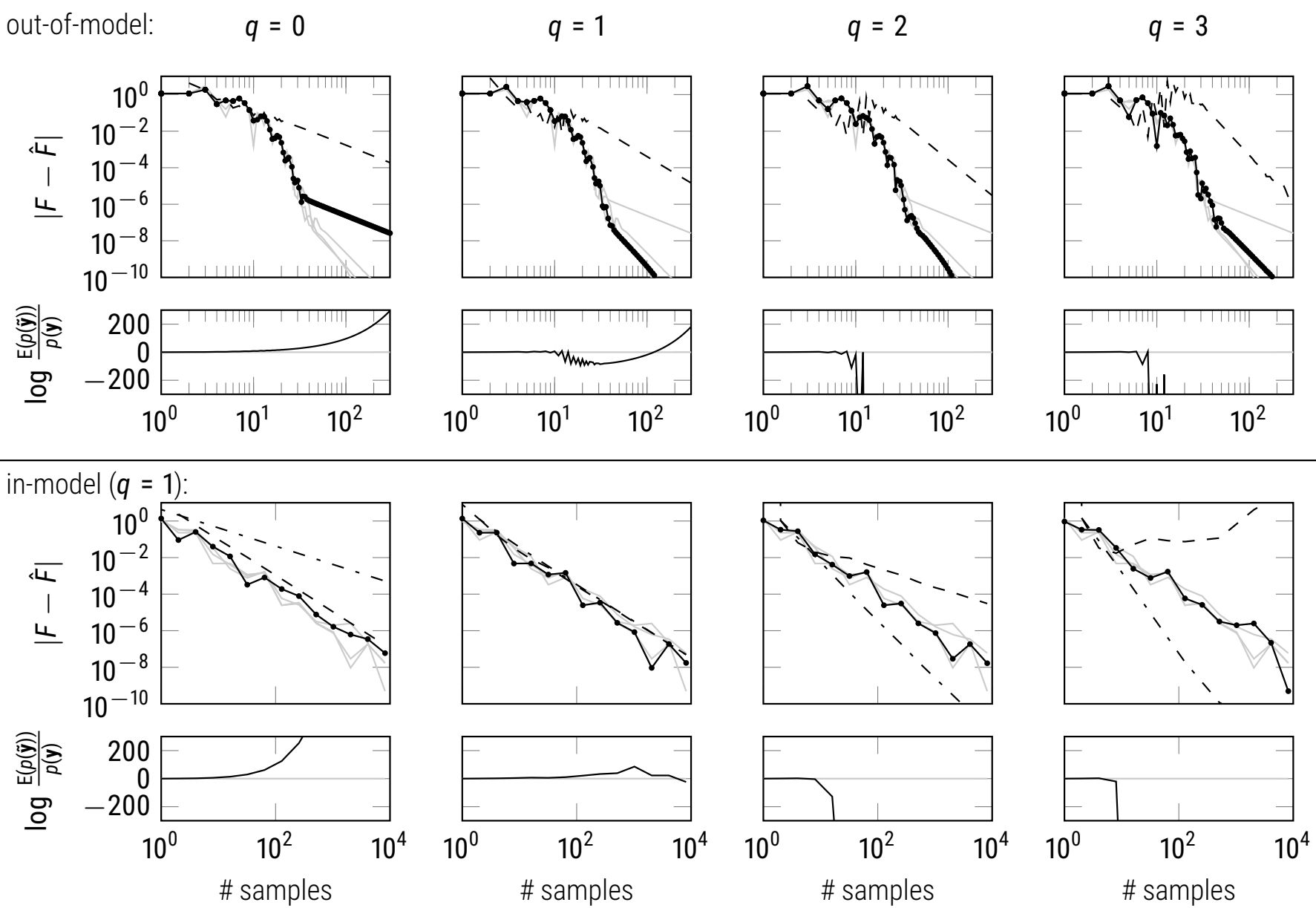
$$[Q(h)]_{ij} = \theta^2 \frac{h^{2q+3-i-j}}{(2q+3-i-j)(q+1-i)!(q+1-j)!}$$

same filter as before (using $[H]_i = \delta_{2i}$)!

Higher Order Filters

polynomial spline quadrature

[cf. Davis & Rabinowitz, 1984, §2.5]



Our first probabilistic numerical method

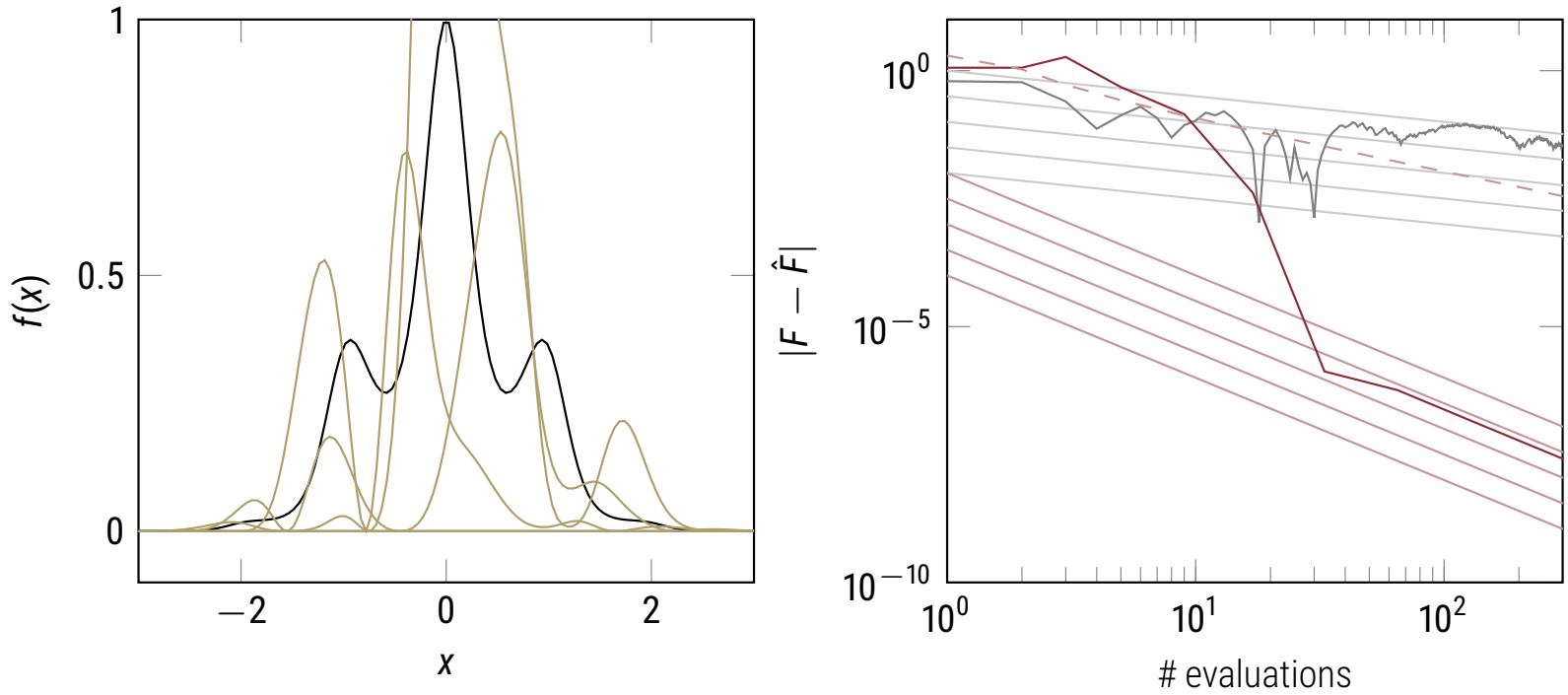
- the **trapezoid rule** arises as the **MAP estimate** under a Wiener process prior on the integrant
- the posterior variance can serve as a conservative notion of **uncertainty**
- hierarchical probabilistic inference gives an adaptive, quantitative **error estimate**
- **regular grids** emerge naturally from an information theoretic perspective.

Some “philosophical” observations:

- no random numbers! probabilistic numerics ≠ stochastic numerics
- **Gaussian measures** provide a very limited notion of uncertainty.
  But they work, and they are **fast**!
- this is basically just a new interpretation of a classic algorithm. But it shows PN methods **exist**, they can be as **fast** as classic methods and satisfy classic convergence requirements

Why? — Example: informative priors

WArped Sequential Active Bayesian Integration (WSABI) [Gunter, Osborne, Garnett, Hennig, Roberts. NIPS 2014]



a prior specifically for integration of probability measures

- $f > 0$ (f is probability measure)
- $f \propto \exp(-x^2)$ (f is product of prior and likelihood terms)
- $f \in \mathcal{C}^{\infty}$ (f is smooth)

Explicit prior knowledge yields reduces complexity.

[cf. **information-based complexity**. E.g. Novak, 1988. Clancy et al. 2013, arXiv 1303.2412v2]

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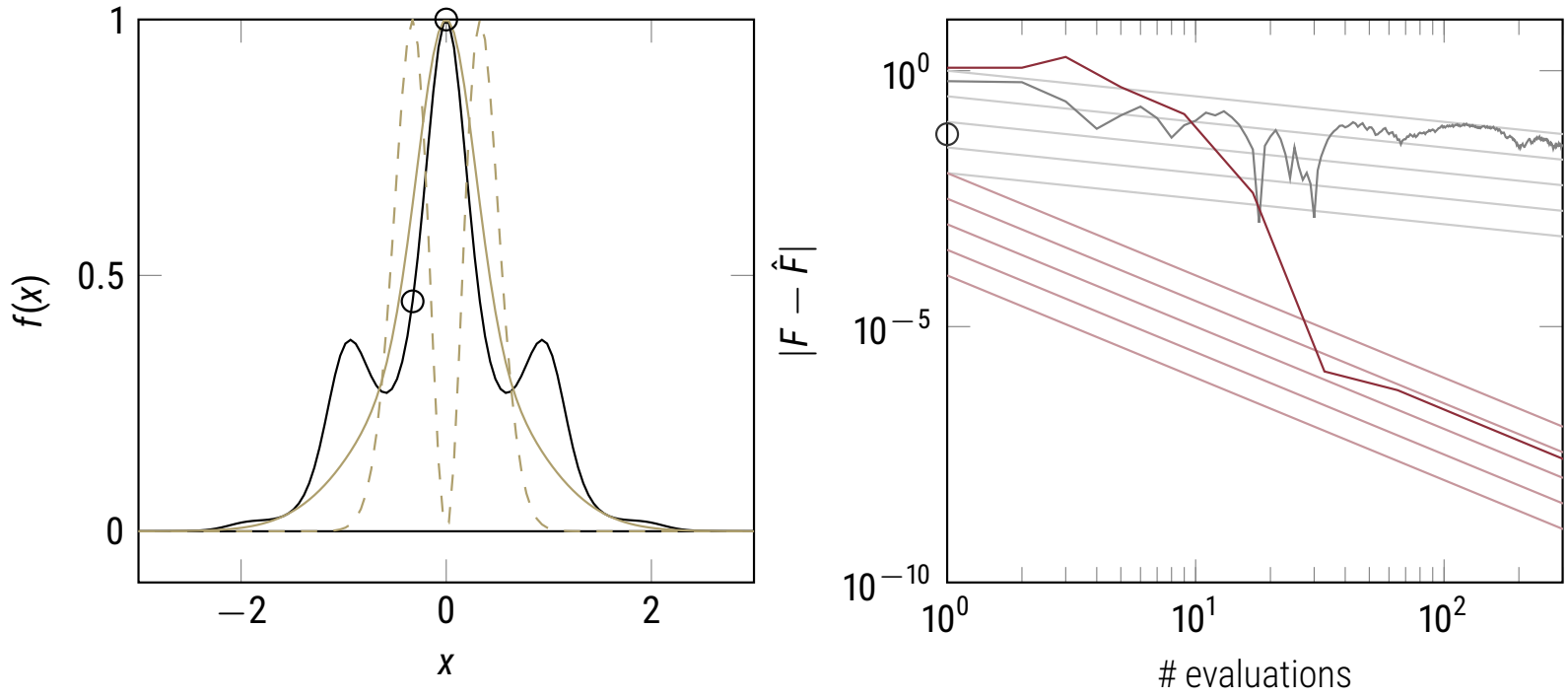

- adaptive node placement
- scales to, in principle, arbitrary dimensions
- faster (in wall-clock time) than MCMC

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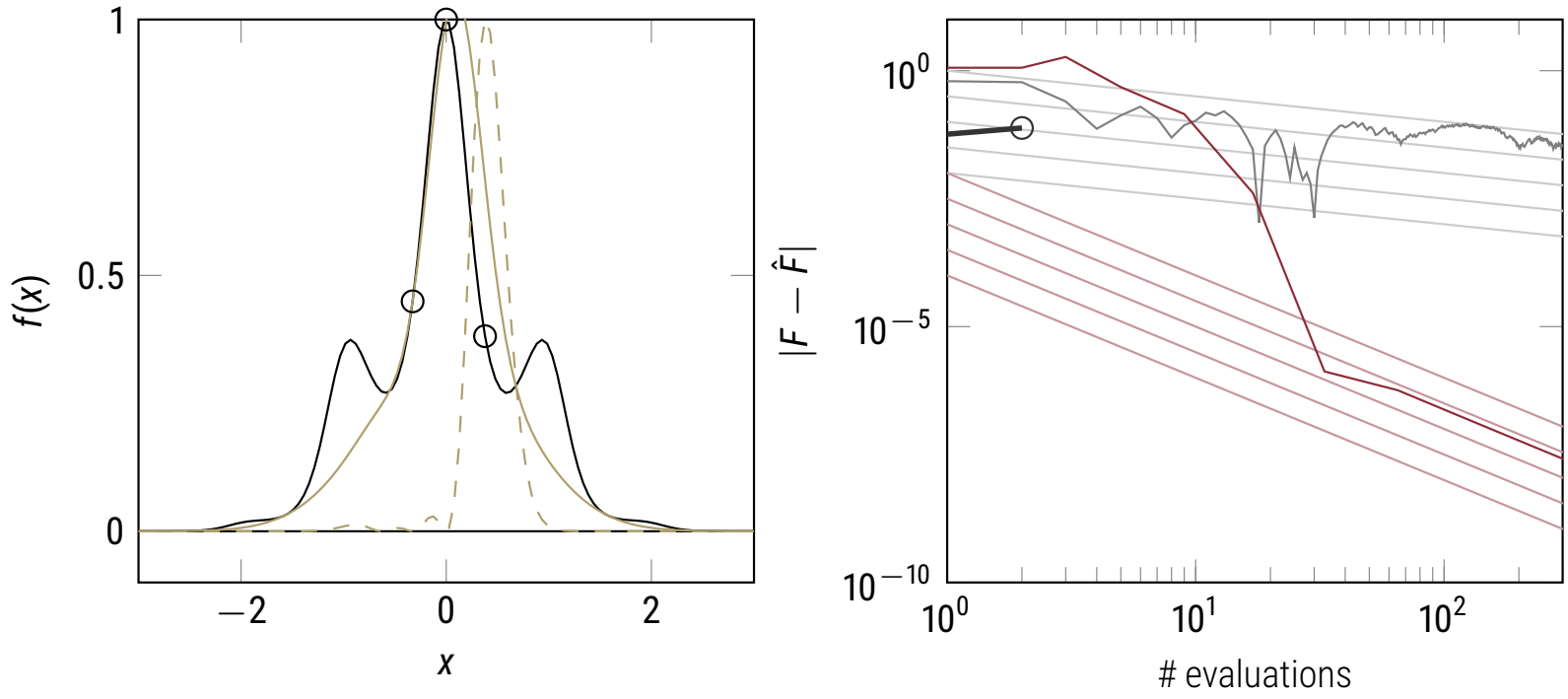

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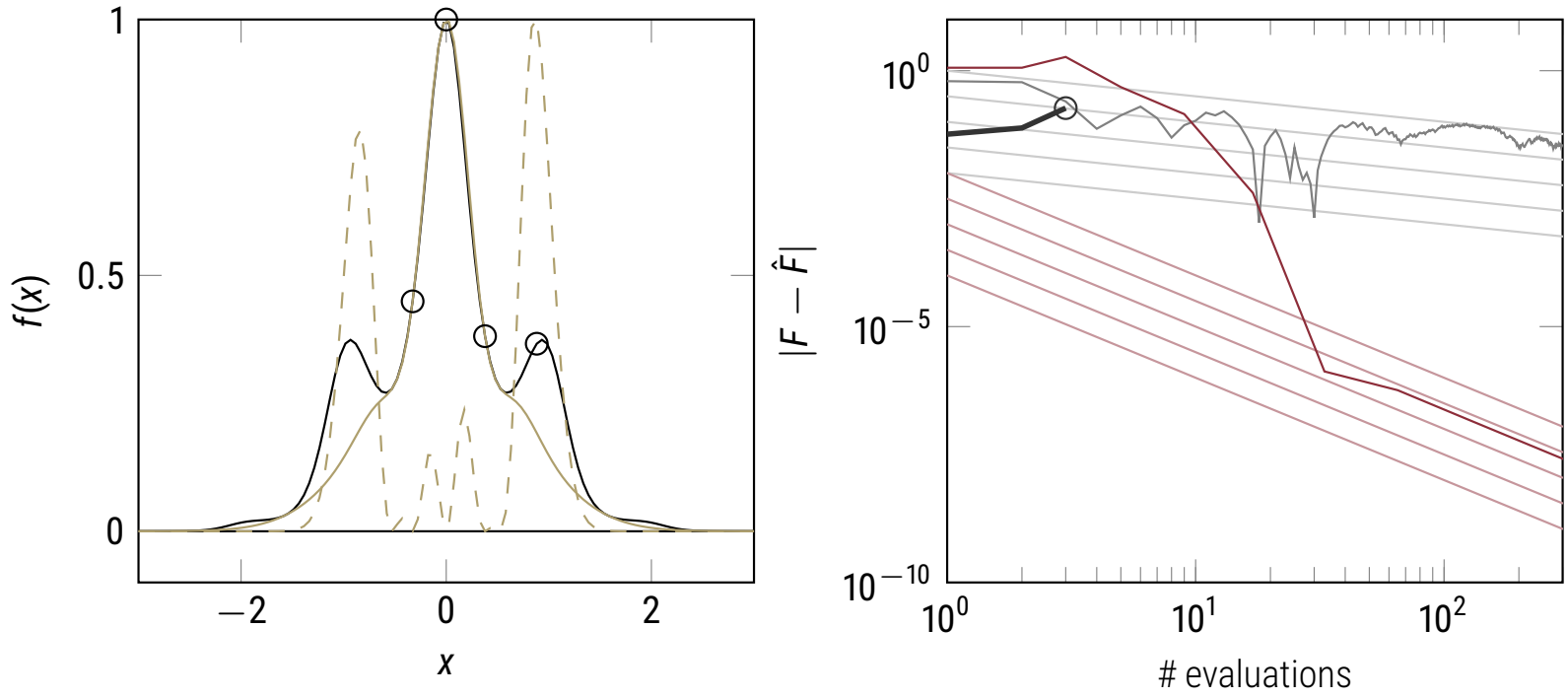

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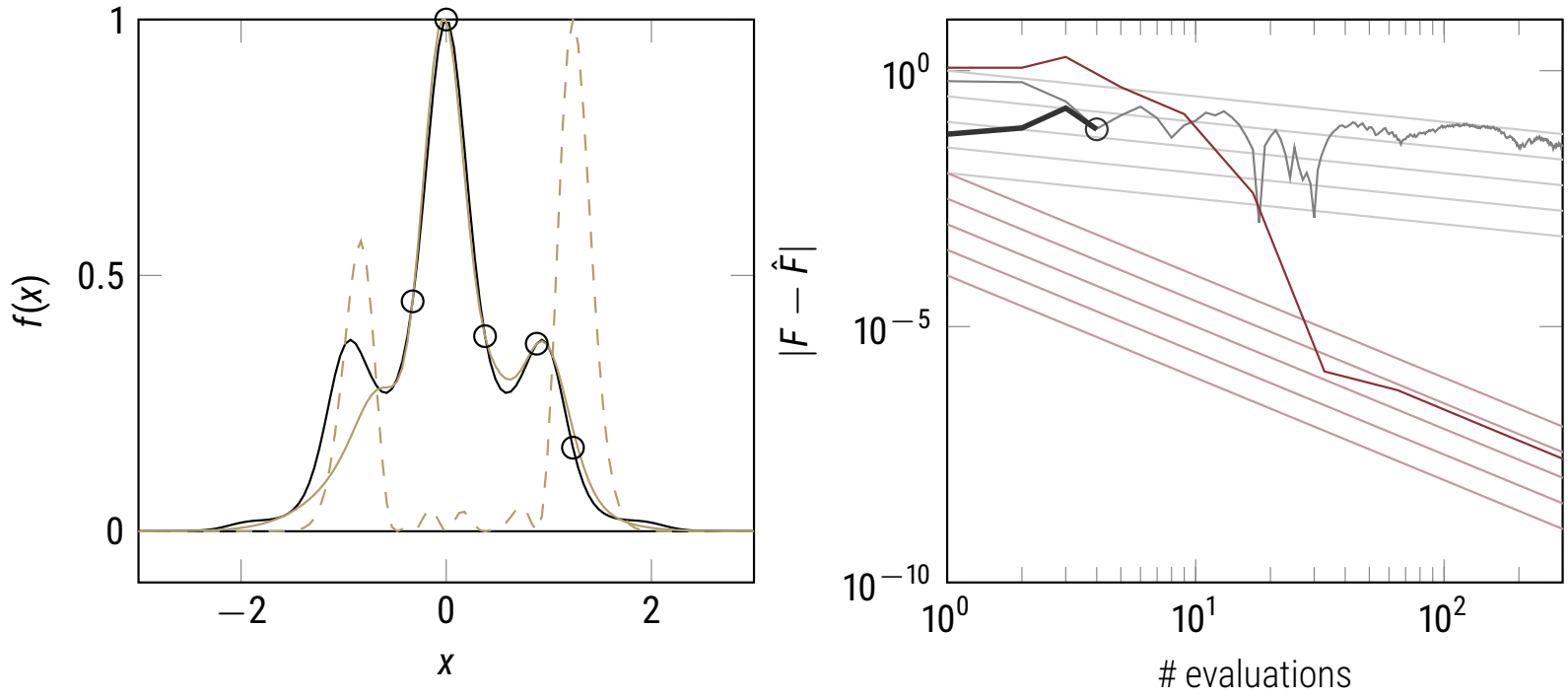

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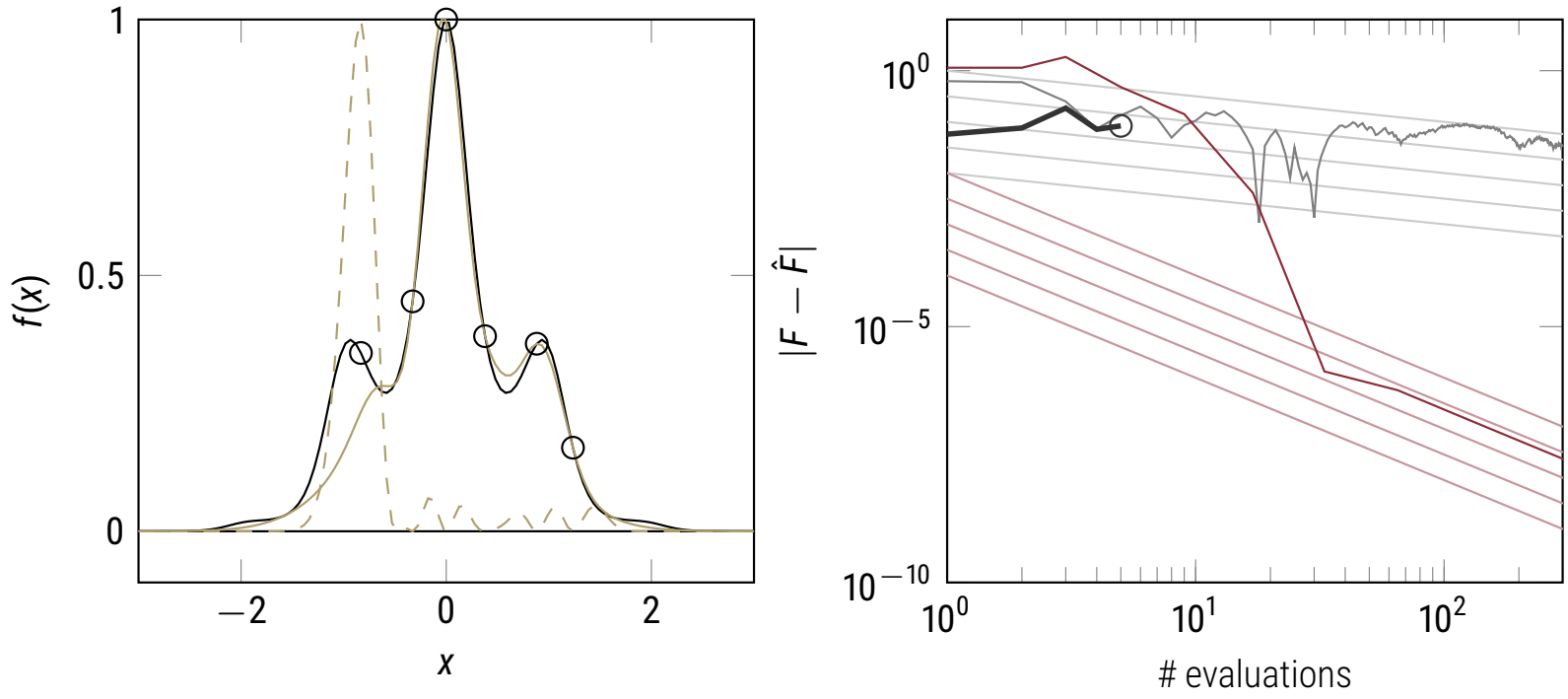

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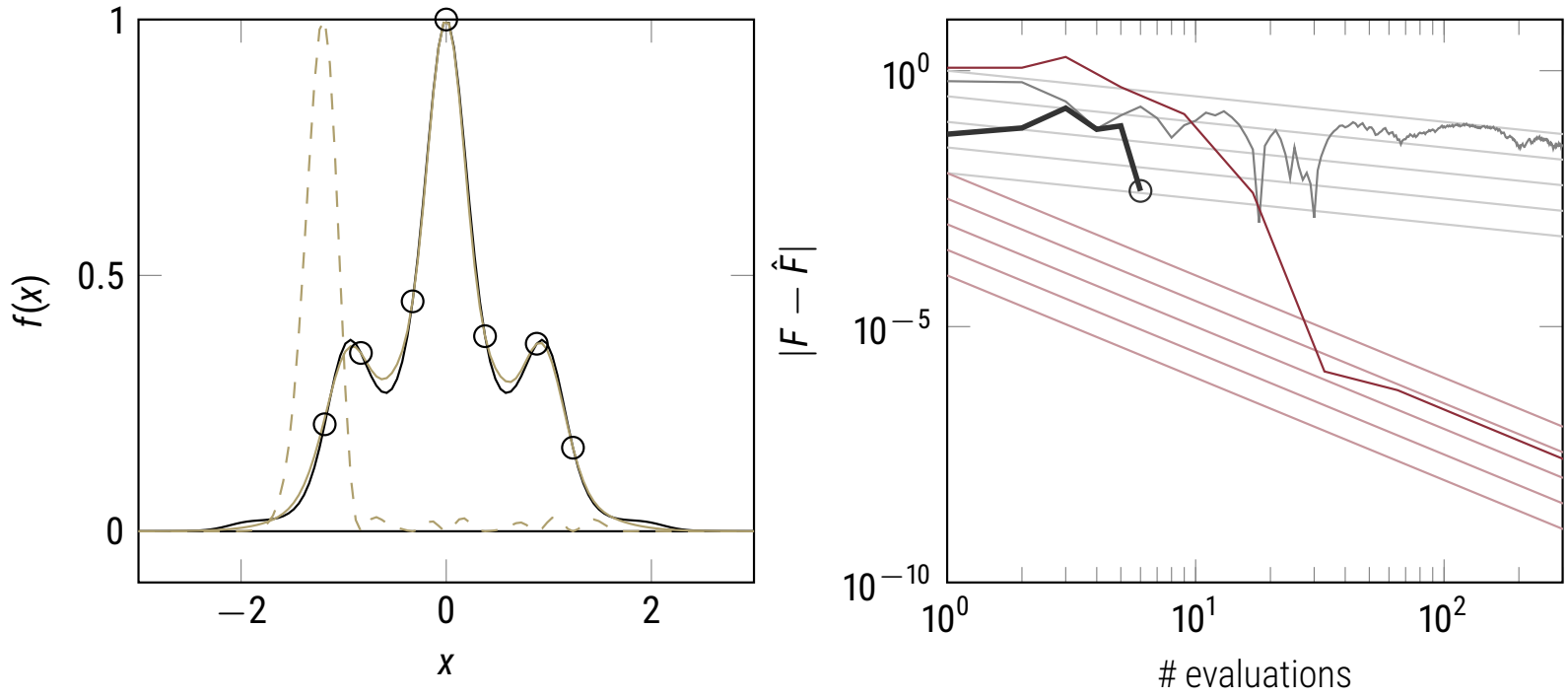

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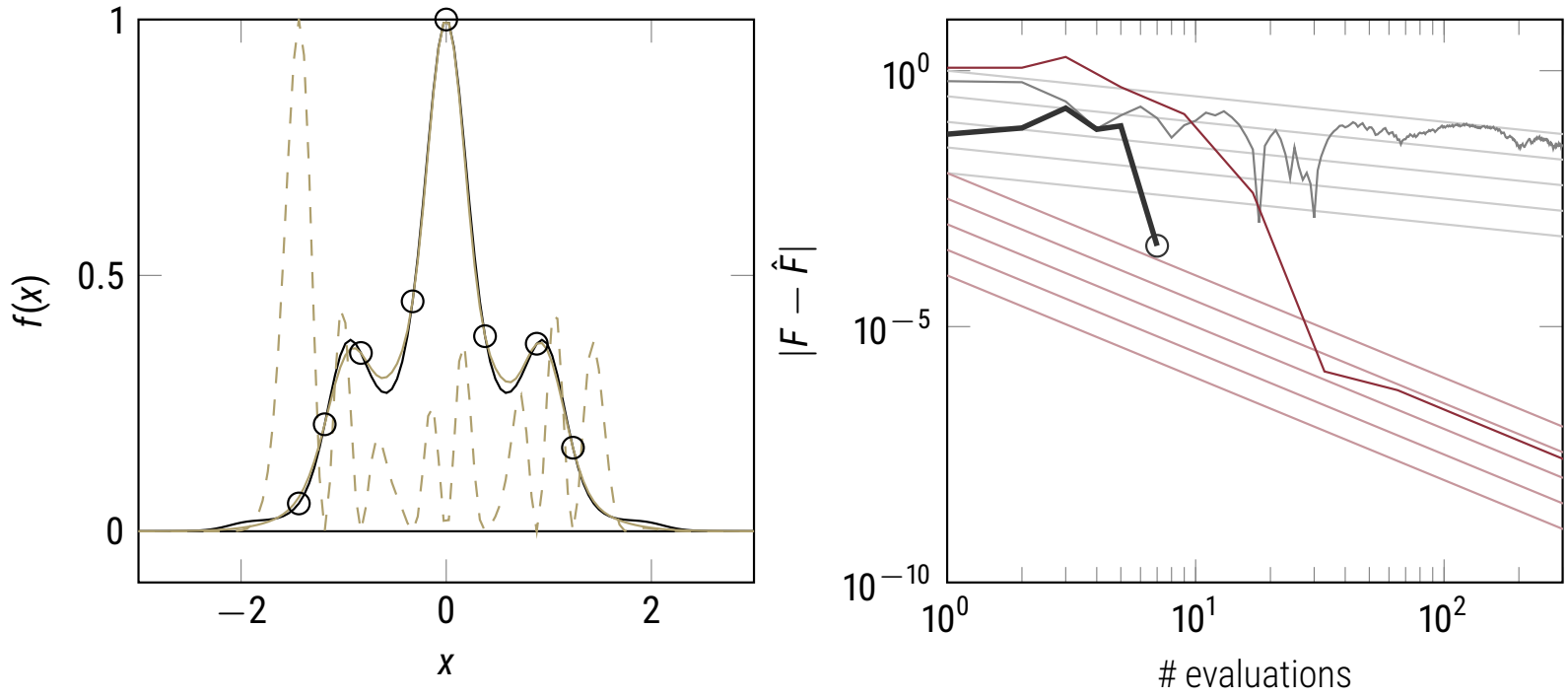

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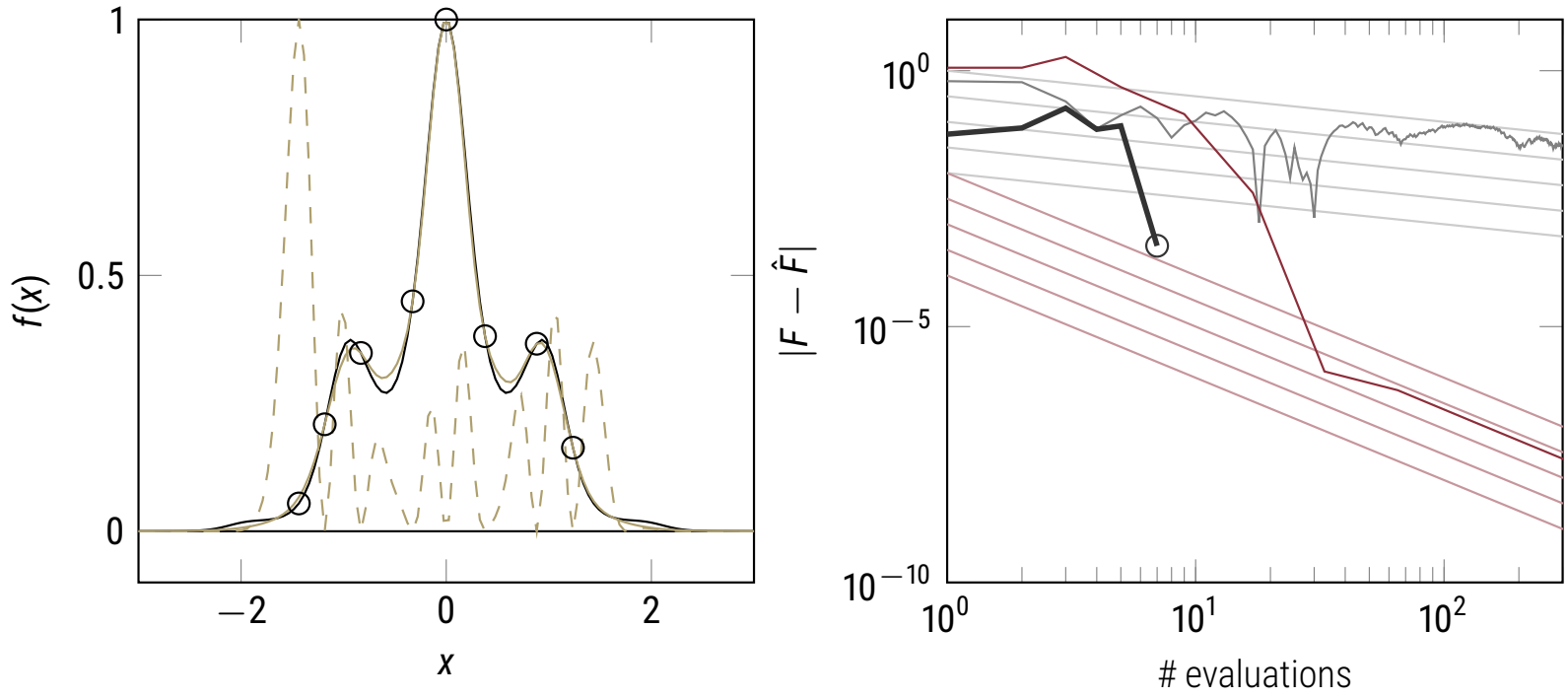

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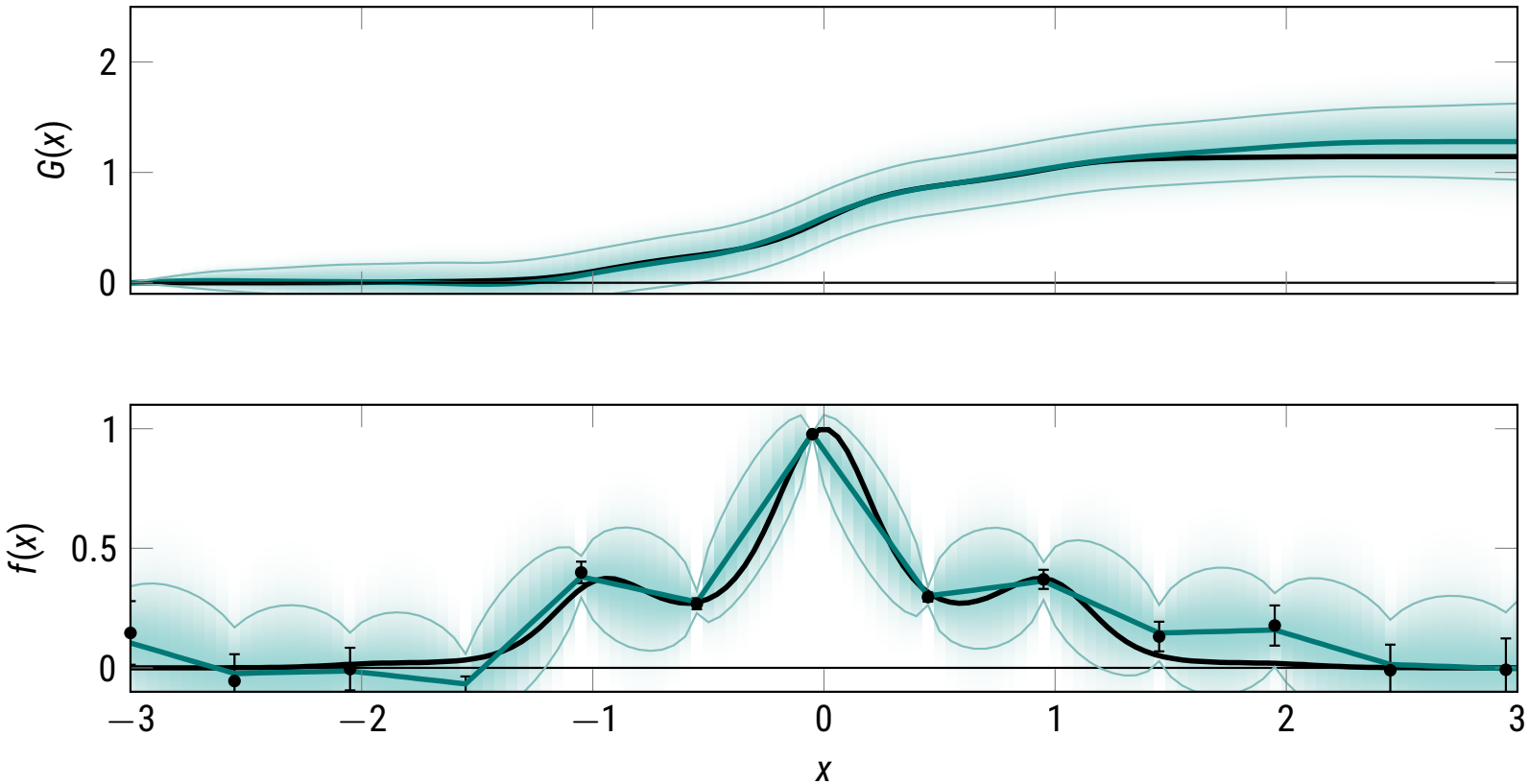
Why? — Arguments for Probabilistic Numerics

systemic uncertainty



- straightforward: just change R!
- obviously, convergence analysis now invalid

- **Gauss-Markov** processes allow linear-time inference in GP models, via **Filtering** and Smoothing
- **Gaussian Quadrature** rules can be interpreted as **MAP** estimators under Gaussian process priors
- **Error estimation** can be performed in closed form for noiseless observations
- **Probabilistic Numerics** formulation allows adaptation of **prior assumptions** and use of **uncertain evaluations**

coming up:

- **ordinary differential equations:** a slightly more challenging setting

These slides can be found at
`http://tinyurl.com/Dobbiaco-Hennig-3`