Numerical Integration

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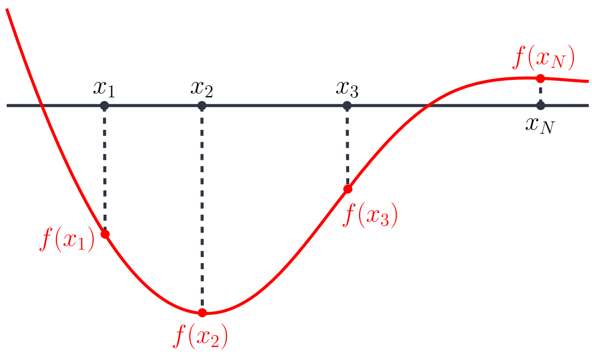
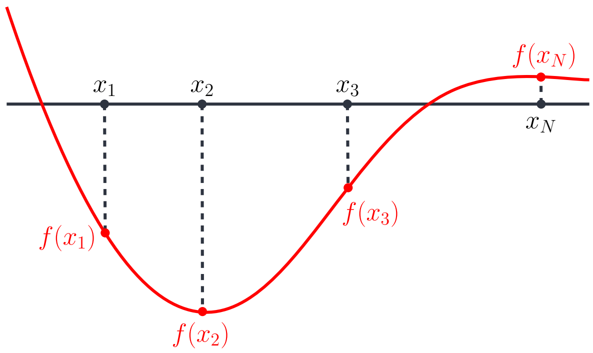
Setting



- Approximate
$$\int_a^b f(x)dx \approx \sum_{n=1}^{N} w_n f(x_n), \quad x \in \mathbb{R}$$
- Nodes x_n and corresponding function values $f(x_n)$

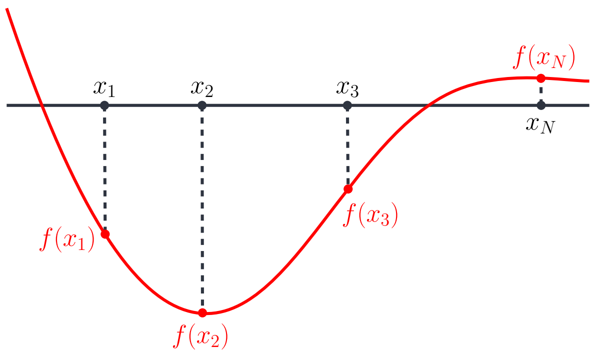
Numerical integration (quadrature)



Key idea

Approximate f using an interpolating function that is easy to integrate (e.g., polynomial)

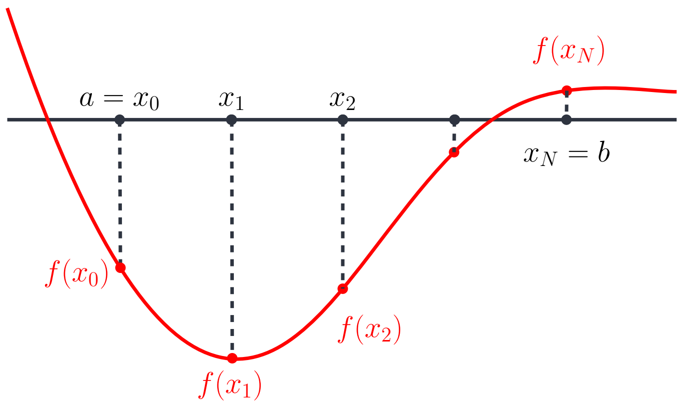
Quadrature approaches



Quadrature	Interpolant	Nodes
Newton–Cotes	low-degree polynomials	equidistant
Gaussian	orthogonal polynomials	roots of polynomial
Bayesian	Gaussian process	user defined

Newton–Cotes Quadrature

Overview



- Equidistant nodes $a = x_0, \ldots, x_N = b$ ⏩ Partition interval $[a, b]$
- Approximate f in each partition with a low-degree polynomial

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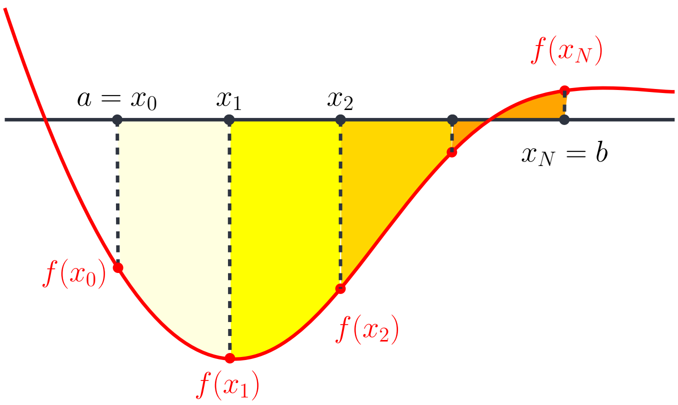
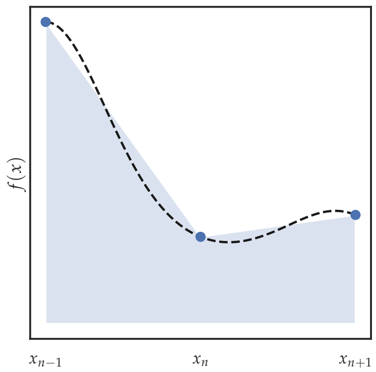


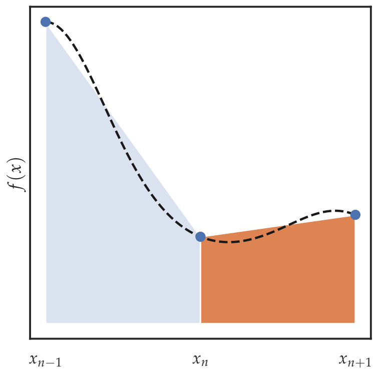
- Equidistant nodes $a = x_0, \dots, x_N = b$ ⏩ Partition interval $[a, b]$
- Approximate f in each partition with a low-degree polynomial
- Compute integral for each partition analytically and sum them up

Trapezoidal rule



- Partition $[a, b]$ into N segments with equidistant nodes x_n
- **Locally linear approximation** of f between nodes

Trapezoidal rule (2)



- Area of a trapezoid with corners $(x_n, x_{n+1}, f(x_{n+1}), f(x_n))$

$$\int_{x_n}^{x_{n+1}} f(x)dx \approx \frac{h}{2}\big(f(x_n) + f(x_{n+1})\big)$$

$h := |x_{n+1} - x_n|$ ▶▶▶Distance between nodes

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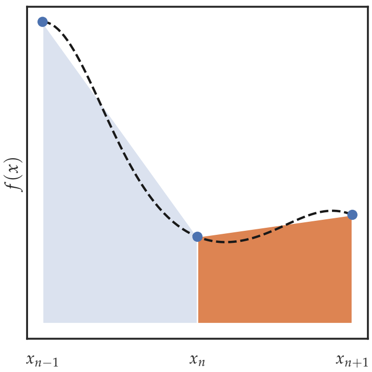

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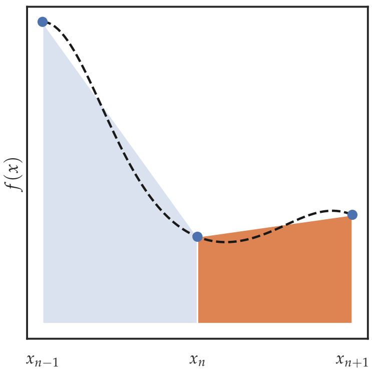

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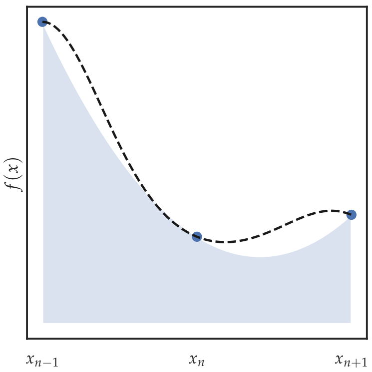
- Full integral:

$$\int_a^b f(x)dx \approx \frac{h}{2}\big(f_0 + 2f_1 + \cdots + 2f_{N-1} + f_N\big), \quad f_n := f(x_n)$$

Simpson's rule



- Partition $[a, b]$ into N segments with equidistant nodes x_n
- **Locally quadratic approximation** of f connecting triplets $\big(f(x_{n-1}), f(x_n), f(x_{n+1})\big)$

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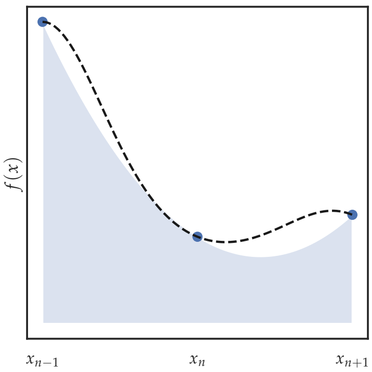

- Area of segment:

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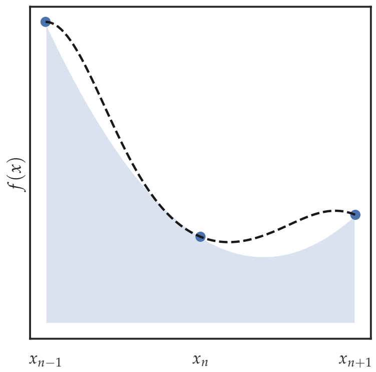

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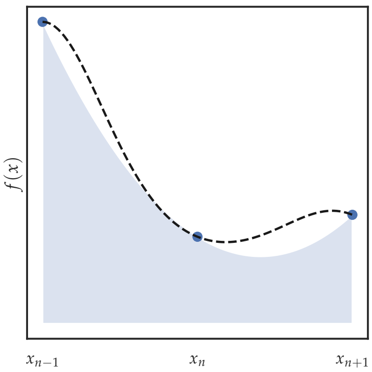

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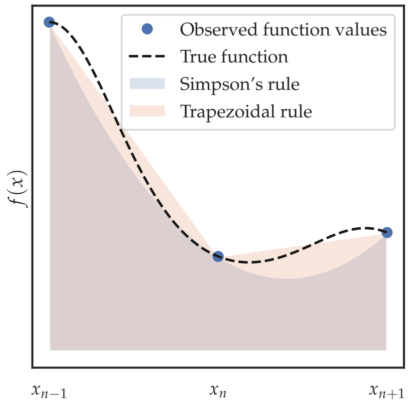
Example

$$\int_0^1 \mathsf{exp}(-x^2 - \mathsf{sin}(3x)^2)dx$$



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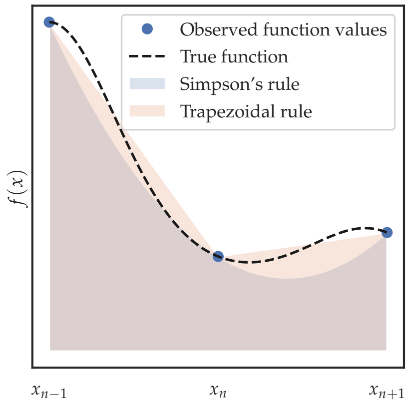
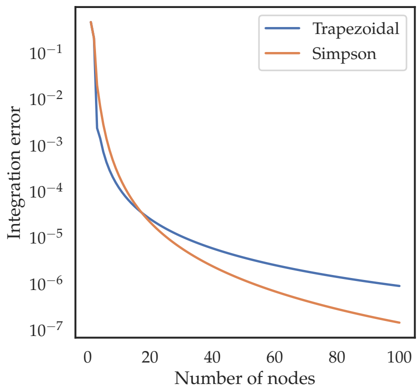
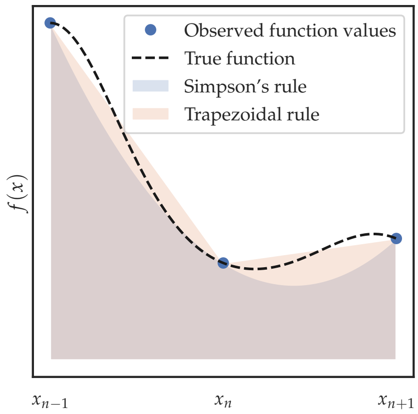




- Simpson's rule yields better approximations
- Very good approximations obtained fairly quickly

Summary: Newton–Cotes quadrature

- Approximate integrand between equidistant nodes with a low-degree polynomial (up to degree 6)
- Trapezoidal rule: linear interpolation
- Simpson's rule: quadratic interpolation
  ⏩ Better approximation and smaller integration error



Gaussian Quadrature

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- Weight function $w(x) \geq 0$ (and some other integration-related properties, which are satisfied if $w(x)$ is a pdf)
- Goal: Find nodes x_n and weights w_n, so that the approximation error is minimized

Central idea

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⏵⏵⏵ Integral can be computed exactly by evaluating f N times at the optimal locations x_n (roots of an orthogonal polynomial) with corresponding optimal weights w_n
⏵⏵⏵ More accurate than Newton–Cotes for the same number of evaluations (with some memory overhead)

Example: Gauß–Hermite quadrature

- Solve

$$\int f(x)\,\underbrace{\exp(-x^2)}_{w(x)}\,dx = \int f(x)\sqrt{2\pi}\mathcal{N}\big(x\big|0,1\big)dx = \mathbb{E}_{x\sim\mathcal{N}(0,1)}[\sqrt{2\pi}f(x)]$$

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- With change-of-variables trick ⏩ Expectation w.r.t. a Gaussian measure

$$\mathbb{E}_{x\sim\mathcal{N}(\mu,\sigma^2)}[f(x)] \approx \frac{1}{\sqrt{\pi}}\sum_{n=1}^{N} w_n f(\sqrt{2}\sigma x_n + \mu).$$

Example: Gauß–Hermite quadrature (2)

- Follow general approximation scheme

$$\int f(x) \underbrace{\mathsf{exp}(-x^2)}_{w(x)} \, dx \approx \sum_{n=1}^{N} w_n f(x_n)$$

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- Nodes $x_1, \ldots, x_N$ are the roots of Hermite polynomial

$$H_N(x) := (-1)^n \exp\left(\frac{x^2}{2}\right) \frac{d^n}{dx^n} \exp(-x^2)$$

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- Weights w_n are

$$w_n := \frac{2^{N-1} N! \sqrt{\pi}}{N^2 H_{N-1}^2(x_n)}$$

Overview (Stoer & Bulirsch, 2002)

$$\int_a^b w(x) f(x) dx \approx \sum_{n=1}^{N} w_n f(x_n)$$

$[a, b]$	$w(x)$	Orthogonal polynomial
$[-1, 1]$	1	Legendre polynomials
$[-1, 1]$	$(1 - x^2)^{-\frac{1}{2}}$	Chebychev polynomials
$[0, \infty]$	$\exp(-x)$	Laguerre polynomials
$[-\infty, \infty]$	$\exp(-x^2)$	Hermite polynomials

Application areas

- Probabilities for rectangular bivariate/trivariate Gaussian and t distributions (Genz, 2004)
- Integrating out (marginalizing) a few hyper-parameters in a latent-variable model (INLA; Rue et al., 2009)
- Predictions with a Gaussian process classifier (GPFlow; Matthews et al., 2017)

Summary: Gaussian quadrature

- Orthogonal polynomials to approximate f
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- **Method of choice** for low-dimensional problems (1–3 dimensions)
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- Only works in low dimensions
- Approaches that scale better with dimensionality
  - **Bayesian quadrature** (up to ≈ 10 dimensions)
  - **Monte Carlo estimation** (high dimensions)

Bayesian Quadrature

Bayesian quadrature: Setting and key idea

$$Z := \int f(\boldsymbol{x})p(\boldsymbol{x})d\boldsymbol{x} = \mathbb{E}_{\boldsymbol{x}\sim p}[f(\boldsymbol{x})]$$

- Function f is expensive to evaluate
- Integration in moderate (≤ 10) dimensions
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Key idea

- Phrase quadrature as a statistical inference problem
  ⏩ Probabilistic numerics (e.g., Hennig et al., 2015; Briol et al., 2015)
- Estimate distribution on Z using a dataset $\mathcal{D} := \{(\boldsymbol{x}_1, f(\boldsymbol{x}_1)), \ldots, (\boldsymbol{x}_N, f(\boldsymbol{x}_N))\}$

Bayesian quadrature: How it works

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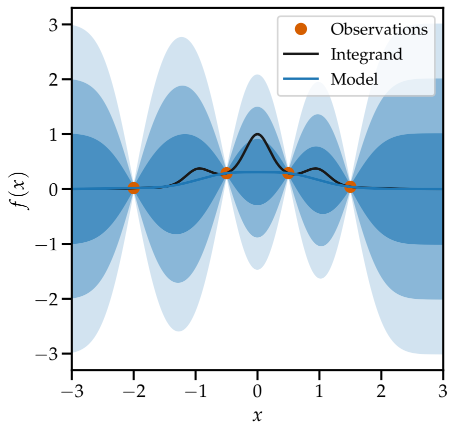

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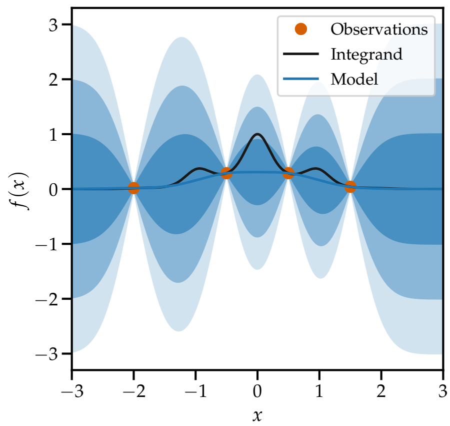
- Place (Gaussian process) prior distribution on f and determine the posterior via Bayes' theorem (Diaconis 1988; O'Hagan 1991; Rasmussen & Ghahramani 2003)
  - Distribution on f induces a distribution on Z



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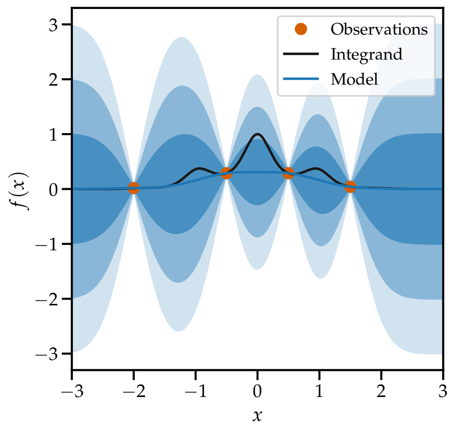
- Generalizes to noisy function observations
$$y = f(\boldsymbol{x}) + \epsilon$$



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$$\sigma_Z^2 = \iint k_{\text{post}}(\boldsymbol{x}, \boldsymbol{x}')p(\boldsymbol{x})p(\boldsymbol{x}')d\boldsymbol{x}d\boldsymbol{x}' = \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'}[k_{\text{post}}(\boldsymbol{x}, \boldsymbol{x}')]$$

Bayesian quadrature: Mean

$$\mathbb{E}_f[Z] = \mu_Z = \overbrace{\mathbb{E}_{\boldsymbol{x}\sim p}[\mu_{\text{post}}(\boldsymbol{x})]}^{\text{expected predictive mean}}$$

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Training data: $\boldsymbol{X}, \boldsymbol{y}$

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Training data: $\boldsymbol{X}, \boldsymbol{y}$

Bayesian quadrature: Variance

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$$= \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'}[k(\boldsymbol{x},\boldsymbol{x}')] - \boldsymbol{z}^\top$$

Bayesian quadrature: Variance

$$\begin{aligned}
\mathbb{V}_f[Z] = \sigma_Z^2 = & \overbrace{\mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'\sim p}[k_{\text{post}}(\boldsymbol{x},\boldsymbol{x}')]}^{\text{expected posterior covariance}} \\
&= \iint \underbrace{k(\boldsymbol{x},\boldsymbol{x}')}_{\text{prior covariance}} - \underbrace{k(\boldsymbol{x},\boldsymbol{X})\boldsymbol{K}^{-1}k(\boldsymbol{X},\boldsymbol{x}')}_{\text{information from training data}} p(\boldsymbol{x})p(\boldsymbol{x}')d\boldsymbol{x}d\boldsymbol{x}' \\
&= \iint k(\boldsymbol{x},\boldsymbol{x}')p(\boldsymbol{x})p(\boldsymbol{x}')d\boldsymbol{x}d\boldsymbol{x}' - \underbrace{\int k(\boldsymbol{x},\boldsymbol{X})p(\boldsymbol{x})d\boldsymbol{x}}_{=\boldsymbol{z}^\top}\boldsymbol{K}^{-1} \\
&= \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'}[k(\boldsymbol{x},\boldsymbol{x}')] - \boldsymbol{z}^\top\boldsymbol{K}^{-1}
\end{aligned}$$

Bayesian quadrature: Variance

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&= \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'}[k(\boldsymbol{x},\boldsymbol{x}')] - \mathbb{E}_{\boldsymbol{x}}[k(\boldsymbol{x},\boldsymbol{X})]\boldsymbol{K}^{-1}\mathbb{E}_{\boldsymbol{x}'}[k(\boldsymbol{X},\boldsymbol{x}')]
\end{aligned}
$$

Computing kernel expectations

$$\mathbb{E}_{\boldsymbol{x}\sim p}[k(\boldsymbol{x}, \boldsymbol{X})], \quad \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'\sim p}[k(\boldsymbol{x}, \boldsymbol{x}')]$$

- Solve a different (easier) integration problem

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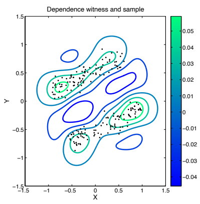
- Solve a different (easier) integration problem

	Input distribution p	
Kernel k	Gaussian	non-Gaussian
RBF/ polynomial/ trigonometric	analytical	analytical via importance-sampling trick
otherwise	Monte Carlo (numerical integration)	Monte Carlo (numerical integration)

Kernel expectations in other areas

$$\mathbb{E}_{\boldsymbol{x}\sim p}[k(\boldsymbol{x}, \boldsymbol{X})], \quad \mathbb{E}_{\boldsymbol{x},\boldsymbol{x}'\sim p}[k(\boldsymbol{x}, \boldsymbol{x}')]$$

- Kernel MMD
  (e.g., Gretton et al., 2012)



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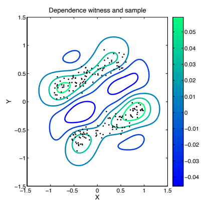

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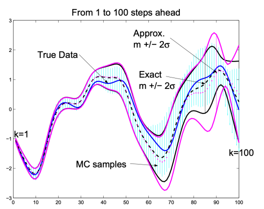

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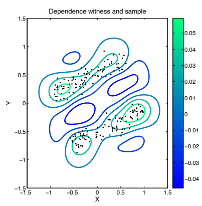

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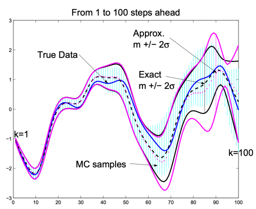

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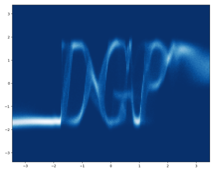
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- Model-based RL with Gaussian processes
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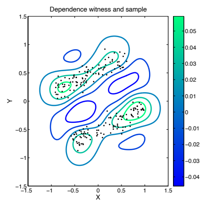

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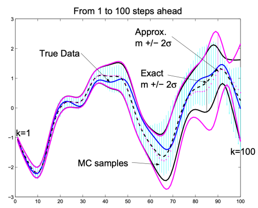

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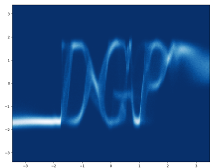

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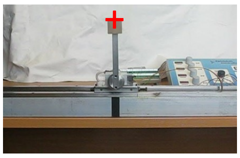

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Iterative procedure: Where to measure f next?

- Define an **acquisition function** (similar to Bayesian optimization)

Iterative procedure: Where to measure f next?

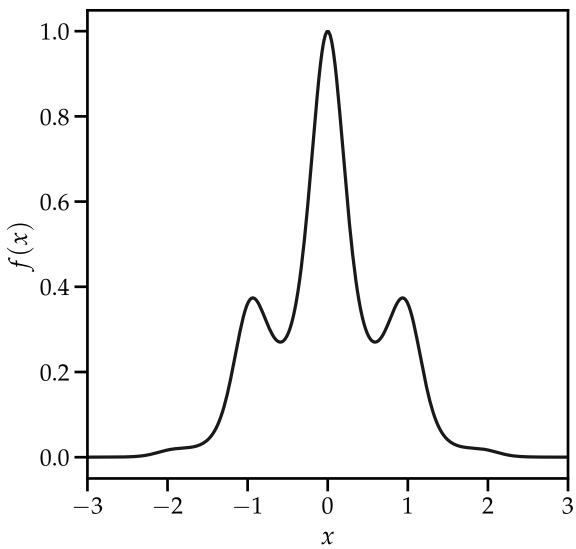
- Define an **acquisition function** (similar to Bayesian optimization)
- Example: Choose next node $\boldsymbol{x}_{n+1}$ so that the variance of the estimator is reduced maximally (e.g., O'Hagan, 1991; Gunter et al., 2014)

$$\boldsymbol{x}_{n+1} = \operatorname{argmax}_{\boldsymbol{x}_*} \overbrace{\mathbb{V}[Z|\mathcal{D}]}^{\text{current variance}} - \overbrace{\mathbb{E}_{y_*}\left[\mathbb{V}[Z|\mathcal{D}\cup\{(\boldsymbol{x}_*, y_*)\}]\right]}^{\text{new variance}}$$

Example with EmuKit (Paleyes et al., 2019)

Compute

$$Z = \int_{-3}^{3} e^{-x^2 - \sin^2(3x)} dx$$



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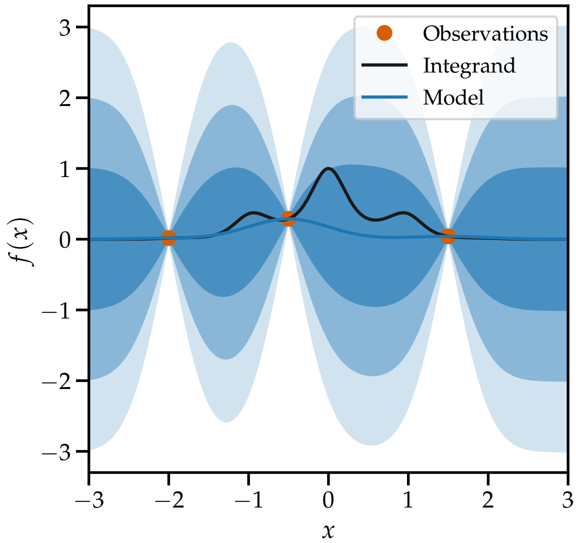

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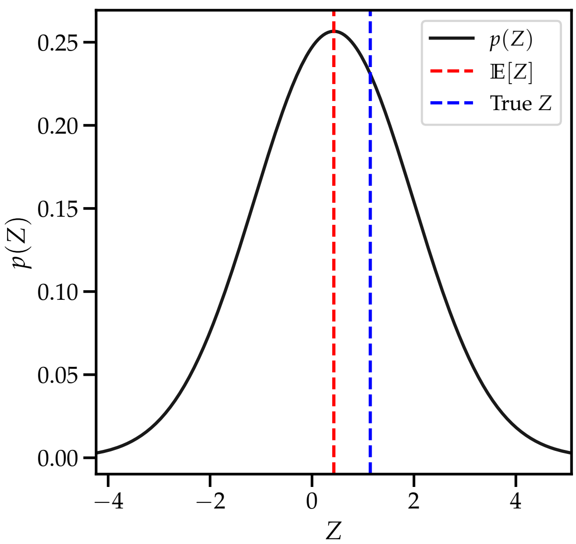
- Determine $p(Z)$



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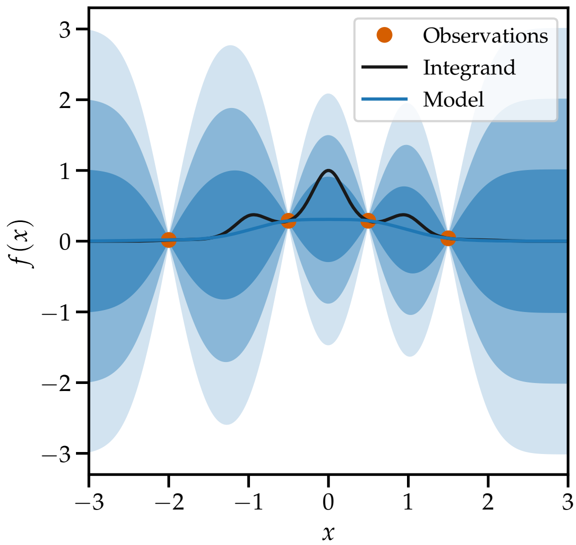
- Determine $p(Z)$
- Find and include new measurement
  1. Find optimal node x_{n+1} by maximizing an acquisition function
  2. Evaluate integrand at x_{n+1}
  3. Update GP with $\big(x_{n+1}, f(x_{n+1})\big)$



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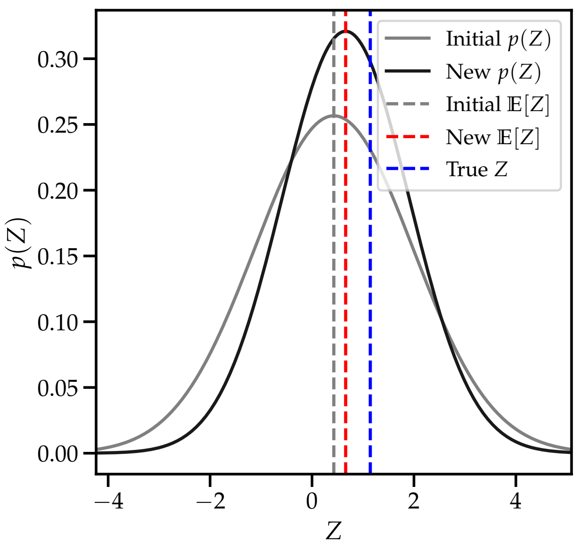

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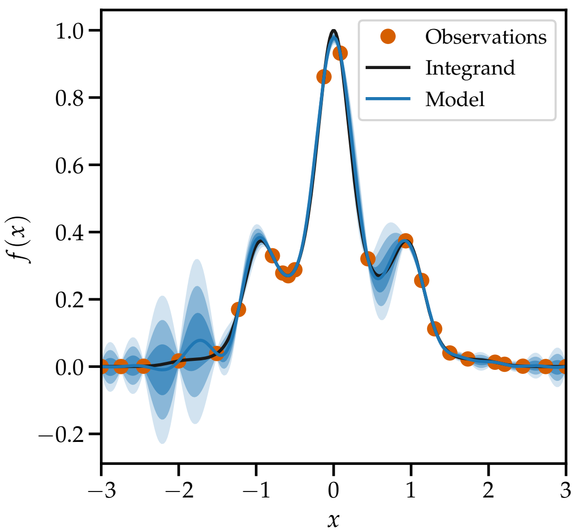
- Compute updated $p(Z)$
- Repeat



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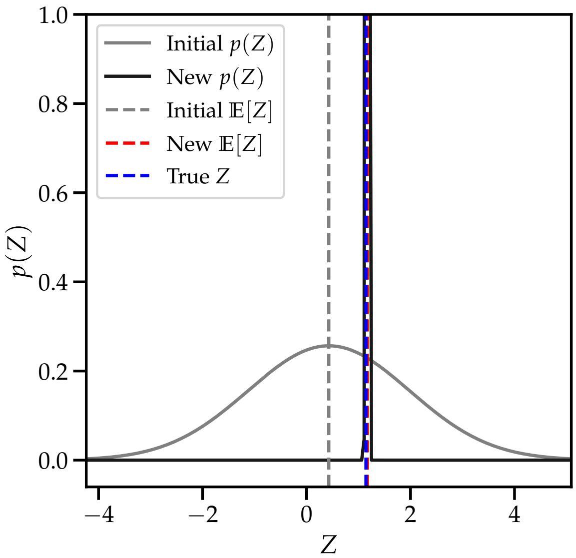
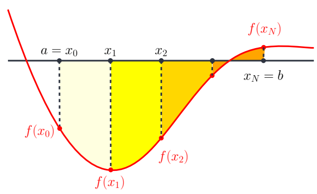


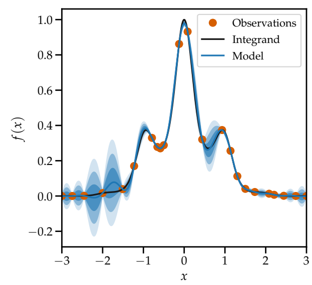
Summary

- Central approximation

$$\int f(\boldsymbol{x})d\boldsymbol{x} \approx \sum_{n=1}^{N} w_n f(\boldsymbol{x}_n)$$



- **Newton–Cotes:** Equidistant nodes $\boldsymbol{x}_n$, low-degree polynomial approximation of f
- **Gaussian quadrature:** Nodes $\boldsymbol{x}_n$ as the roots of interpolating orthogonal polynomials of f
- **Bayesian quadrature:** Integration as a statistical inference problem; Global approximation of f using a Gaussian process; scales to moderate dimensions



Numerical integration is a really good idea in low dimensions

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