Monte-Carlo Methods and Sampling for Computing

Monte-Carlo Integration

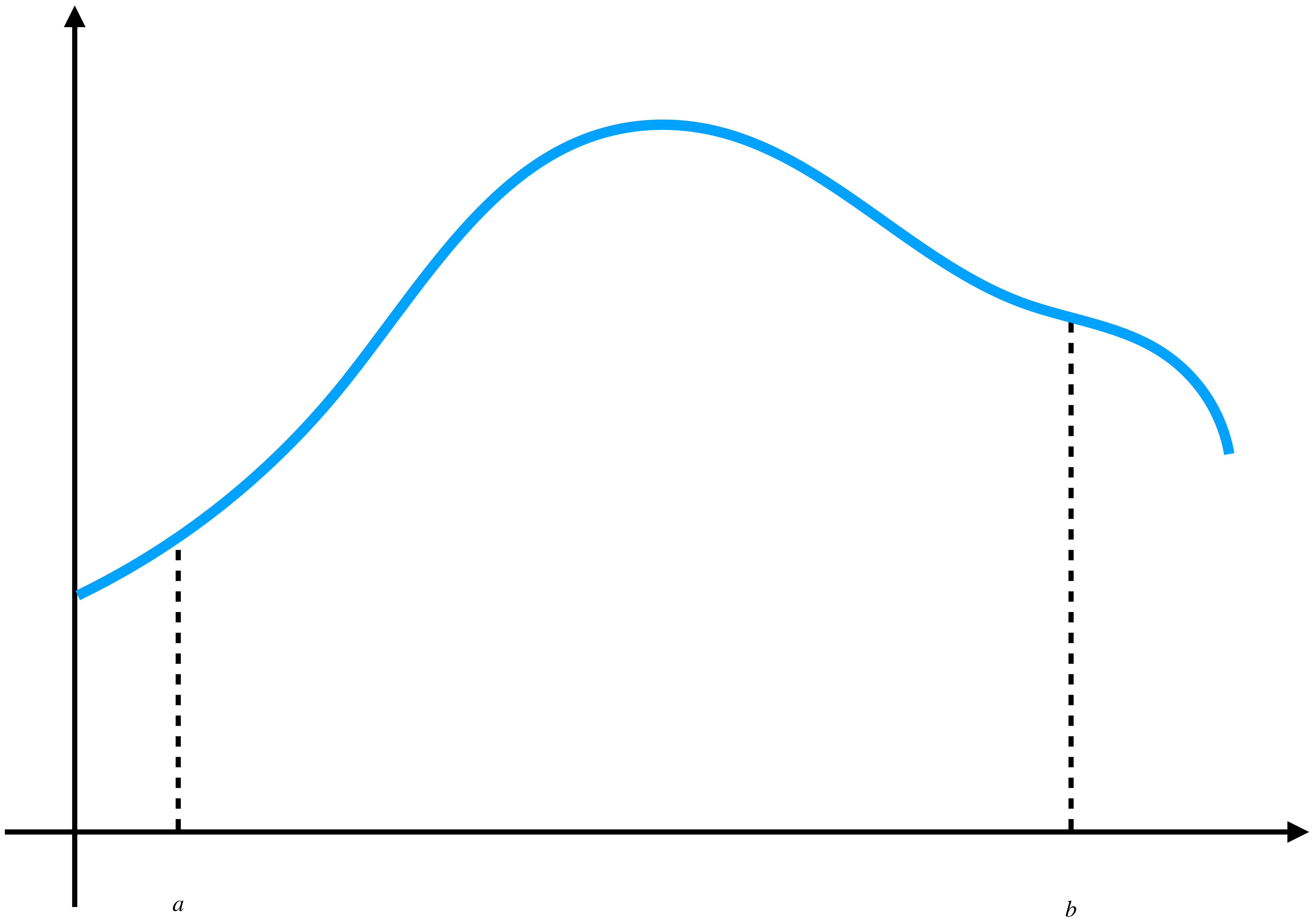
Francesco Banterle, Ph.D.

Monte-Carlo Integration
Quadrature Rules

- Quadrature rules are efficient for 1D smooth functions:
  - Midpoint rule;
  - Trapezoidal rule;
  - Simpson rule;
  - Gauss rule;
  - etc.

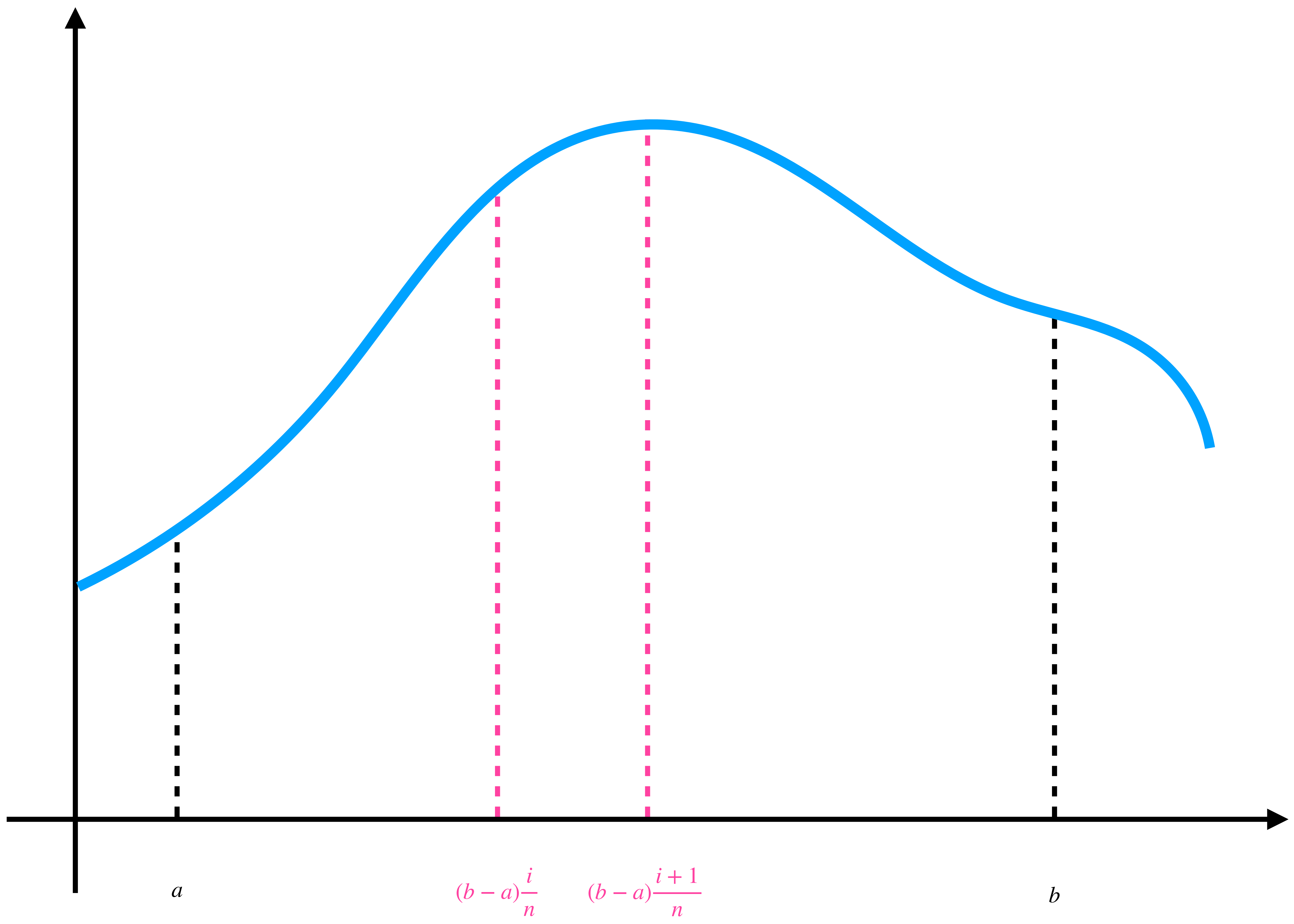
Monte-Carlo Integration

Quadrature Rules: Midpoint Rule



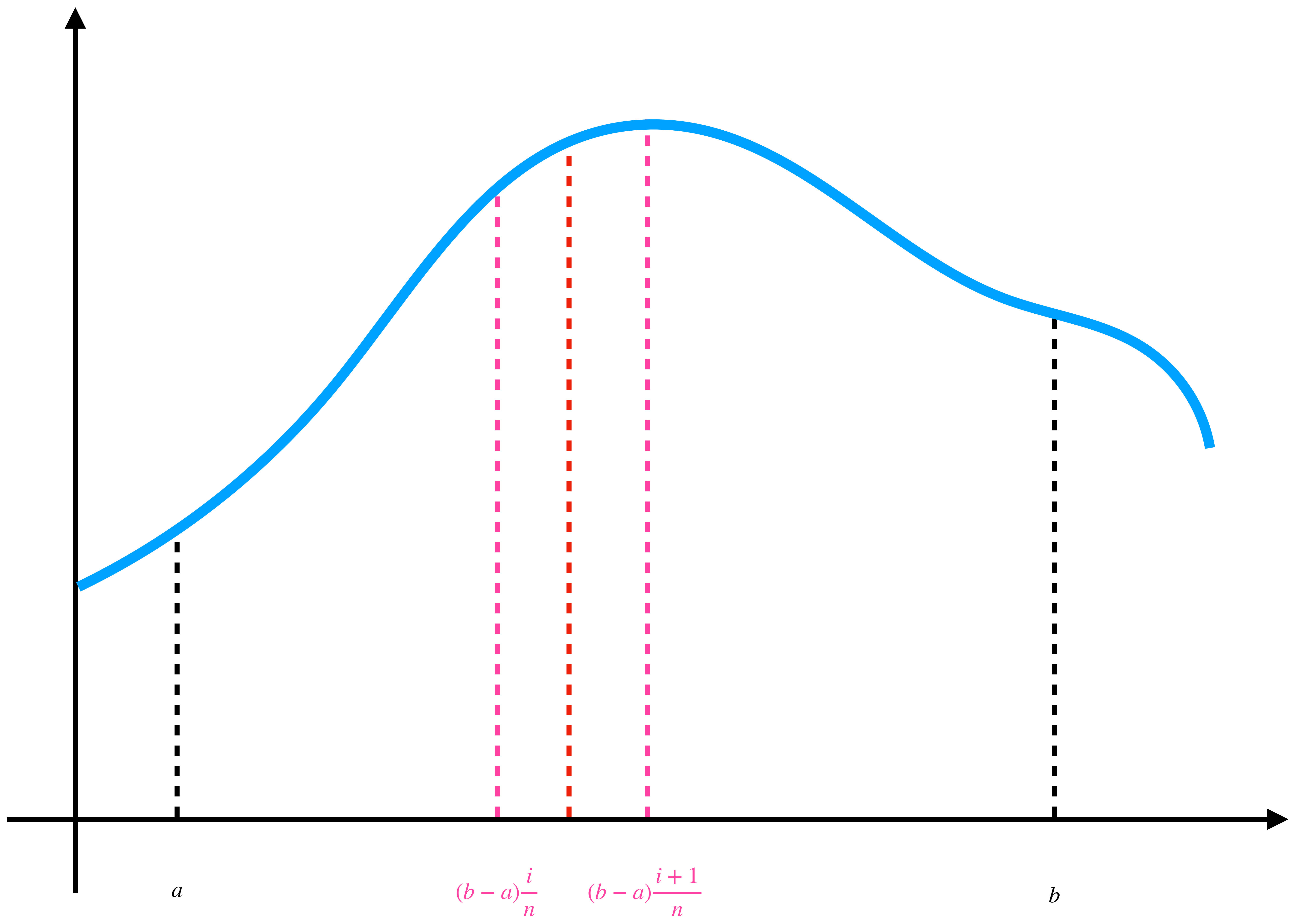
Monte-Carlo Integration

Quadrature Rules: Midpoint Rule



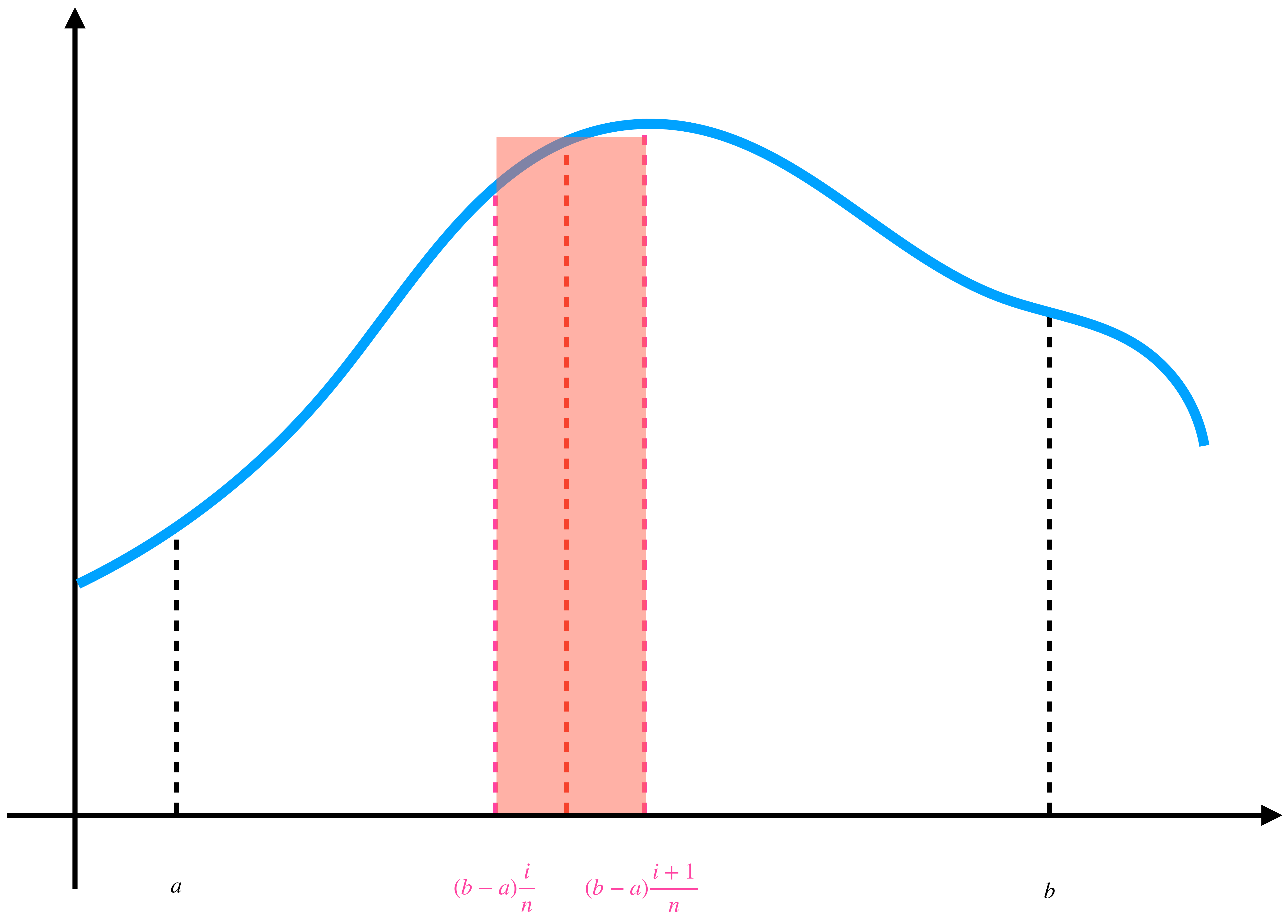
Monte-Carlo Integration

Quadrature Rules: Midpoint Rule



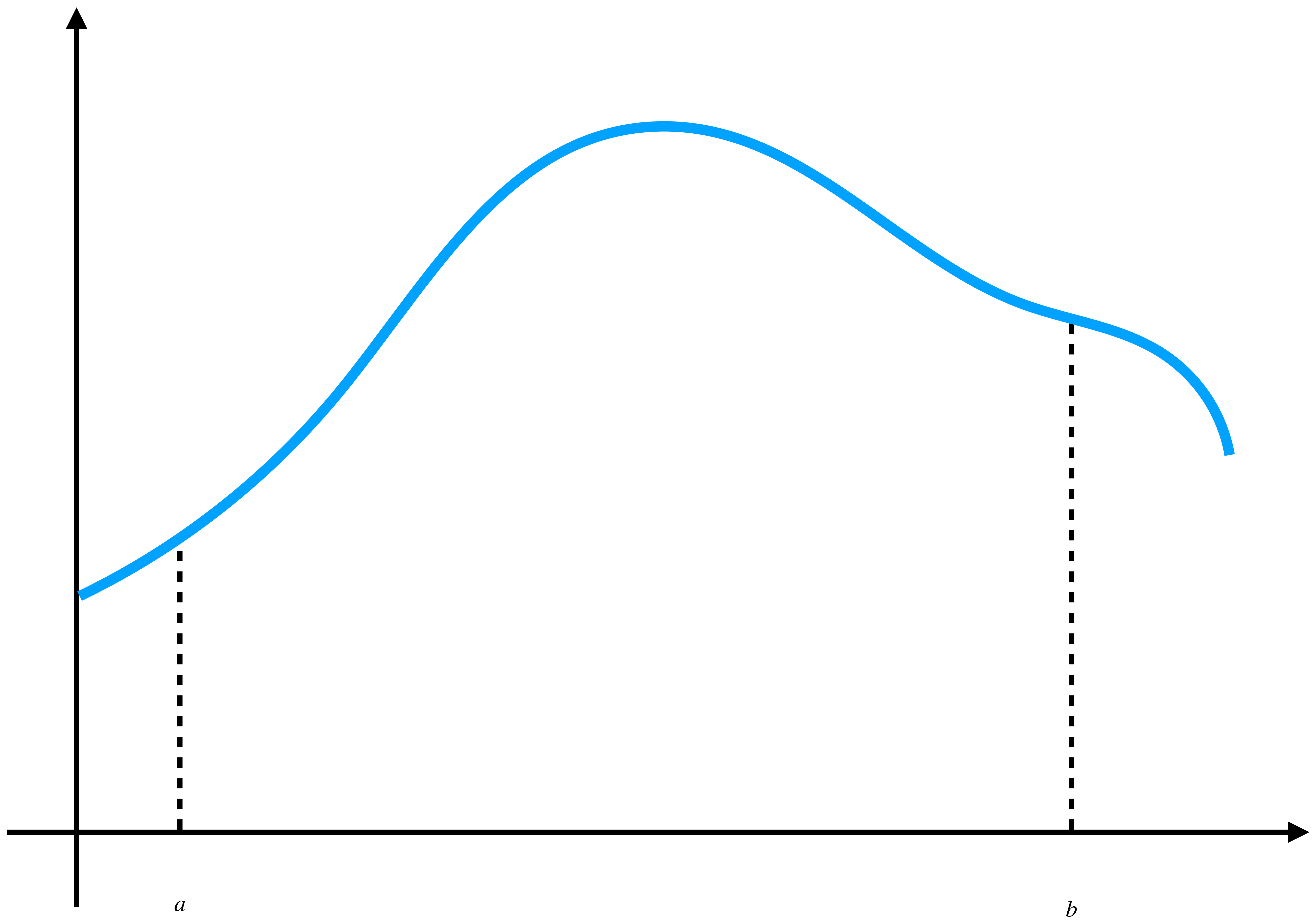
Monte-Carlo Integration

Quadrature Rules: Midpoint Rule



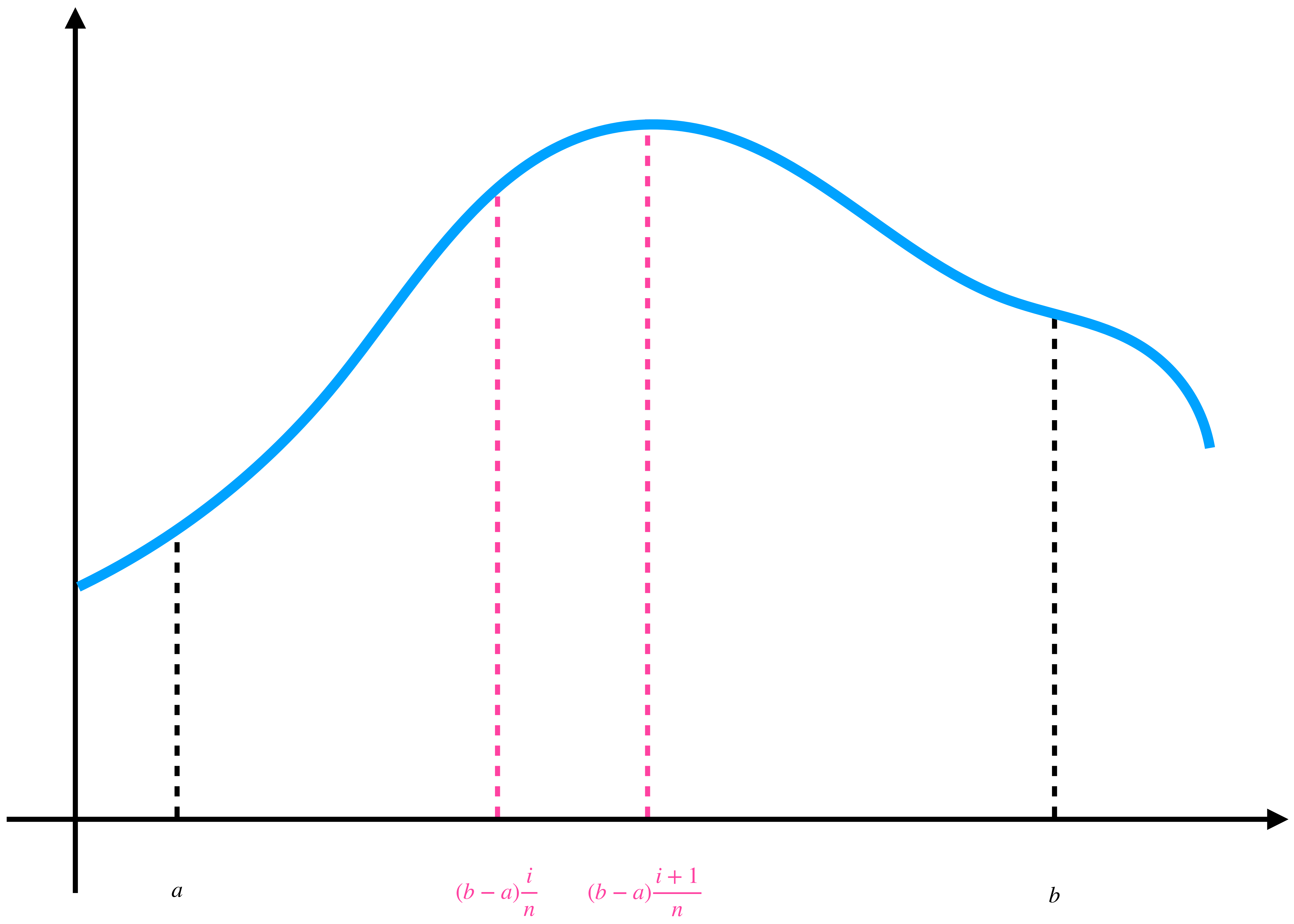
Monte-Carlo Integration

Quadrature Rules: Trapezoidal Rule



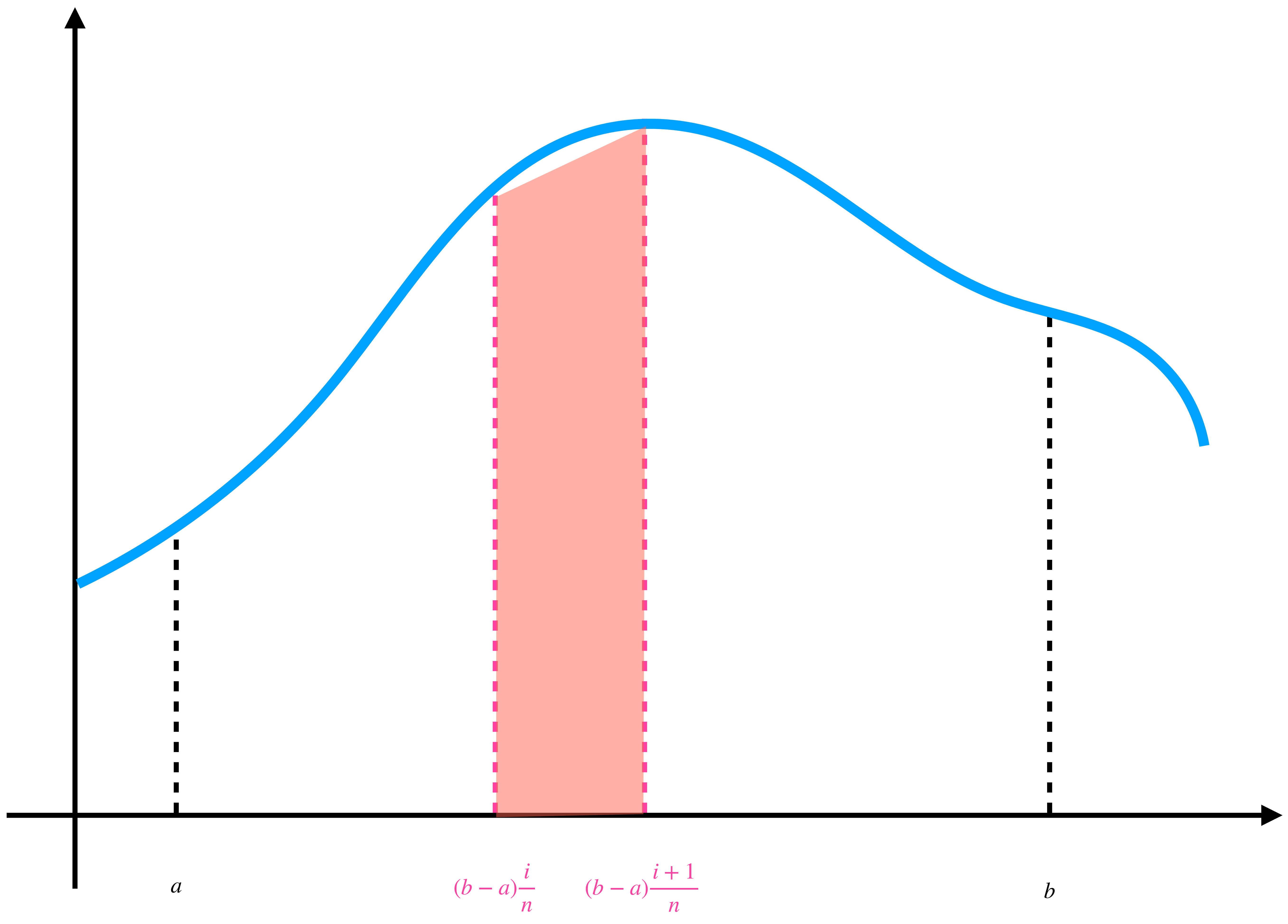
Monte-Carlo Integration

Quadrature Rules: Trapezoidal Rule



Monte-Carlo Integration

Quadrature Rules: Trapezoidal Rule



Monte-Carlo Integration

Quadrature rules

- In general, all quadrature rules can be distilled into the following equation:

$$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i),$$

  where w_i are the weights of a polynomial.

- The error is $O(n^{-r})$ where r depends on:
  - The quadrature rule.
  - How smooth f is.

Monte-Carlo Integration

The Curse of Dimensionality

- However, when we have multidimensional integrals, quadrature methods generate samples on a multidimensional grid:
  - Reduced accuracy!
- Let's see a quadrature rule for a d-dimensional integral:

$$\int_{a_1}^{b_1} \dots \int_{a_d}^{b_d} f(x_1, \dots, x_d) dx_1 \dots dx_d \approx \sum_{i_1=1}^{n_1} \dots \sum_{i_1=d}^{n_d} \left(\prod_{j=1}^{d} w_{ji_j} \right) f(x_{i_1}, \dots, x_{i_d}).$$

- Note that we apply a 1-dimensional rule for each dimension. Therefore the error becomes:

$$O\left(n^{-\frac{r}{d}}\right).$$

- Note that increasing r would not help much.

Monte-Carlo Integration

Basics

- Our goal is to compute this integral:

$$I = \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}, \text{ where } f : \mathbb{R}^d \rightarrow \mathbb{R}$$

- We defined a new function:

$$g(\mathbf{x}) = \frac{f(\mathbf{x})}{p(\mathbf{x})}, \text{ and } p \text{ is a PDF.}$$

- The expected value of $g(\mathbf{x})$ is:

$$\mathbb{E}[g(\mathbf{x})] = \mu = \int_{\mathbb{R}^d} g(\mathbf{x}) p(\mathbf{x}) d\mathbf{x} = \int_{\mathbb{R}^d} f(\mathbf{x}) d\mathbf{x}.$$

- We approximate it as:

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^{n} \frac{f(\mathbf{x}_i)}{p(\mathbf{x}_i)} \qquad \mathbf{x}_i \sim^{\text{i.i.d.}} p.$$

Monte-Carlo Integration

An Example

- Let's compute the integral of $f(x) = -x^2 + 2$ in the interval $[0,2]$:
- As first step, we need to define a PDF to use.
- Since we need to compute the integral in $[0,2]$ and we can draw uniform samples in that interval or $[a, b]$ in general, p is going to be uniform:

$$p(x) = \frac{1}{b-a} = \frac{1}{2}.$$

- Now let's draw random samples according to $p(x)$:

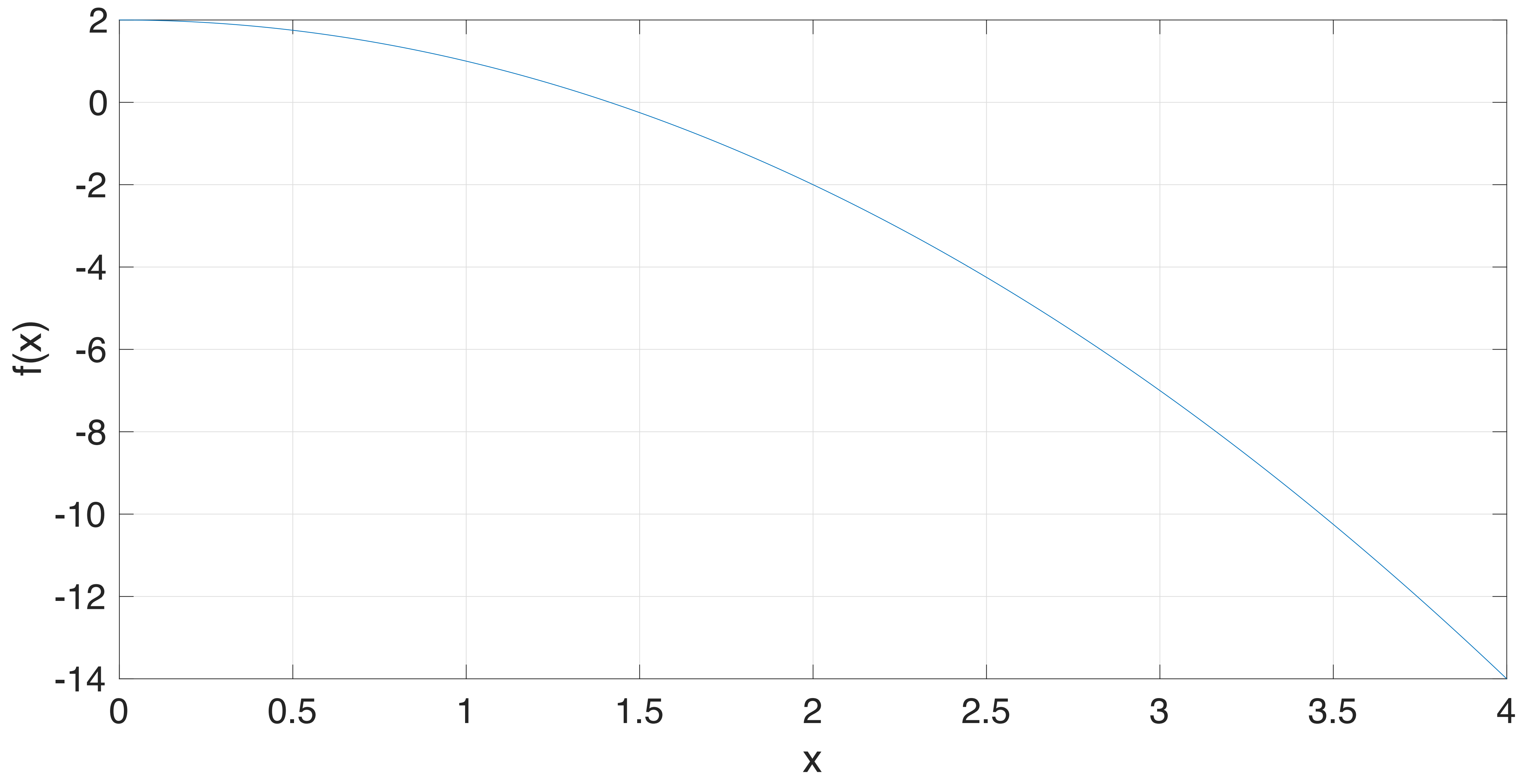
$$x_i = (a-b)u_i + b \qquad u_i \in \mathbf{U}(0,1).$$

Monte-Carlo Integration

An Example

- Let's compute the integral of $f(x) = -x^2 + 2$ in the interval $[0,2]$:

$$\int_0^2 (-x^2 + 2)dx \approx \frac{1}{N}\sum_{i=1}^{n}\frac{f(x_i)}{p(x_i)} = \frac{1}{N}\sum_{i=1}^{n}\frac{(-x^2+2)}{\frac{1}{2}} = \frac{2}{N}\sum_{i=1}^{n}(-x_i^2+2) \qquad p(x) = \frac{1}{2}.$$



Monte-Carlo Integration

An Example

- In this simple case, if we draw 100,000 samples we will get as integral value **1.3**xxx, with only two stable decimals.
  - Note that the result of this integral is $\frac{4}{3}$.
  - This is not a great performance.
  - How many samples do we need?

Monte-Carlo Integration

An Example

- We can compute σ_0^2 for $g(x) = f(x)p(x)$:

$$Var(g(x)) = \mathbb{E}(g(x)^2) - \mathbb{E}(g(x))^2 = \int_0^2 g(x)^2 p(x) dx - \left(\int_0^2 g(x)p(x)dx\right)^2$$

$$= \int_0^2 \left(2(-x^2+2)\right)^2 \frac{1}{2} dx - \left(\int_0^2 \left(2(-x^2+2)\right)\frac{1}{2}\right)^2 = \frac{256}{45} = 5.689$$

.

- So, with an error $\epsilon = 0.01$, and a confidence level α at 99%, we need:

$$n \geq \frac{\sigma_0^2}{\epsilon^2}\frac{1}{1-\alpha} = \frac{5.689}{0.01^2}\frac{1}{1-0.99} = 5{,}689{,}000.$$

Monte-Carlo Integration

Conclusions

- Quadrature Rule Error:

$$O\left(n^{-\frac{r}{d}}\right)$$

  - Monte-Carlo Error:

$$O\left(n^{-\frac{1}{2}}\right)$$

Bibliography

- Art Owen. “Chapter 1: Introduction” from the book “Monte Carlo theory, methods and examples”. 2013.
- Art Owen. “Chapter 2: Simple Monte Carlo” from the book “Monte Carlo theory, methods and examples”. 2013.
- Art Owen. “Chapter 7: Other Integration Methods” from the book “Monte Carlo theory, methods and examples”. 2013.
- Peter Shirley, Changyaw Wang, Kurt Zimmerman. “Monte Carlo Techniques for Direct Lighting Calculations”. ACM Transactions on Graphics. Volume 15. Issue 1. Jan. 1996.

Thank you for your attention!