

Monte-Carlo Methods and Sampling for Computing

Monte-Carlo Integration

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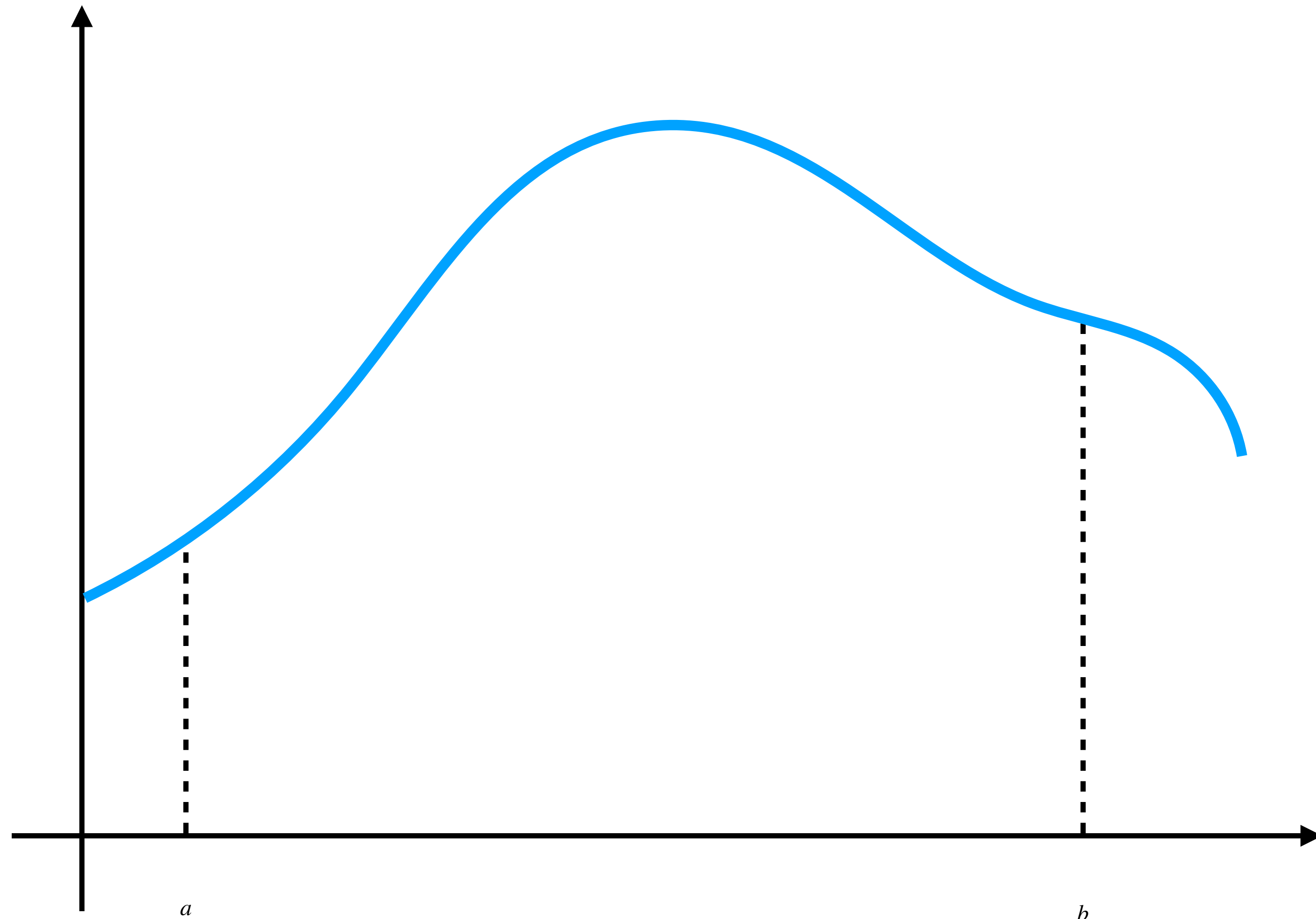
Monte-Carlo Integration

Quadrature Rules

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

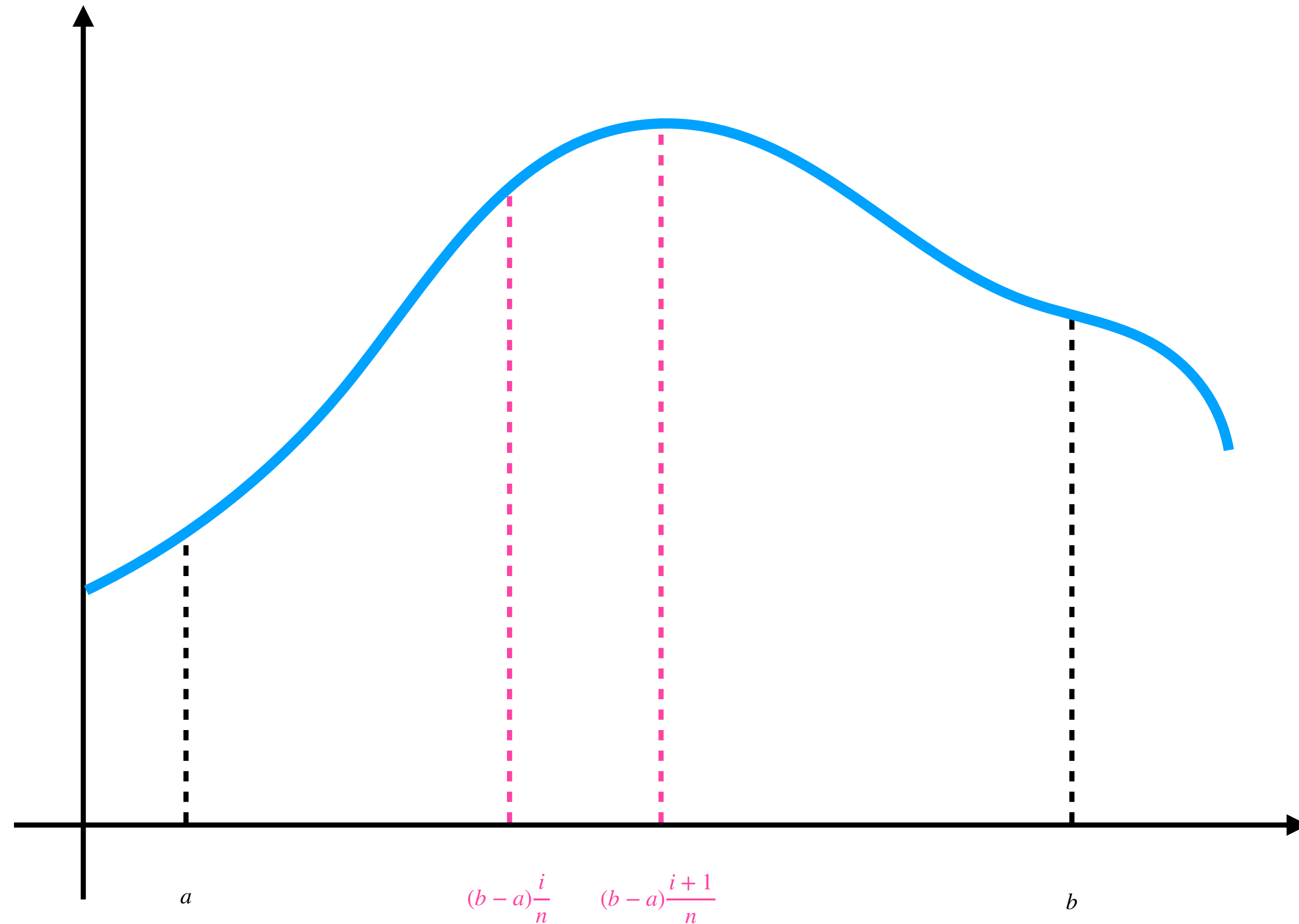
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Quadrature Rules: Midpoint Rule



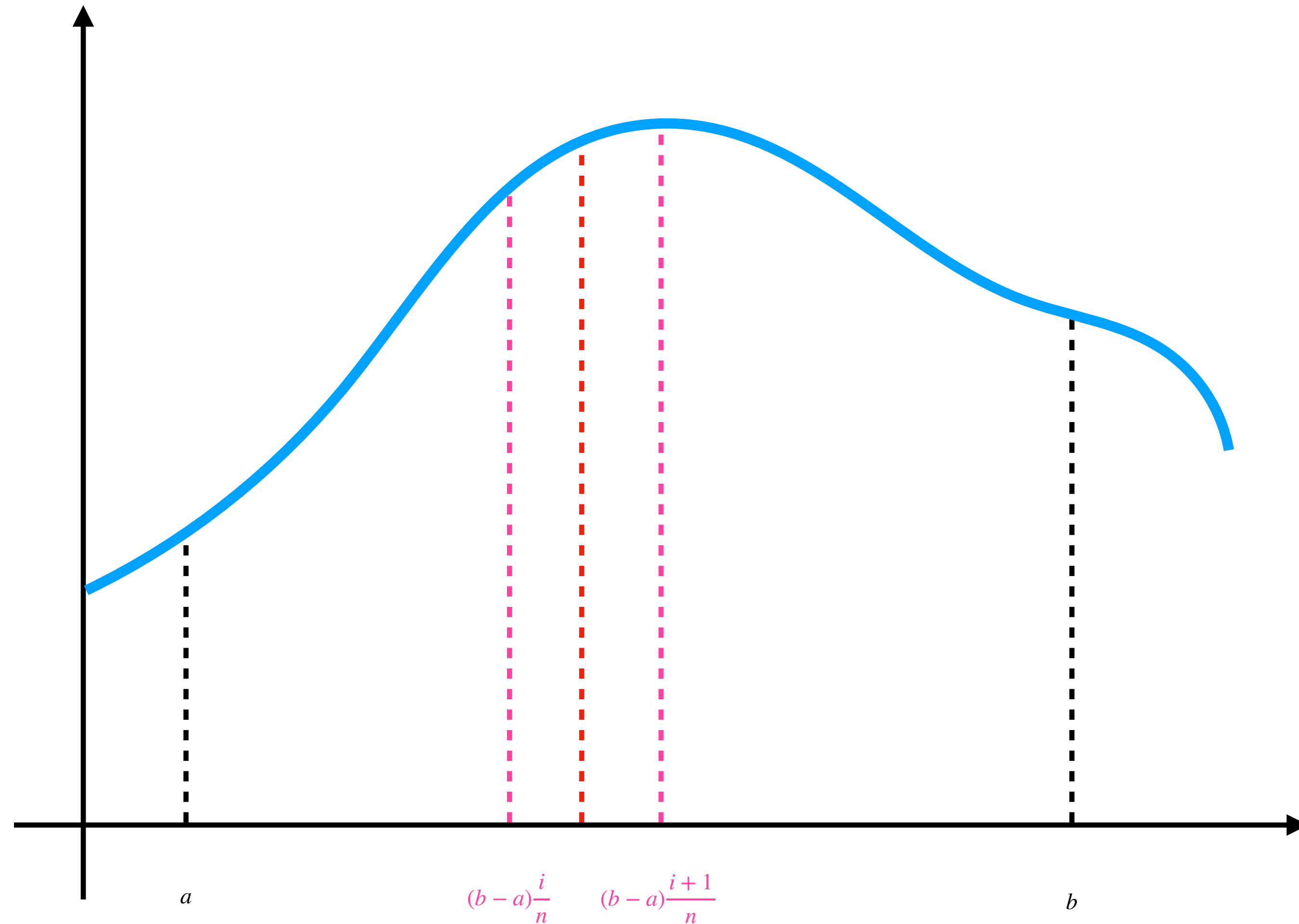
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Quadrature Rules: Midpoint Rule



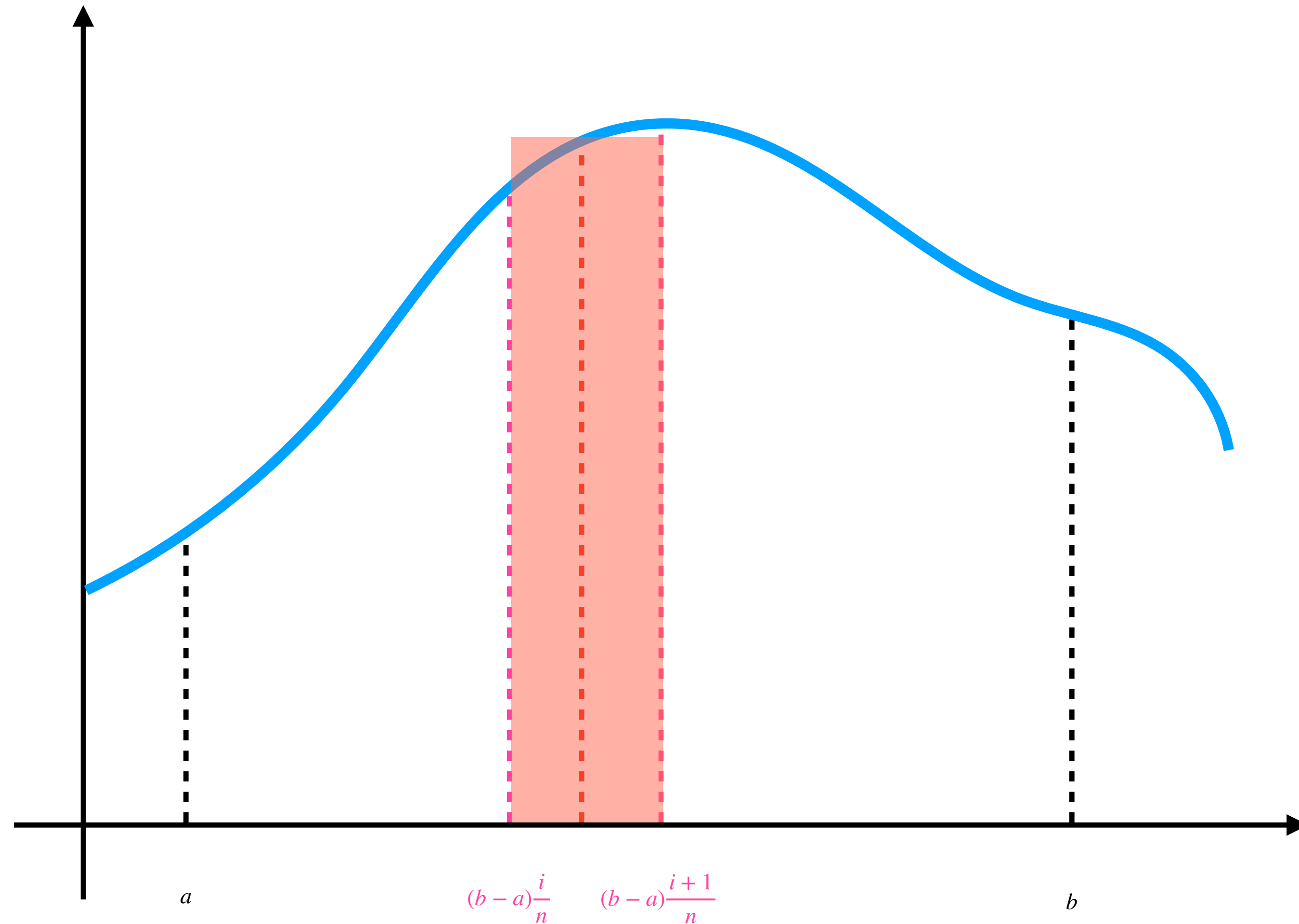
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Quadrature Rules: Midpoint Rule



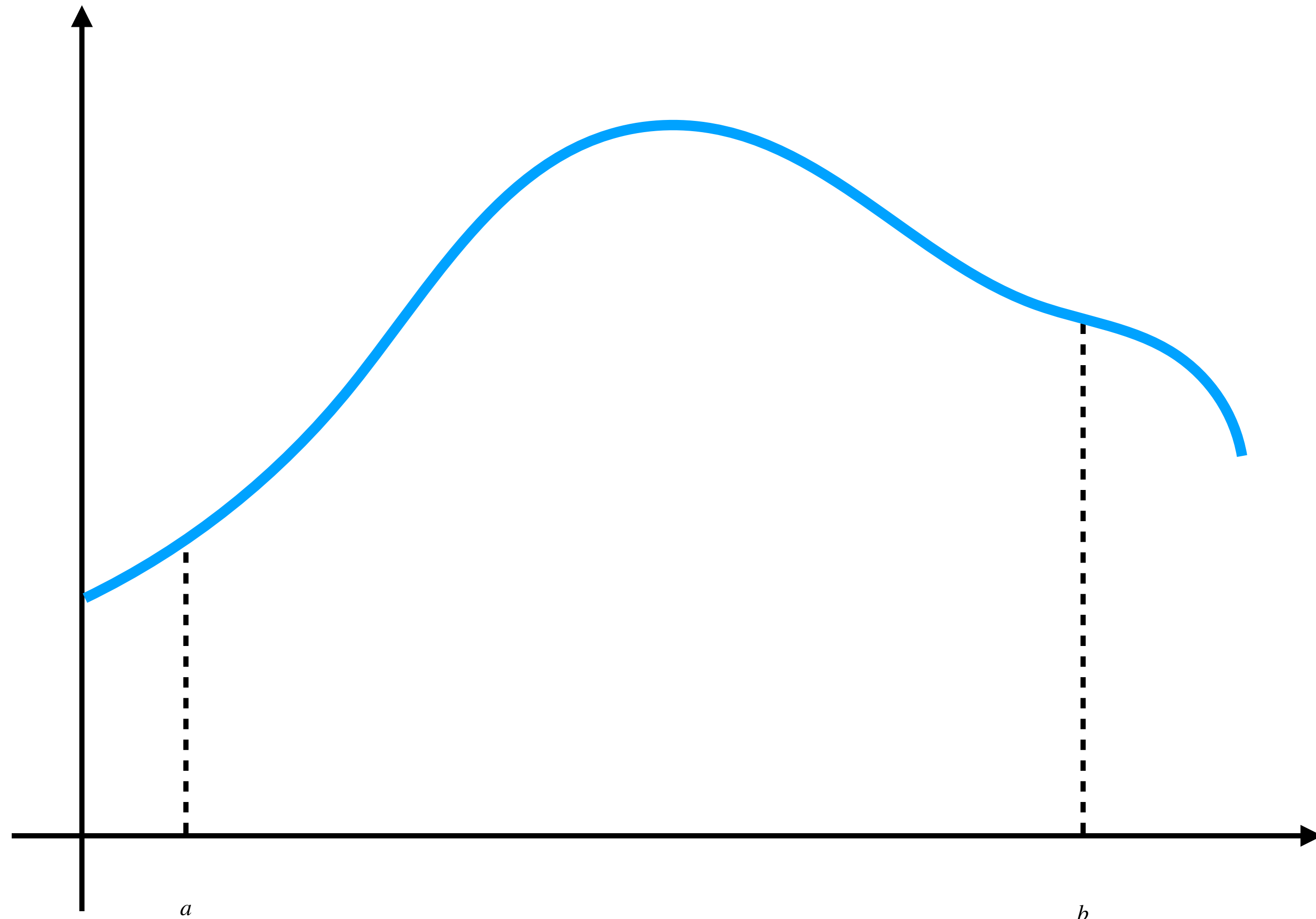
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Quadrature Rules: Midpoint Rule



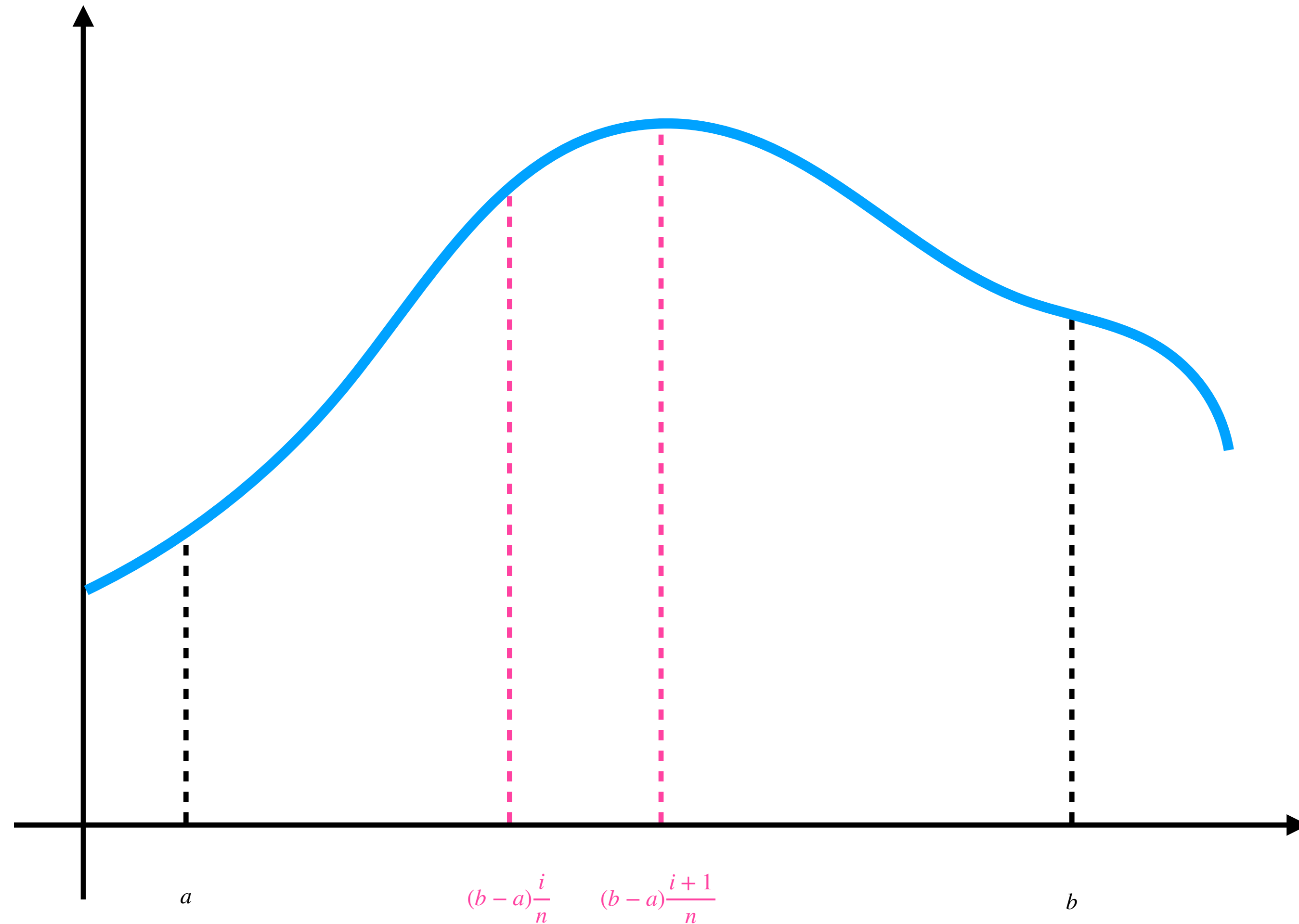
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Quadrature Rules: Trapezoidal Rule



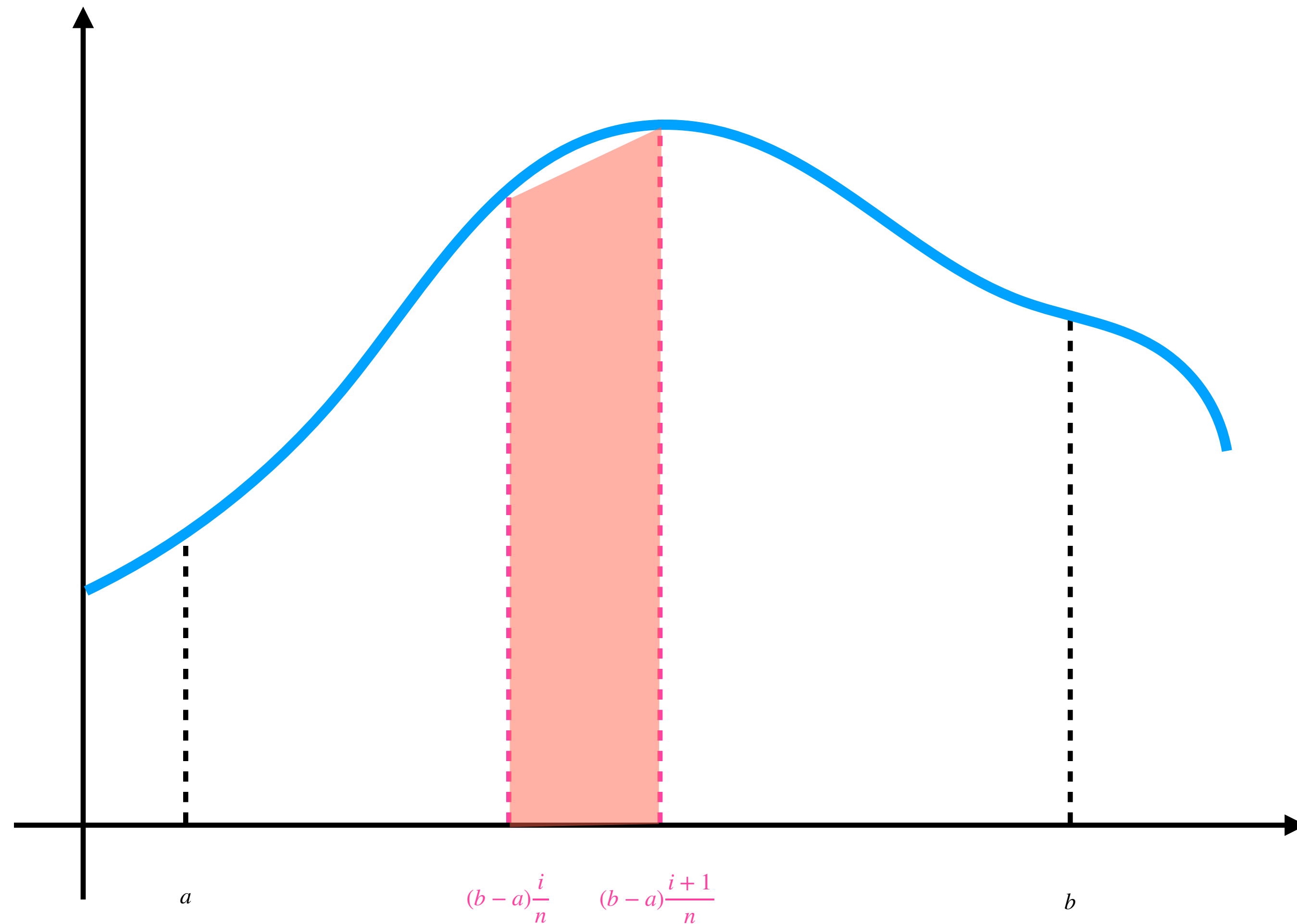
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Quadrature Rules: Trapezoidal Rule



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.

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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:

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

- 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.

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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:

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

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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 $p(x)$:

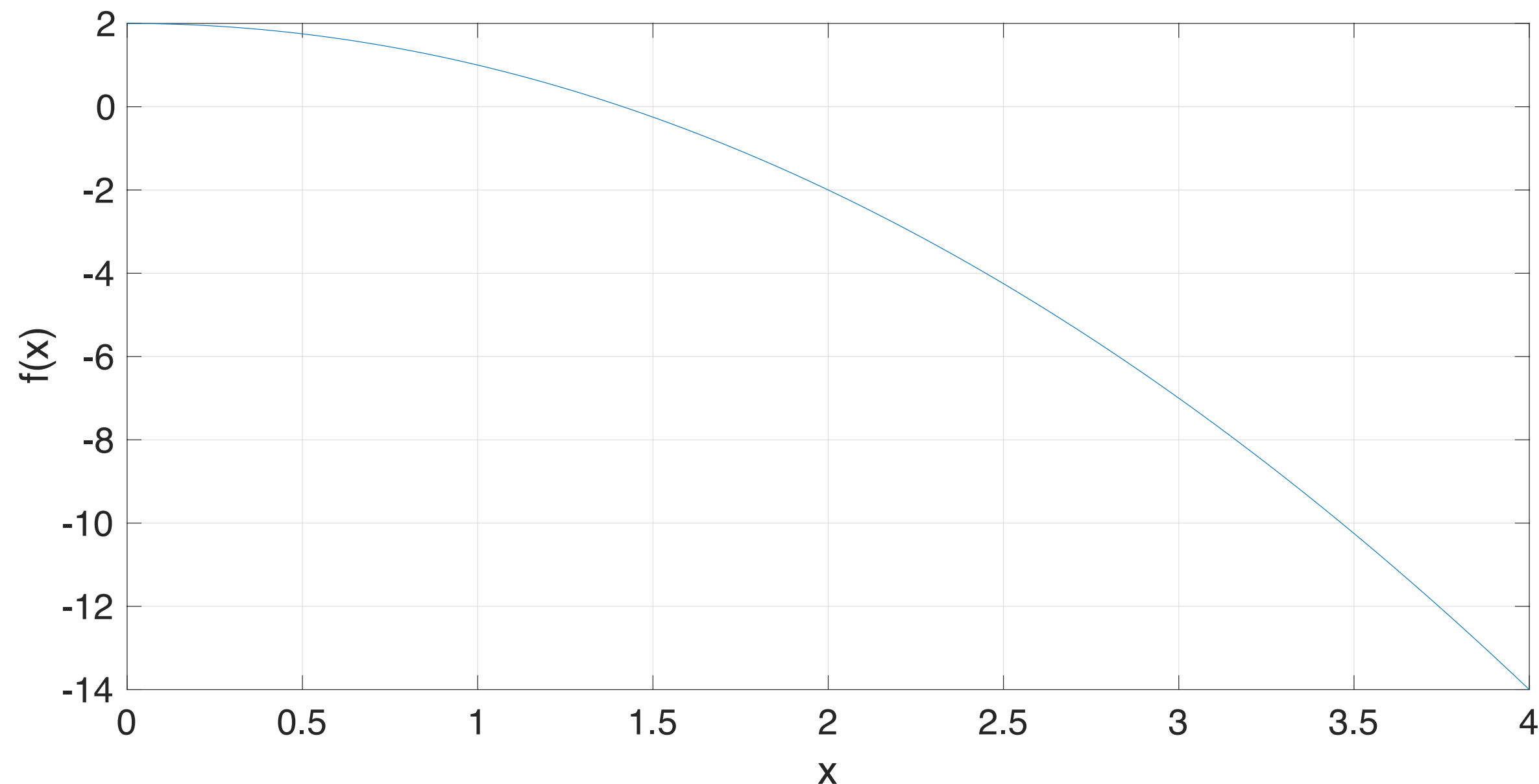
$$x_i = (a - b)u_i + b \quad u_i \in \mathbf{U}(0,1).$$

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An Example

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

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



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An Example

- In this simple case, if we draw 100,000 samples we will get as integral value **1.3xxx**, 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?

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An Example

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

$$\begin{aligned} \text{Var}(g(x)) &= \mathbb{E}(g(x)^2) - \mathbb{E}(g(x))^2 = \int_0^2 g(x)^2 p(x) dx - \left(\int_0^2 g(x) p(x) dx \right)^2 \\ &= \int_0^2 (2(-x^2 + 2))^2 \frac{1}{2} dx - \left(\int_0^2 (2(-x^2 + 2)) \frac{1}{2} dx \right)^2 = \frac{256}{45} = 5.689 \end{aligned}$$

.

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

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

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Conclusions

- Quadrature Rule Error:

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

- Monte-Carlo Error:

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

Bibliography

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Thank you for your attention!