Computational Physics I - Lecture 2, part 1

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Integrals and Derivatives

Integrals: $$I(a,b) = \int_a^b f(x)dx$$

- integrals occur widely in physics
- some integrals can be done analytically, most cannot!
- integration is one of the most important applications in computational physics

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- most derivatives can be done analytically
- we still often need numerical derivatives

Integrals and Derivatives

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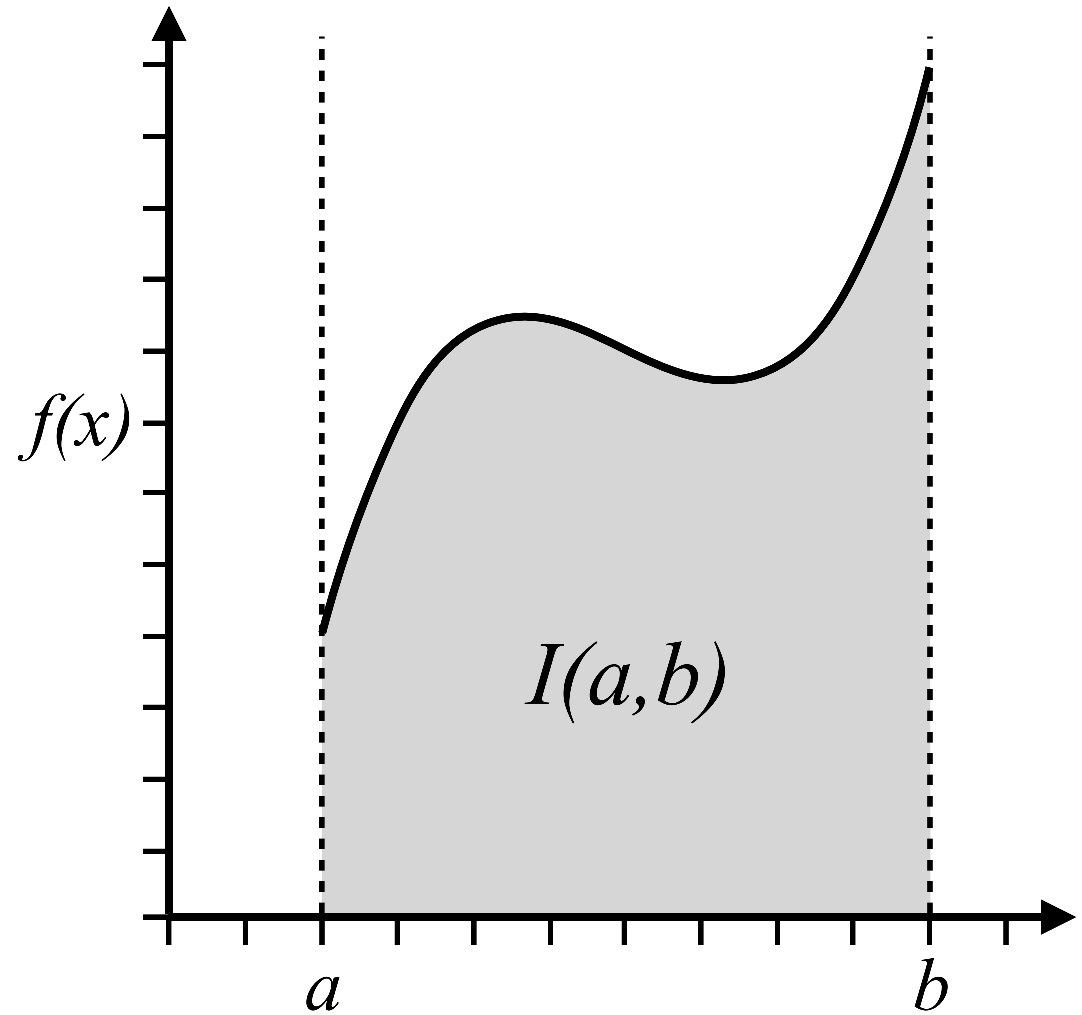
- programs like Maple or Mathematic can do symbolic integration to find *F(y)*
- symbolic integration is not a topic in this course

Definite Integrals

Definite integral: $I(a,b) = \int_a^b f(x)dx$

- we wish to know the numeric value of *I(a,b)*
- but computers are not good at continuous variables…



Integrals - Discretisation

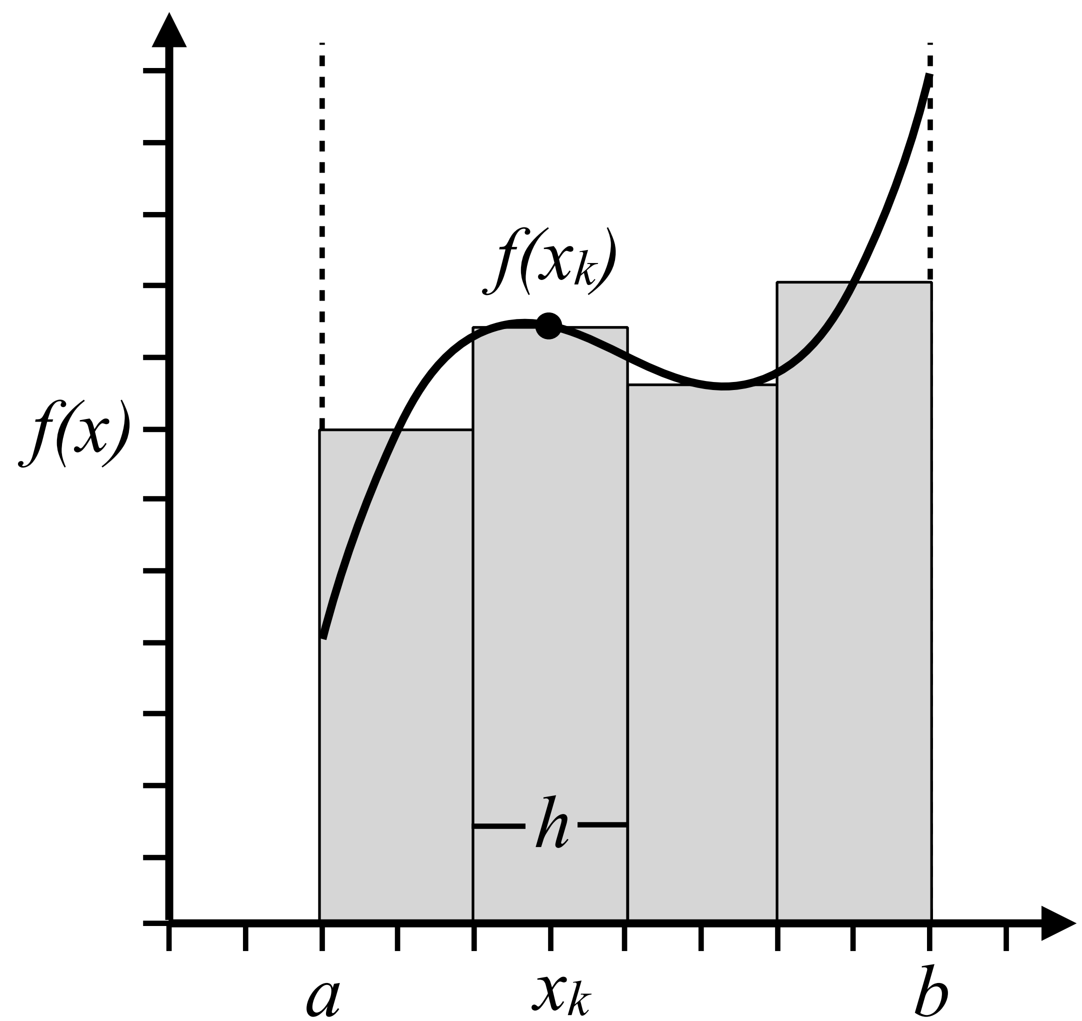
Definite integral: $I(a,b) = \int_a^b f(x)dx$

- instead: discretise
- divide interval *[a,b]* into *N* equal segments

$$h = (b-a)/N$$

$$x_k = a + (k - \frac{1}{2})h$$

$$I(a,b) \approx \sum_{k=1}^{N} f(x_k)h$$

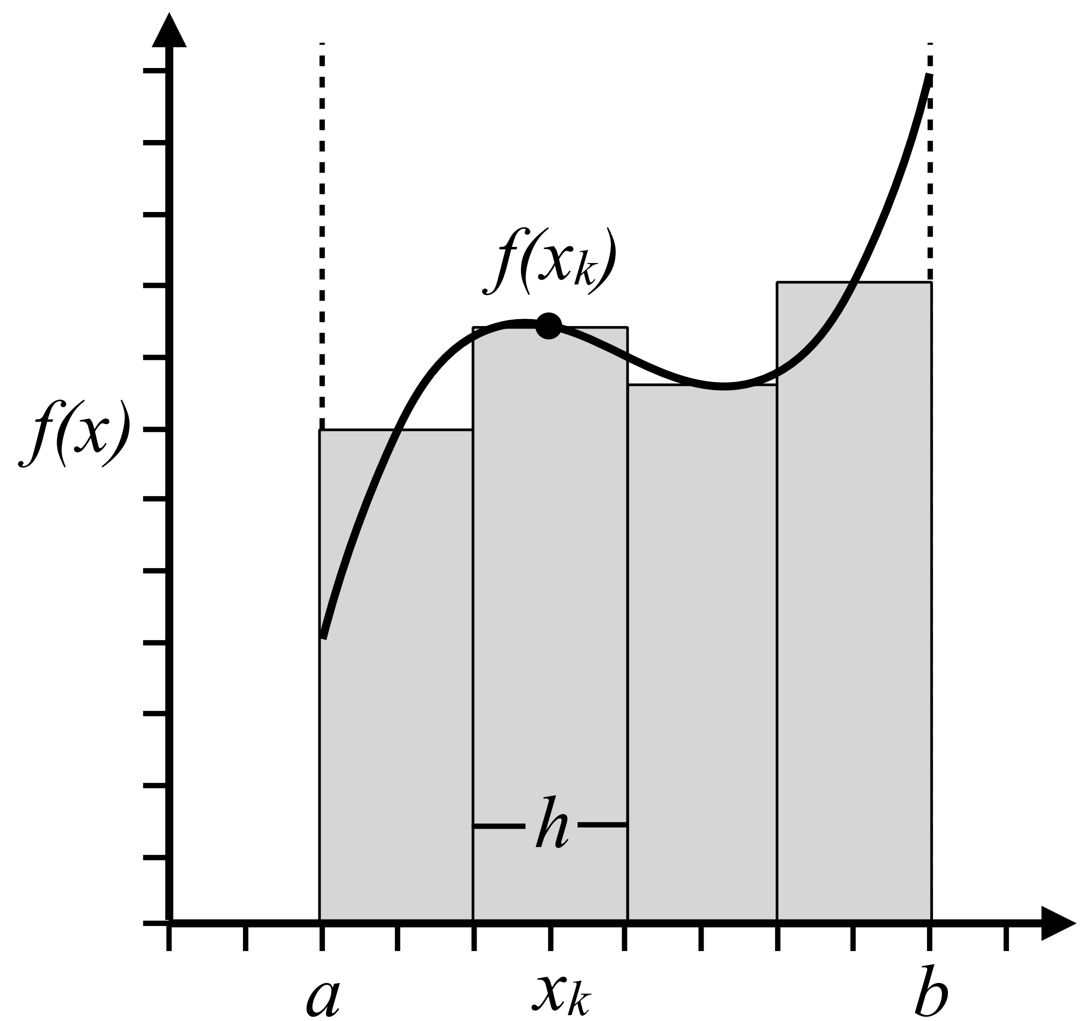


Integrals - Discretisation

Definite integral: $$I(a,b) = \int_a^b f(x)dx$$

Key concept: discretisation

Discretisation is a very common technique to make continuous variables tractable for a computer.



Integrals - Example 1

Integrate: $$\int_0^2 (x^4 - 2x + 1)dx$$

Integrals - Exercise 1

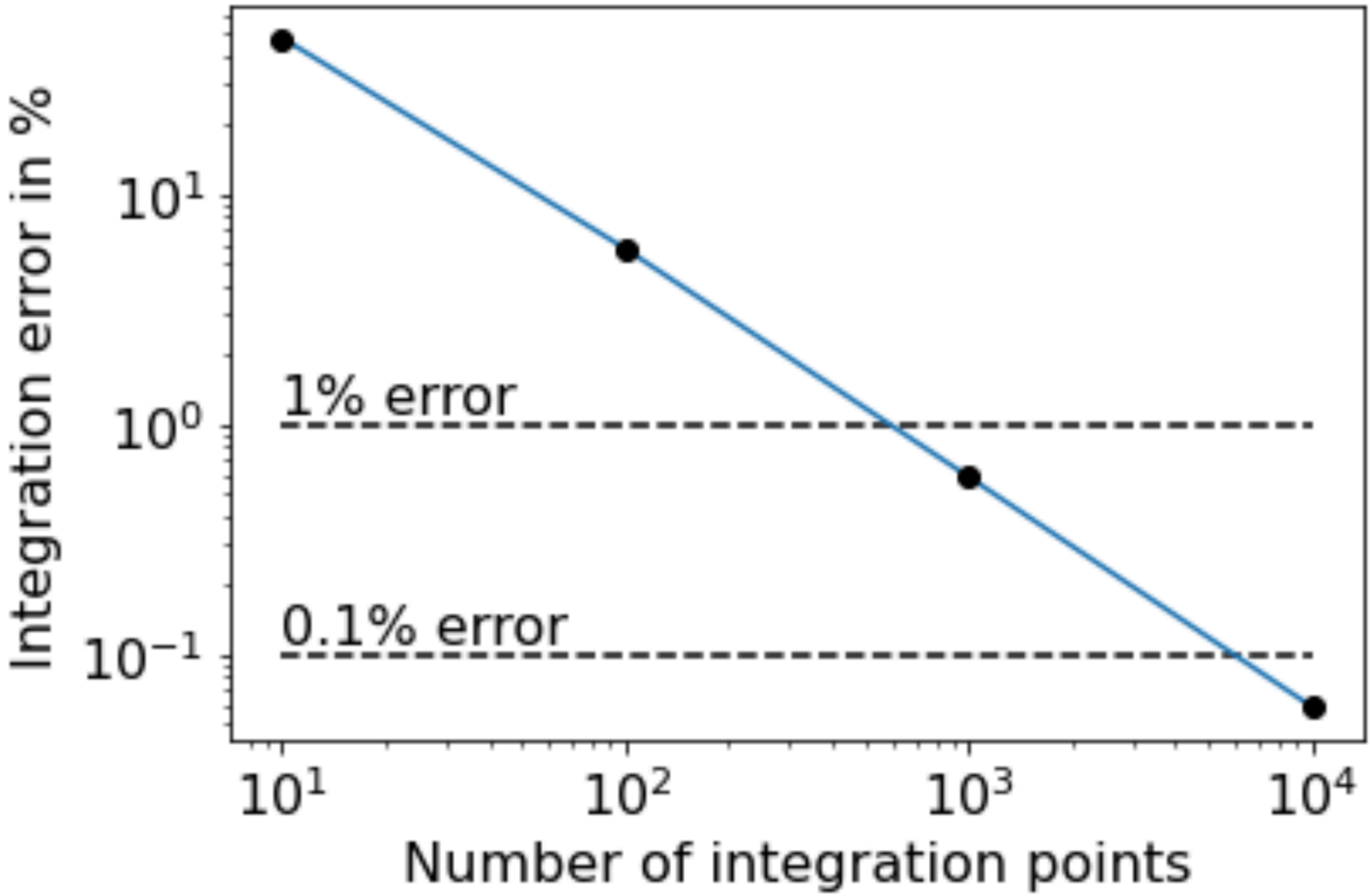
Integrate: $\int_0^2 (x^4 - 2x + 1)dx = 4.4$

1. Plot the function $f(x) = (x^4 - 2x + 1)$
2. Change the example integration program to add a loop over the number of discretisation points.
3. Plot the value of the integral and/or the integration error as a function of integration points.

Talking points:

1. **What do you observe?**
2. **How many points do you need for 1% accuracy and how many for 0.1% accuracy?**
3. **How can we do better?**

Integrals - Exercise 1 - Observation



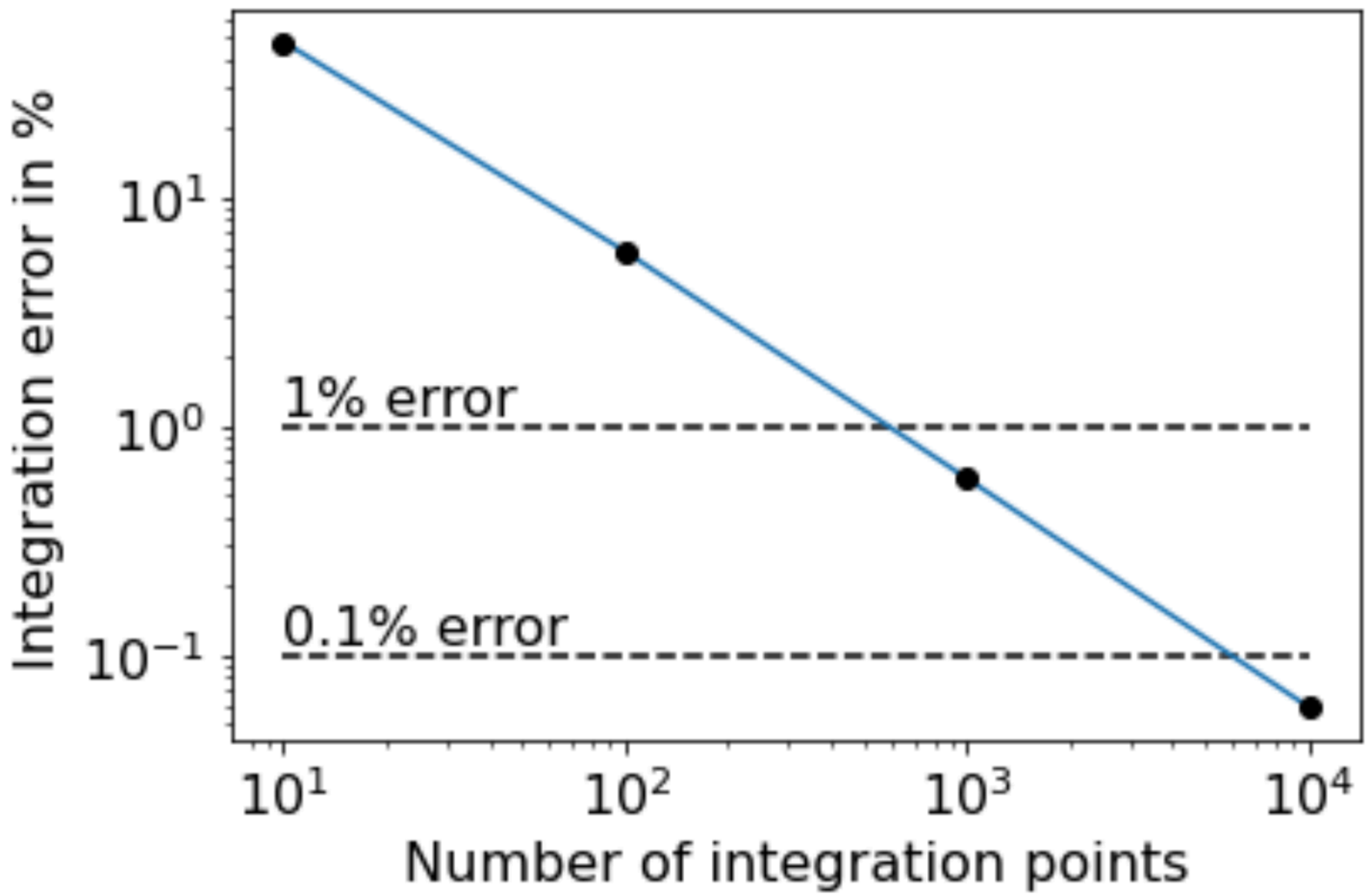
Integration rules - number of points & errors

Method	1% error	0.1% error
Naive	589	5907

Integrals - Convergence

Key concept: convergence

The result of a computation should not depend on the computational parameters within a tolerable accuracy. The results have then *converged* to their final value.



Integrals - Trapezoidal rule

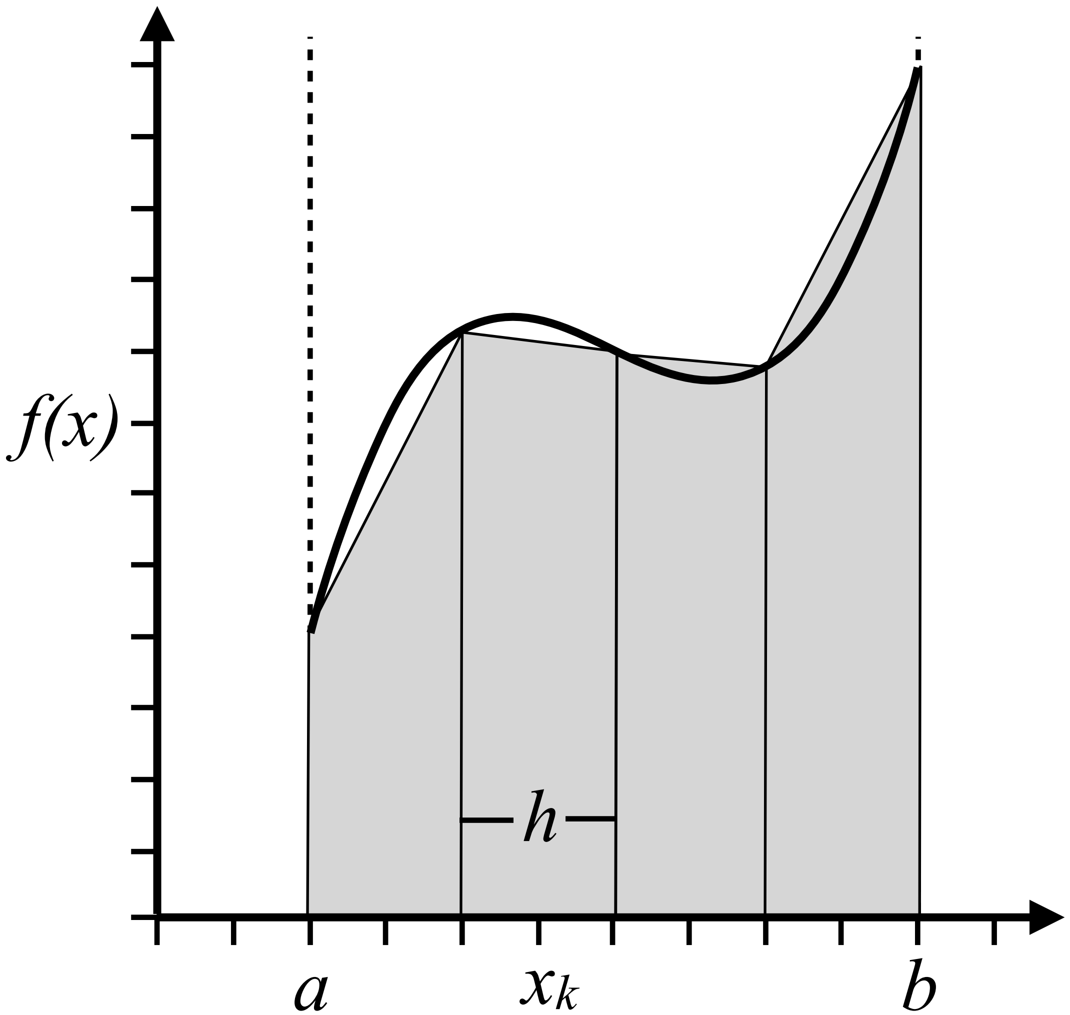
Replace constant by line that goes through endpoints.

- two endpoints of interval:

  $a + (k-1)h$ and $a + kh$

- area of segment:

$$A_k = \frac{1}{2} h \left[f(a + (k-1)h) \right.$$
$$\left. + f(a + kh) \right]$$



Integrals - Trapezoidal rule

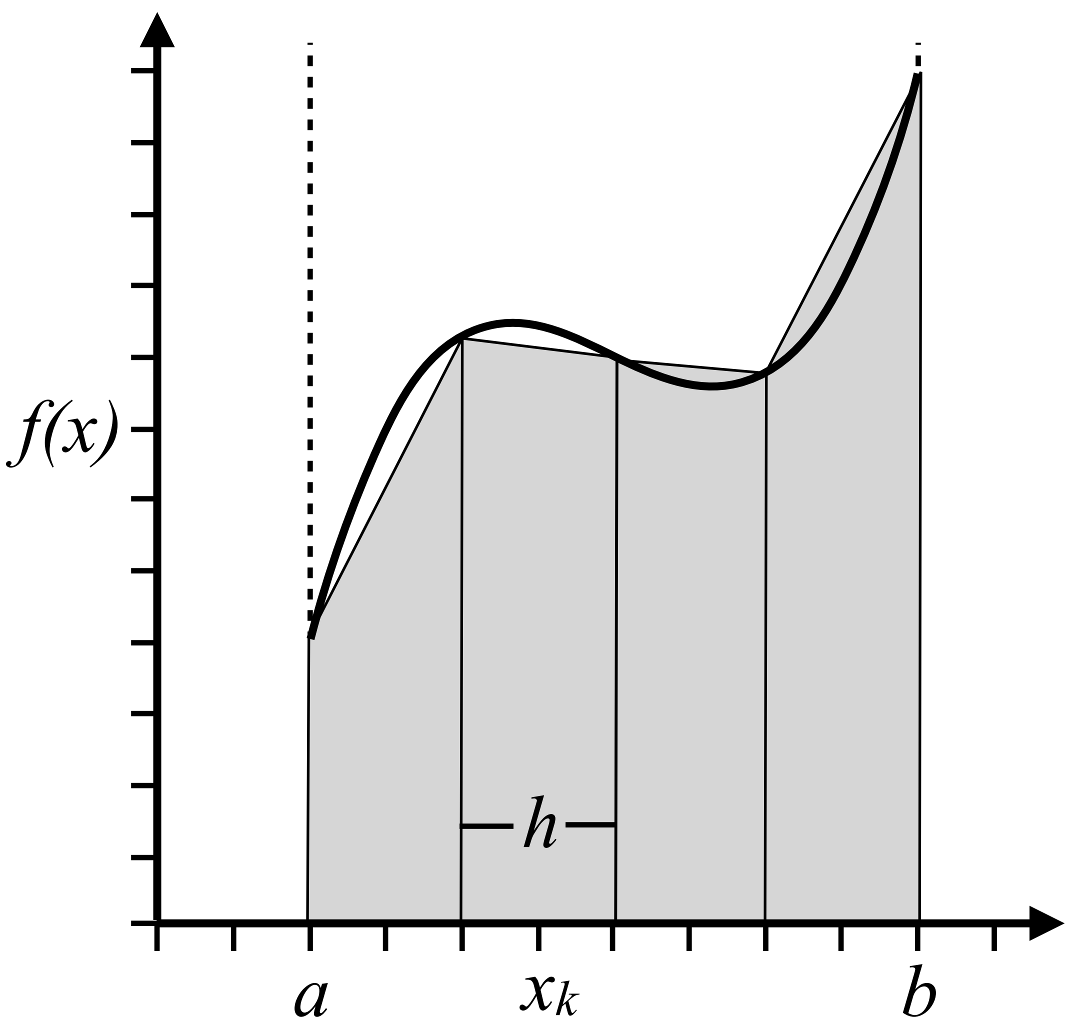
Replace constant by line that goes through endpoints.

- sum up segments for integral

$$I(a,b) \approx \sum_{k=1}^{N} A_k$$

$$= \frac{1}{2} h \sum_{k=1}^{N} \left[f(a+(k-1)h) + f(a+kh) \right]$$

$$= h \left[\frac{1}{2} f(a) + \frac{1}{2} f(b) + \sum_{k=1}^{N-1} f(a+kh) \right]$$



Integrals - Exercise 2

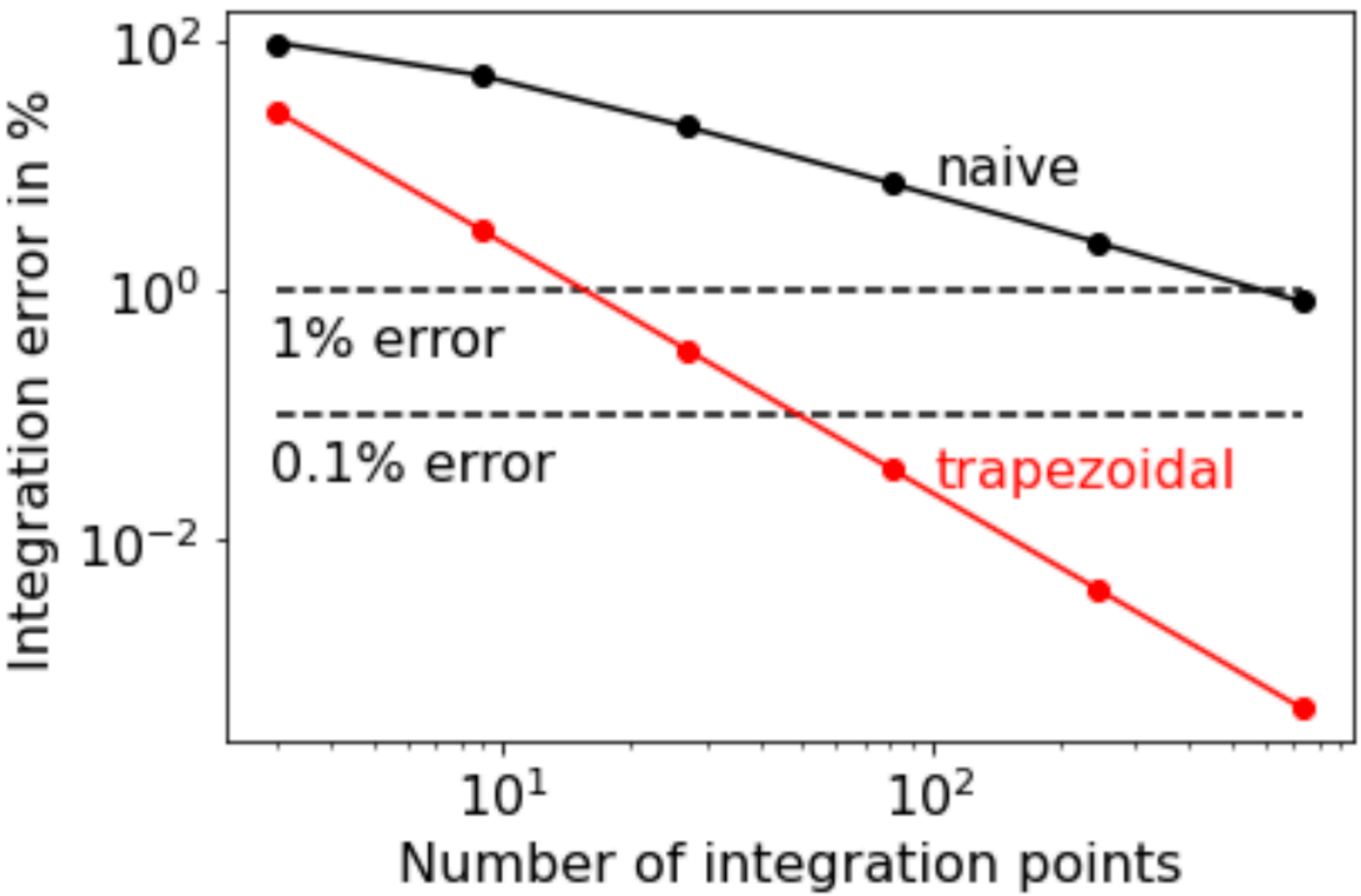
Integrate: $$\int_0^2 (x^4 - 2x + 1)dx = 4.4$$

1. Change your integration program to the trapezoidal rule. Loop over the number of discretisation points.
2. Plot the value of the integral and/or the integration error as a function of integration points.

Talking points:

1. **What changes with the trapezoidal rule?**
2. **How many points do you need for 1% accuracy and how many for 0.1% accuracy?**
3. **How could we do even better?**

Integrals - Exercise 2 - Observation

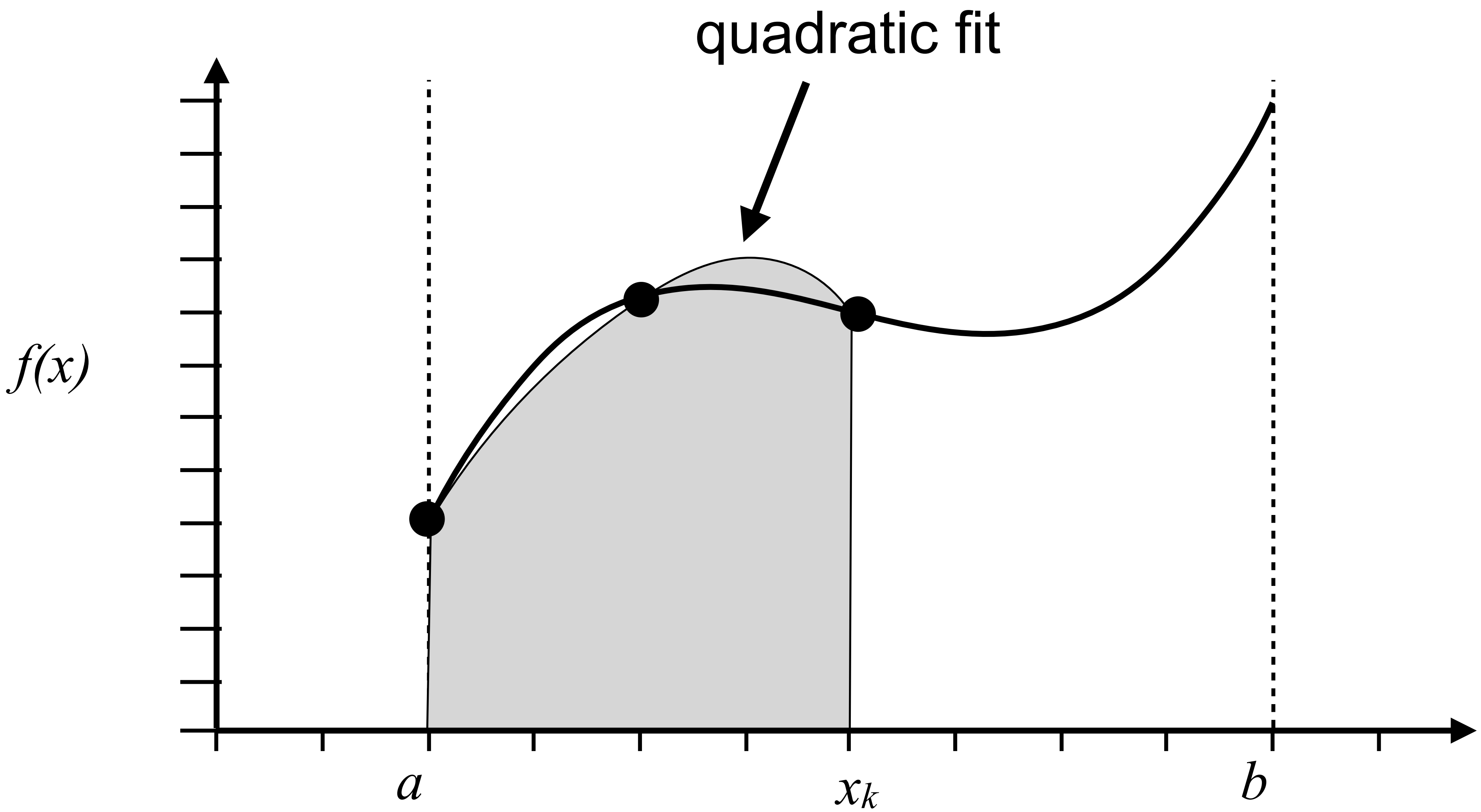


Integration rules - number of points & errors

Method	1% error	0.1% error
Naive	589	5907
Trapezoidal	16	50

Integrals - Simpson's rule

Do a Taylor expansion (to 2nd order) for the curve



Integrals - Simpson's rule

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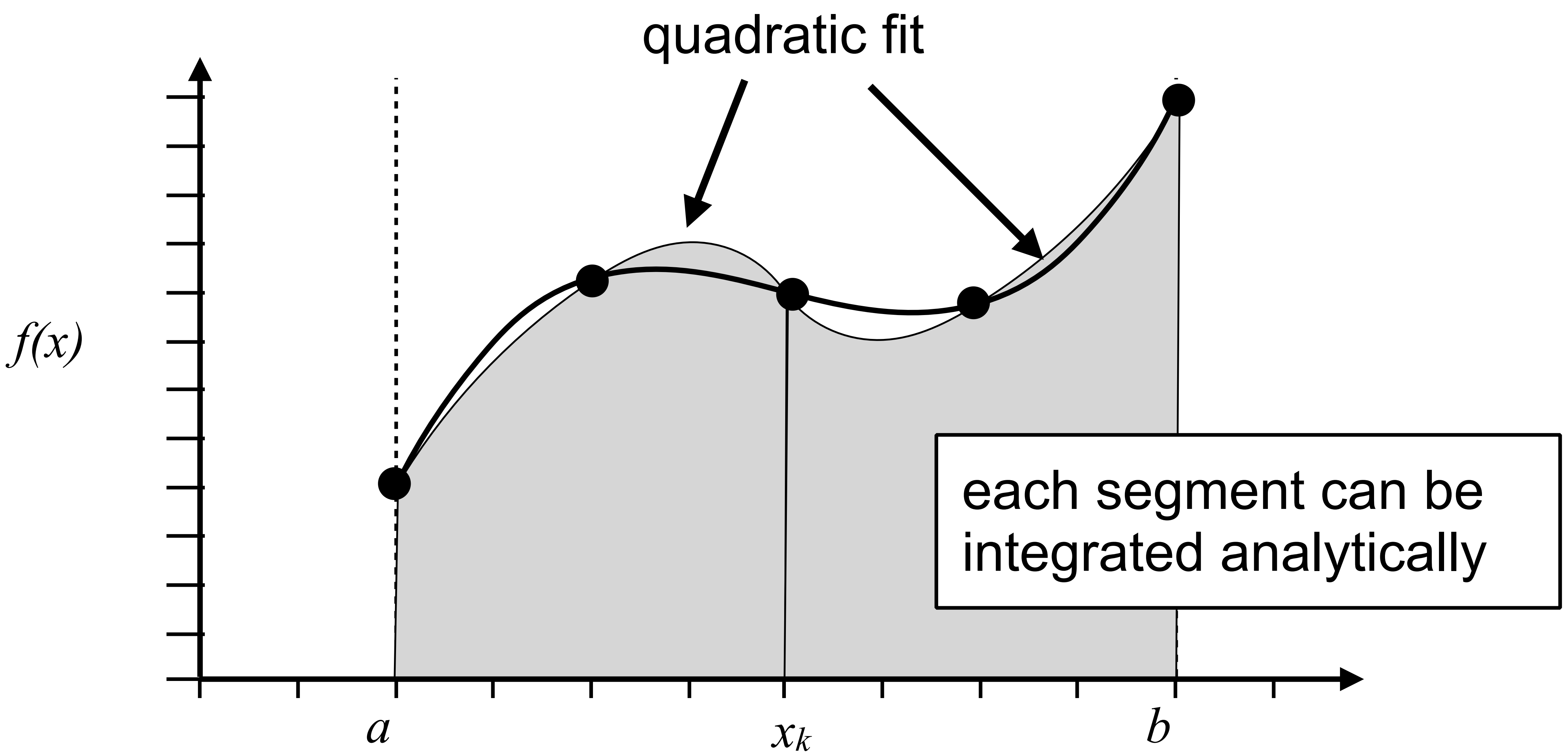

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Integrals - Simpson's rule

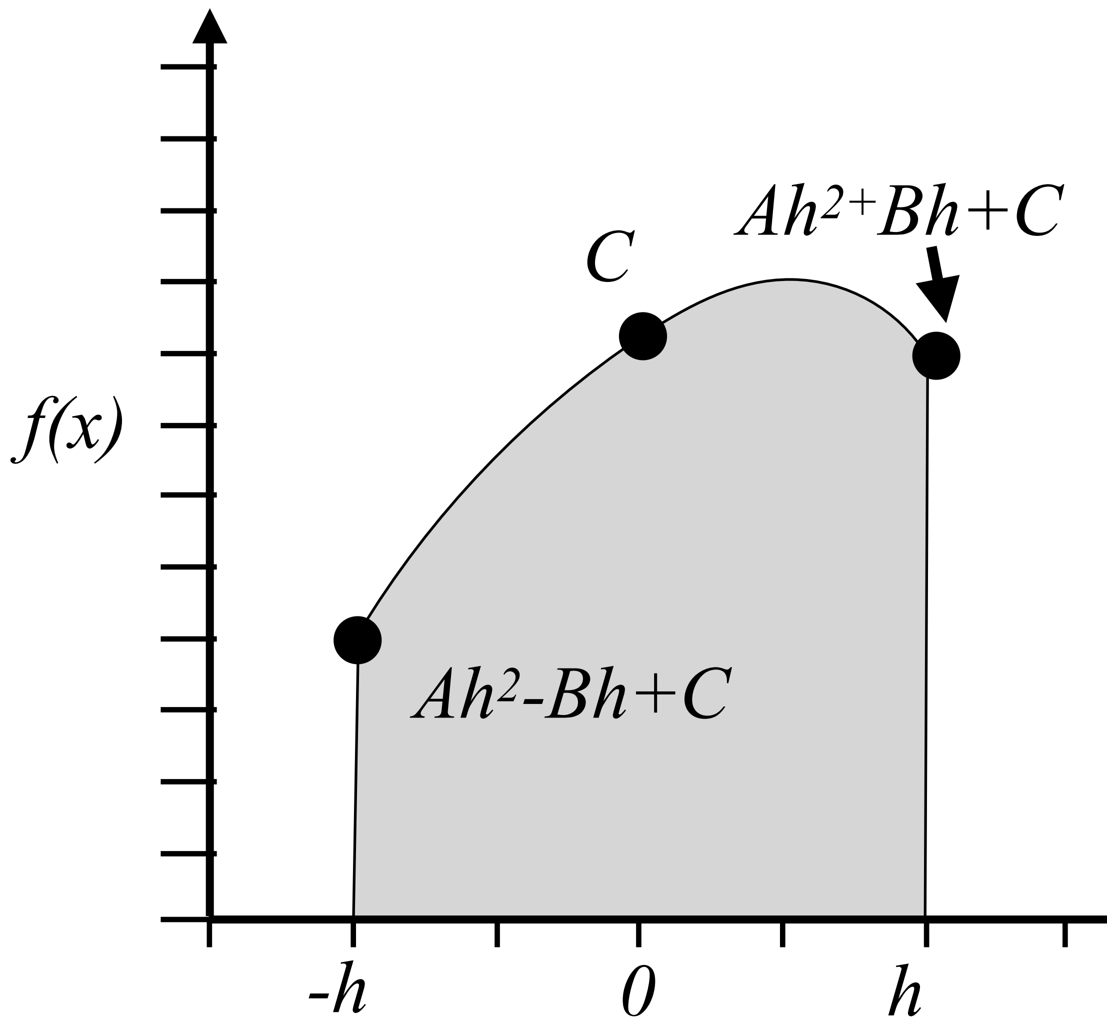
- we fit the function $Ax^2 + Bx + C$ to the points *-h*, *0* and *h*

- the solution is:

$$A = \frac{1}{h^2}\left[\frac{1}{2}f(-h) - f(0) + \frac{1}{2}f(h)\right]$$

$$B = \frac{1}{2h}\left[f(h) - f(-h)\right]$$

$$C = f(0)$$



Integrals - Simpson's rule

- with A, B, and C determined
  we can integrate:

$$
\begin{aligned}
\int_{-h}^{h} (Ax^2 + Bx + C)dx &= \frac{2}{3}Ah^3 + 2Ch \\
&= \frac{1}{3}\left[f(-h) + 4f(0) + f(h)\right]
\end{aligned}
$$

Integrals - Simpson's rule

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$$\int_{-h}^{h} (Ax^2 + Bx + C)dx = \frac{2}{3}Ah^3 + 2Ch$$
$$= \frac{1}{3}\left[f(-h) + 4f(0) + f(h)\right]$$

- Now generalize to incorporate also the remaining segments:

a, $a+h$ and $a+2h$ $\longrightarrow$ $a+2h$, $a+3h$ and $a+4h$

Integrals - Simpson's rule

- Now generalize to incorporate also the remaining segments:

a, $a+h$ and $a+2h$ ⟶ $a+2h$, $a+3h$ and $a+4h$

- The integral becomes:

$$\begin{aligned} I(a,b) \approx & \frac{h}{3}\left[f(a) + 4f(a+h) + f(a+2h)\right] \\ & + \frac{h}{3}\left[f(a+2h) + 4f(a+3h) + f(a+4h)\right] + \ldots \\ & + \frac{h}{3}\left[f(a+(N-2)h + 4f(a+(N-1)h) + f(b)\right] \end{aligned}$$

Integrals - Simpson's rule

- Rearranging terms gives:

$$I(a,b) \approx \frac{h}{3}\left[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \ldots + f(b)\right]$$

$$= \frac{h}{3}\left[f(a) + f(b) + 4\sum_{\substack{k \text{ odd} \\ 1\ldots N-1}} f(a+kh) + 2\sum_{\substack{k \text{ even} \\ 2\ldots N-2}} f(a+kh)\right]$$

- Simpson's rule requires an even number of points.

Integrals - Simpson's rule

- Rearranging terms gives:

$$
\begin{aligned}
I(a,b) &\approx \frac{h}{3}\left[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \ldots + f(b)\right] \\
&= \frac{h}{3}\left[f(a) + f(b) + 4\sum_{\substack{k \text{ odd} \\ 1\ldots N-1}} f(a+kh) + 2\sum_{\substack{k \text{ even} \\ 2\ldots N-2}} f(a+kh)\right] \\
&= \frac{h}{3}\left[f(a) + f(b) + 4\sum_{k=1}^{N/2} f(a+(2k-1)h) + 2\sum_{k=1}^{N/2-1} f(a+2kh)\right]
\end{aligned}
$$

- Simpson's rule requires an even number of points.

Integrals - Exercise 3

Integrate: $$\int_0^2 (x^4 - 2x + 1)dx = 4.4$$

1. Change your integration program to the Simpson's rule. Loop over the number of discretisation points.
2. Plot the value of the integral and/or the integration error as a function of integration points.

Talking points:
1. **What changes with the Simpson's rule?**
2. **How many points do you need for 1% accuracy and how many for 0.1% accuracy?**
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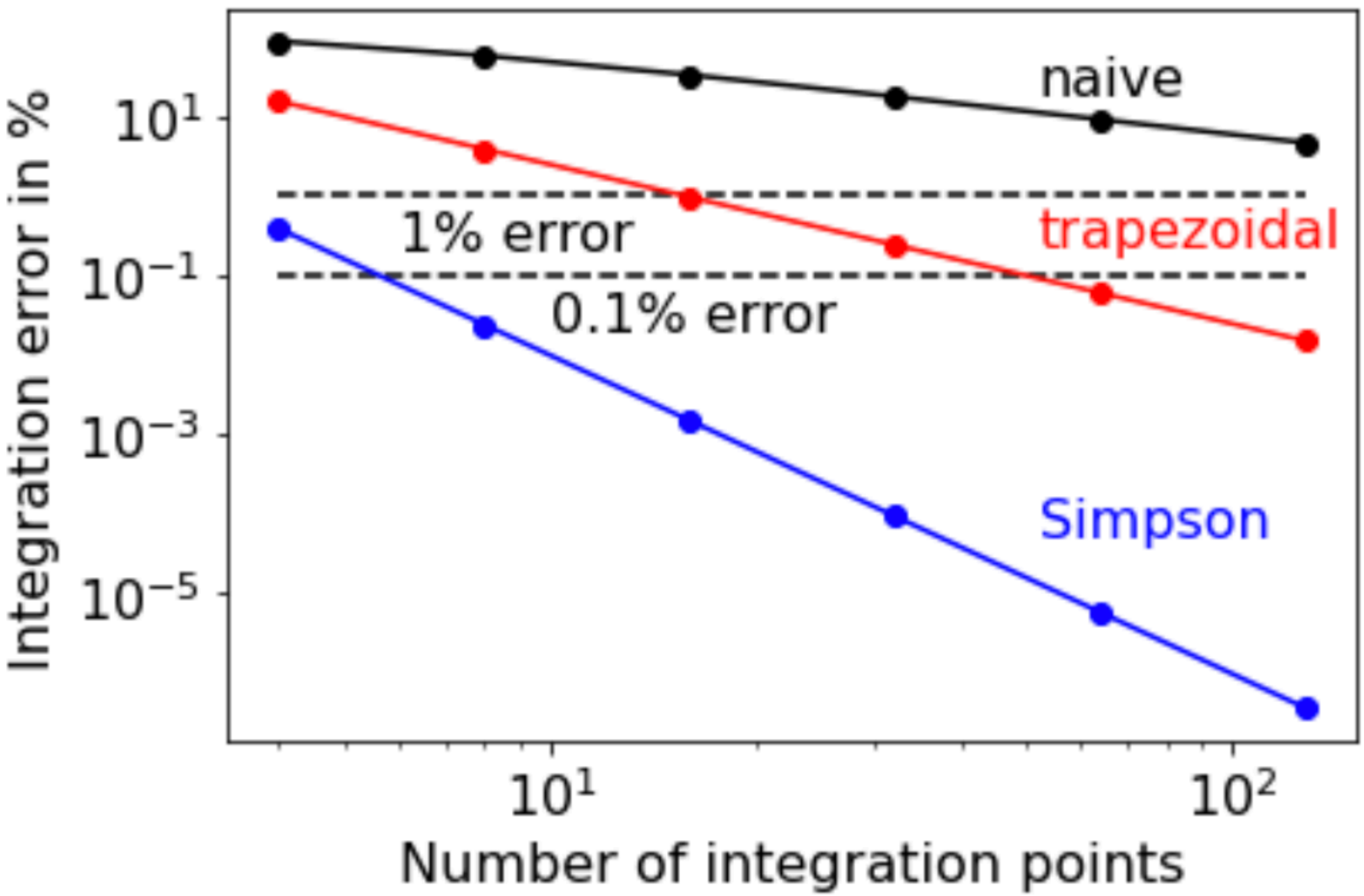
Integrals - Exercise 3 - Observation



Integration rules - number of points & errors

Method	1% error	0.1% error	order
Naive	589	5907	0th
Trapezoidal	16	50	1st
Simpson	2	6	2nd

Integrals - integration weights

- general integral expression

integration weights

$$\int_a^b f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$

integration points

Key concept: integration weights

Integrals are a sum over integration weights and function values. The weights depend on the integration method and can be precomputed.

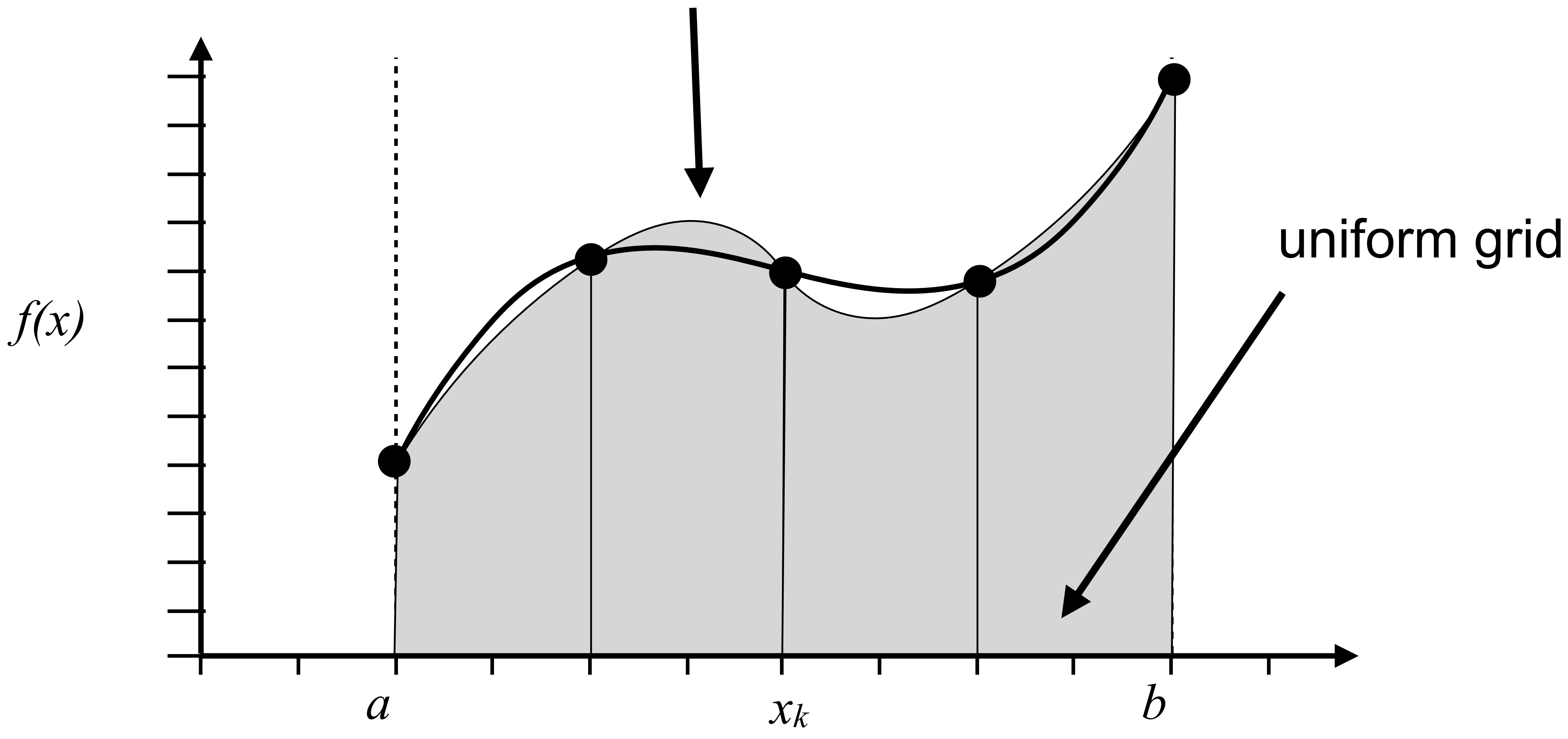
Integrals - integration weights

$$\int_a^b f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$

Order	Polynomial	Weights ($\{w_k\}$)
0 (naive)	constant	$1, 1, 1, \ldots, 1$
1 (trapezoidal rule)	straight line	$\frac{1}{2}, 1, 1, \ldots, 1, \frac{1}{2}$
2 (Simpson's rule)	quadratic	$\frac{1}{3}, \frac{4}{3}, \frac{2}{3}, \frac{4}{3}, \ldots, \frac{4}{3}, \frac{1}{3}$
3	cubic	$\frac{3}{8}, \frac{9}{8}, \frac{9}{8}, \frac{3}{4}, \frac{9}{8}, \frac{9}{8}, \frac{3}{4}, \ldots, \frac{9}{8}, \frac{3}{8}$
4	quartic	$\frac{14}{45}, \frac{64}{45}, \frac{8}{15}, \frac{64}{45}, \frac{28}{45}, \frac{64}{45}, \frac{8}{15}, \frac{64}{45}, \ldots, \frac{64}{45}, \frac{14}{45}$

Integrals - non uniform integration grids

So far we improved approximations for the integrand.



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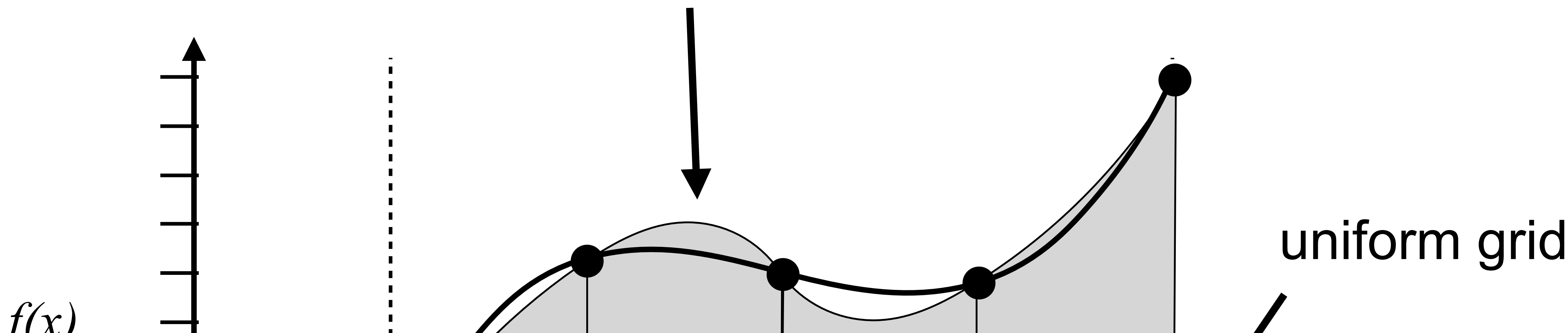

Question:

Could we position the integration points in an optimal way?

Integrals - non uniform integration grids

- We want to find the integration points and weights for:

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$

degree 2N-1 degree N-1 degree N-1

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Integrals - non uniform integration grids

- We want to find the integration points and weights for:

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$

- For simplicity we assume that *f* is a polynomial of degree *2N-1*
- We then divide *f* by a Legendre polynomial $P_N(x)$ of degree *N*

$$\underbrace{f(x)}_{\text{degree } 2N-1} = \underbrace{q(x)}_{\text{degree } N-1} P_N(x) + \underbrace{r(x)}_{\text{degree } N-1}$$

Integrals - Legendre polynomials

- Legendre polynomials satisfy the following properties

1. $\int_{-1}^{1} x^k P_N(x)dx = 0$ for all k between *0* and *N*

2. For all *N*, $P_N(x)$ has *N* real roots in *[-1,1]*

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2. For all *N*, $P_N(x)$ has *N* real roots in *[-1,1]*

- this gives:

$$\underbrace{f(x)}_{\text{degree } 2N-1} = \underbrace{q(x)}_{\text{degree } N-1} P_N(x) + r(x)$$

$$\int_{-1}^{1} f(x)dx = \underbrace{\int_{-1}^{1} q(x)P_N(x)dx}_{0} + \int_{-1}^{1} r(x)dx = \int_{-1}^{1} r(x)dx$$

Integrals - finding grid points

- insert $f = q * P_N + r$ into sum over points expression:

$$\sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} q(x_k) P_N(x_k) + \sum_{k=1}^{N} w_k r(x_k)$$

The integral is zero. Now we have to ensure that also this sum is zero.

- We know $P_N(x_k)=0$ if x_k are the roots of P_N:

$$\sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} w_k r(x_k) = \int_{-1}^{1} r(x)dx = \int_{-1}^{1} f(x)dx$$

Integrals - Gauss Legendre grid points

- If x_k are the roots of $P_N(x)$ then:

$$\int_{-1}^{1} f(x)dx = \sum_{k=1}^{N} w_k f(x_k)$$

Note, this is not approximate, but should be exact!

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- Algorithms exist that find the roots of functions. We will learn about them later in the course. For now, we can assume that the roots of $P_N(x)$ can be found with a subroutine.

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- Algorithms exist that find the roots of functions. We will learn about them later in the course. For now, we can assume that the roots of $P_N(x)$ can be found with a subroutine.
- Next we need to find the integration points.

Integrals - Gauss Legendre weights

- We assume that we can find a single polynomial of degree N-1 to fit the function $f(x)$. For this we use an *interpolating polynomial*:

$$\phi_k(x) = \prod_{\substack{m=1\ldots N \\ m\neq k}} \frac{(x - x_m)}{(x_k - x_m)}$$

$$= \frac{(x - x_1)}{(x_k - x_1)} \times \ldots \times \frac{(x - x_{k-1})}{(x_k - x_{k-1})} \frac{(x - x_{k+1})}{(x_k - x_{k+1})} \times \ldots \times \frac{(x - x_N)}{(x_k - x_N)}$$

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- $\phi_k(x)$ is a polynomial of degree N-1 with the property:

$$\phi_k(x_m) = \delta_{km}$$

Integrals - Gauss Legendre weights

- We now use $\phi_k(x)$ to define a surrogate function for *f(x)*:

$$\Phi(x) = \sum_{k=1}^{N} f(x_k)\phi_k(x)$$

Integrals - Gauss Legendre weights

- We now use $\phi_k(x)$ to define a surrogate function for $f(x)$:

$$\Phi(x) = \sum_{k=1}^{N} f(x_k)\phi_k(x)$$

- $\Phi(x)$ is identical to $f(x)$ at our $(\{x_m\})$:

$$\Phi(x_m) = \sum_{k=1} f(x_k)\phi_k(x_m) = \sum_{k=1} f(x_k)\delta_{km} = f(x_m)$$

Integrals - Gauss Legendre weights

- We now insert $\Phi(x)$ into our integral:

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} \Phi(x)dx = \int_{-1}^{1} \sum_{k=1}^{N} f(x_k)\phi_k(x)dx$$

$$= \sum_{k=1}^{N} f(x_k) \int_{-1}^{1} \phi_k(x)dx = \sum_{k=1}^{N} f(x_k)w_k$$

Integrals - Gauss Legendre weights

- We now insert *Φ(x)* into our integral:

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} \Phi(x)dx = \int_{-1}^{1} \sum_{k=1}^{N} f(x_k)\phi_k(x)dx$$

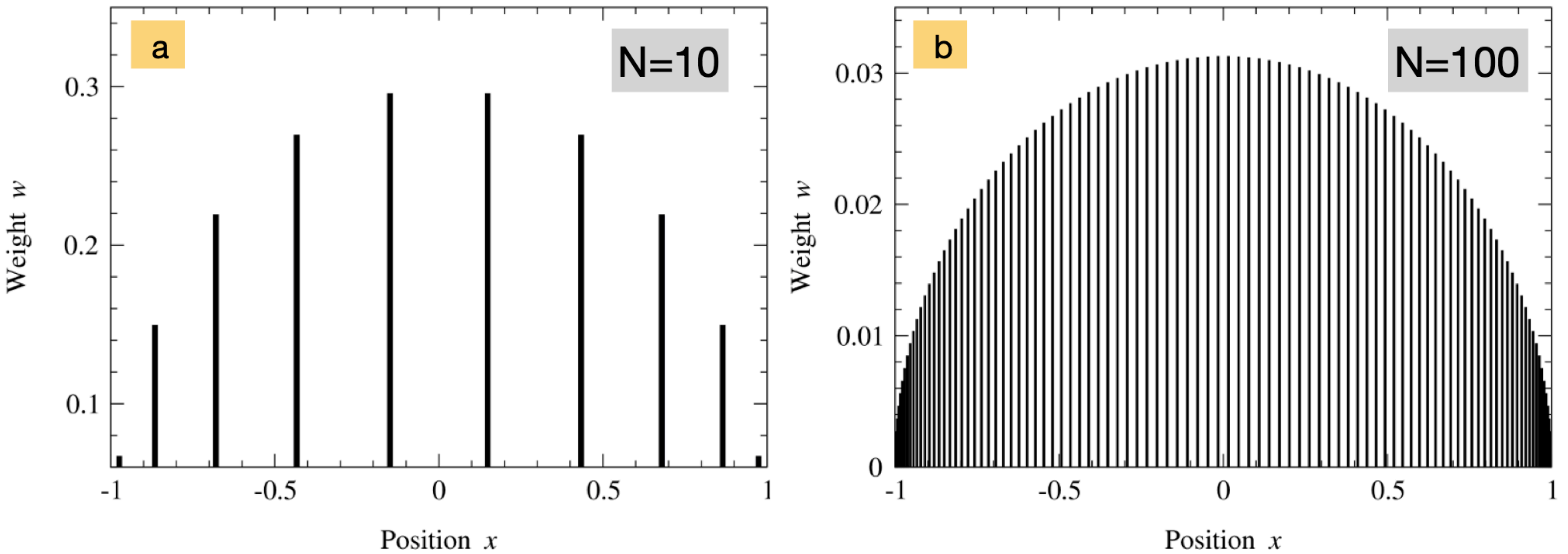
$$= \sum_{k=1}^{N} f(x_k) \int_{-1}^{1} \phi_k(x)dx = \sum_{k=1}^{N} f(x_k)w_k$$

- The weights are given as integral over $\phi_k(x)$:

$$w_k = \int_{-1}^{1} \phi_k(x)dx$$

- These integrals are tedious analytically but can be done numerically. Routines for this exist.

Integrals - Gauss Legendre points and weights



Integrals - Gauss Legendre summary

- Gauss-Legendre integration:

$$\int_{-1}^{1} f(x)dx = \sum_{k=1}^{N} w_k f(x_k)$$

roots of Legendre polynomial $P_N(x)$

given by interpolating polynomial: $w_k = \int_{-1}^{1} \phi_k(x)dx$

Key concept: Gauss-Legendre integration

With N integration points, any polynomial of degree $2N$-1 can be integrated exactly!

Integrals - Rescaling integration domain

- To change the integration domain from *[-1,1]* to *[a,b]* we need to rescale the integration points and weights as follows:

$$
\begin{aligned}
x'_k &= \frac{1}{2}(b-a)x_k + \frac{1}{2}(b+a) \\
w'_k &= \frac{1}{2}(b-a)w_k
\end{aligned}
$$

Integrals - Exercise 4

Integrate: $$\int_0^2 (x^4 - 2x + 1)dx = 4.4$$

1. Change your integration program to use Gauss-Legendre integration. The example notebook shows you how to call the **gaussxw** python package. Use N=*3* integration points.
2. Test what happens when you increase the number of integration points.

Talking points:

1. **What changes with Gauss-Legendre integration?**
2. **Do you still need to verify convergence?**

Integration rules - number of points & errors

Method	1% error	0.1% error	order
Naive	589	5907	0th
Trapezoidal	16	50	1st
Simpson	2	6	2nd
		exact	
Gauss Legendre		3	

Integration - Summary II

Choosing the right integration method

Method	complexity	accuracy	noisy data	pathological integrals
Trapezoidal	low	low	yes	yes
Simpson	medium	medium	less suitable	less suitable
Gauss Legendre	high	high	less suitable	less suitable

Integration - Summary I

Key concept: numeric integration

Integrals over finite ranges can be solved numerically as sum over function values at grid points with appropriate weights.

$$\int_a^b f(x)dx \approx \sum_{k=1}^{N} w_k f(x_k)$$