Computational Physics I - Lecture 2, part 2

Adam Foster, Dorothea Golze, Patrick Rinke
Levi Keller, Yashasvi Ranawat, Ygor Morais Jaques

Aalto University
School of Science
Department of Applied Physics

Integrals and Derivatives

Integrals: $$I(a,b) = \int_a^b f(x)dx$$ Last week / Some more today

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

Derivatives: $$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$ Today

- derivatives occur widely in physics
- most derivatives can be done analytically
- we still often need numerical derivatives

Definite Integrals

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

- we know now how to calculate the numeric value of *I(a,b)*

Question:

Can we also treat infinite integrals?

$$I = \int_0^\infty f(x)dx$$

Infinite Integrals

Infinite integral: $I = \int_0^\infty f(x)dx$

- we could brute force the problem with a finite integral

$$I = \lim_{b\to\infty} \int_0^b f(x)dx$$

and then make b larger and larger.

Infinite Integrals

Infinite integral: $I = \int_0^\infty f(x)dx$

- we could brute force the problem with a finite integral

$$I = \lim_{b \to \infty} \int_0^b f(x)dx$$

  and then make b larger and larger.

- This works, when $f(x)$ goes to 0 with increasing x.
- However, we introduce a new convergence parameter, b, and the integral may converge badly.
- Maybe we can do something more clever.

Infinite Integrals

Infinite integral: $I = \int_0^\infty f(x)dx$

- we make a variable transformation

$$z = \frac{x}{1+x} \quad \text{or equivalently} \quad x = \frac{z}{1-z}$$

Infinite Integrals

Infinite integral: $I = \int_0^\infty f(x)dx$

- we make a variable transformation

$$z = \frac{x}{1+x} \quad \text{or equivalently} \quad x = \frac{z}{1-z}$$

- with $dx = dz/(1-z)^2$ we obtain:

$$\int_0^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f(\frac{z}{1-z})dz$$

- this integral can be solved with the techniques we learned

Infinite Integrals

Infinite integral: $I = \int_a^{\infty} f(x)dx$

- now we make two transformations - first $y=x\text{-}a$ and then the one we made on the previous slide:

$$z = \frac{x-a}{1+x-a} \quad \text{or equivalently} \quad x = \frac{z}{1-z} + a$$

Infinite Integrals

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- with $dx = dz/(1-z)^2$ we obtain:

$$\int_a^{\infty} f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f(\frac{z}{1-z} + a)dz$$

Infinite Integrals

Infinite integral: $I = \int_{-\infty}^{\infty} f(x)dx$

- we could break this integral up into two: $\int_{-\infty}^{0} + \int_{0}^{\infty}$

Infinite Integrals

Infinite integral: $I = \int_{-\infty}^{\infty} f(x)dx$

- we could break this integral up into two: $\int_{-\infty}^{0} + \int_{0}^{\infty}$

- or make a single substitution:

$$x = \frac{z}{1-z^2}, \quad dx = \frac{1+z^2}{(1-z^2)^2}dz$$

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-1}^{1} \frac{1+z^2}{(1-z)^2} f(\frac{z}{1-z^2})dz$$

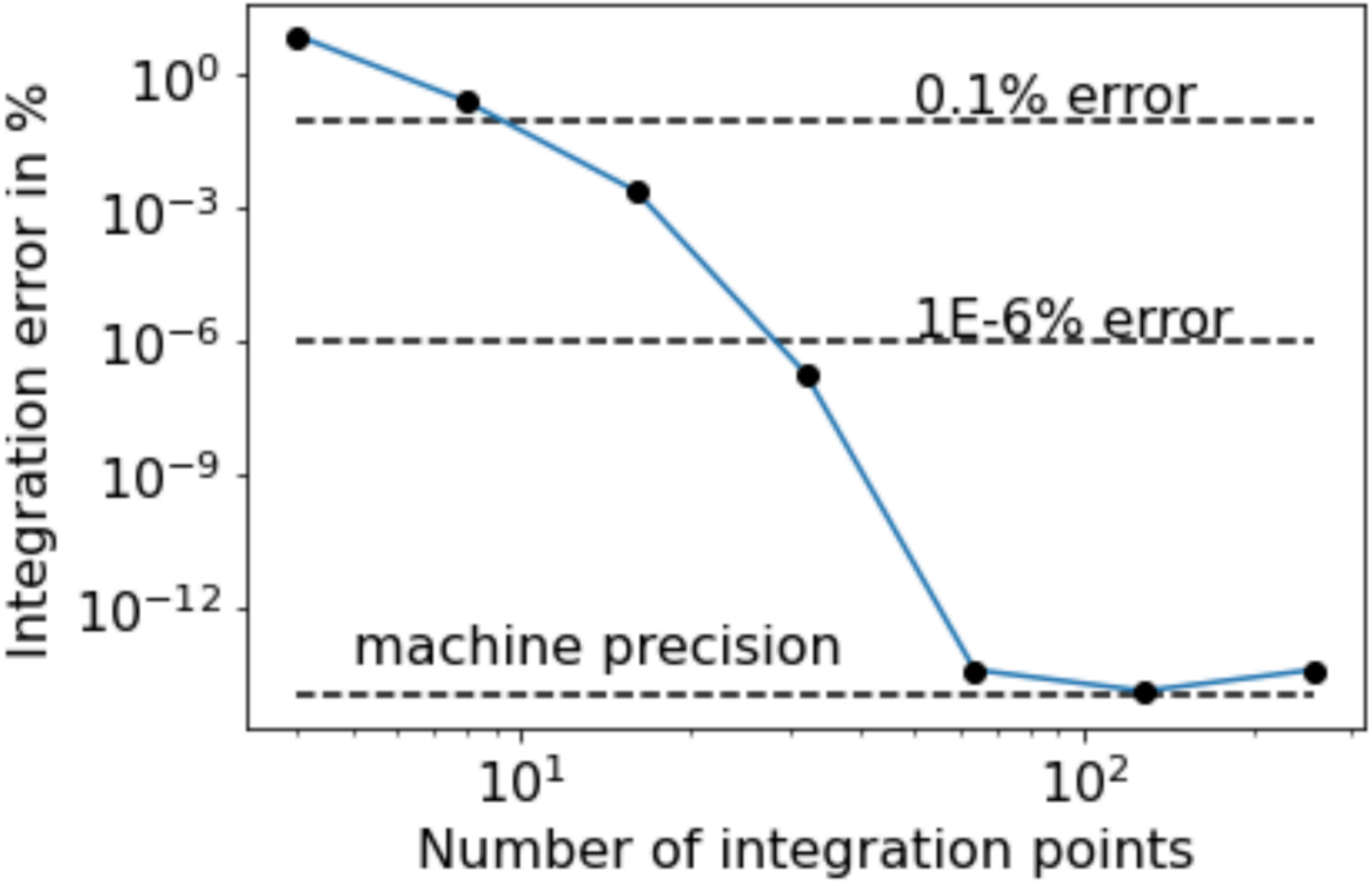
Integrals - Exercise 1

Integrate: $$\int_0^\infty e^{-t^2} dt = \frac{1}{2}\sqrt{\pi} = 0.886226925453\ldots$$

1. Make the transformation $z = t/(1+t)$
   The integral becomes: $$\int_0^1 \frac{e^{-z^2/(1-z)^2}}{(1-z)^2} dz$$
2. Plot the old and the new integrant.
3. Integrate with your Gauss-Legendre integration program.
4. Plot the error as a function of integration points.

Talking points:
1. **What do you observe?**
2. **How many points do you need for 0.1% or 10^{-6}% accuracy?**

Infinite integrals - number of points & errors



Integration rules - number of points & errors

Method	0.1% error	1E-6 % error
Gauss Legendre	9	27

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Key concept: variable transformation

Through *variable transformation* we can turn an infinite into a finite integral and thus make it tractable numerically.

Multiple Integrals

Multiple integral: $$I = \int_0^1 \int_0^1 f(x, y)dxdy$$

- We perform the integrals sequentially. We define:

$$F(y) = \int_0^1 f(x, y)dx$$

- Then our integral becomes:

$$I = \int_0^1 F(y)dy$$

Multiple Integrals

Multiple integral: $$I = \int_0^1 \int_0^1 f(x,y)\,dx\,dy$$

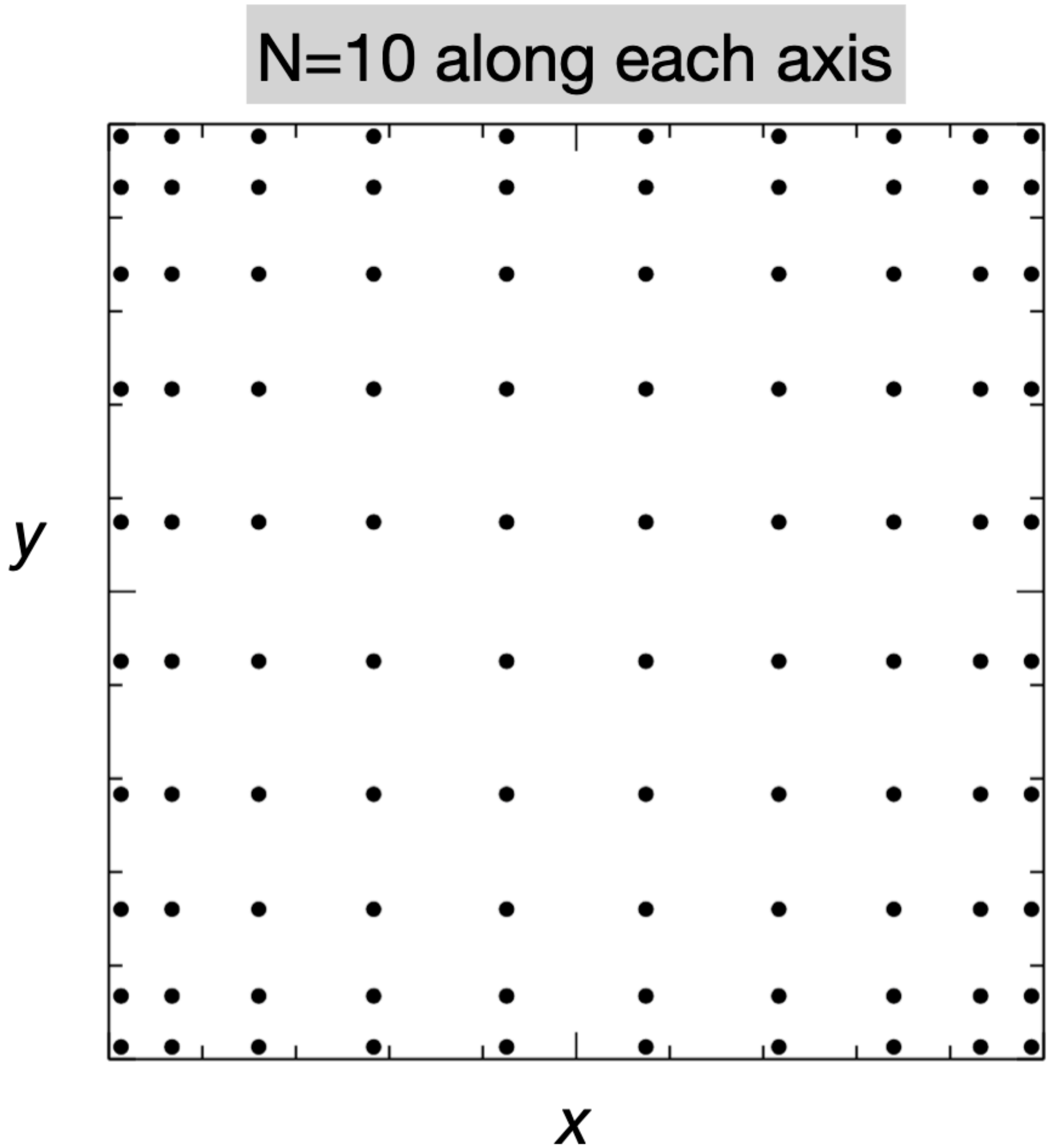
- Applying our numeric integration formula:

$$F(y) \approx \sum_{i=1}^{N} w_i f(x_i, y) \quad \text{and} \quad I \approx \sum_{j=1}^{N} w_j F(y_j)$$

- As expected, we obtain a double sum over the x and y coordinates of a 2 dimensional grid:

$$I \approx \sum_{i=1}^{N} \sum_{j=1}^{N} w_i w_j f(x_i, y_j)$$

Multiple Integrals - 2D Gauss Legendre grid



Integrals - Exercise 2

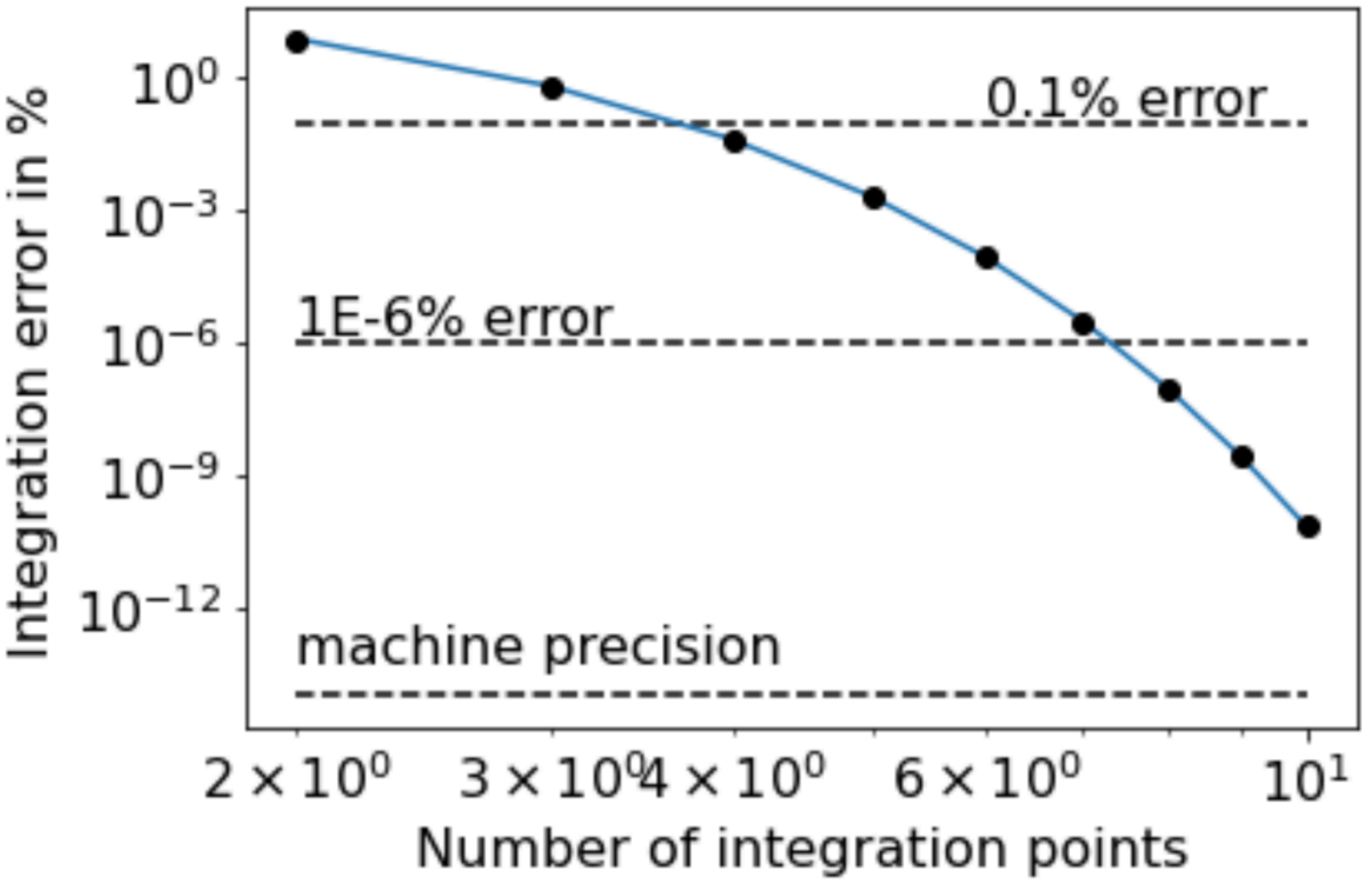
Integrate: $$\int_{-1}^{1}\int_{-1}^{1} e^{(-x^2-y^2)}\,dx\,dy = \pi\,\mathrm{erf}(1)^2$$

1. Plot the function $e^{(-x^2-y^2)}$.
2. Adapt your Gauss-Legendre integration program to solve this integral.
3. Plot the error as a function of integration points.

Talking points:

1. **What do you observe?**
2. **How many points do you need for 0.1% or 10^{-6}% accuracy?**

Multiple integrals - number of points & errors



Multiple Integrals - Note on convergence

Multiple integral: $$I \approx \sum_{i=1}^{N_i} \sum_{j=1}^{N_j} w_i w_j f(x_i, y_j)$$

- Normally we would have one convergence parameter per dimension, as N_i is typically not the same as N_j.

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- Normally we would have one convergence parameter per dimension, as N_i is typically not the same as N_j.

$$\int_{-1}^{1} \int_{-1}^{1} e^{(-x^2-y^2)} dx dy = \pi \, \mathrm{erf}(1)^2$$

- However, the integral in our example had the same x and y dimensions, so $N_i = N_j = N$ is justified.

Multiple integrals - number of points & errors

Method	0.1% error	1E-6 % error
Gauss Legendre	5x5=25	8x8=64

Multiple integrals - number of points & errors

Method	0.1% error	1E-6 % error
Gauss Legendre	5x5=25	8x8=64

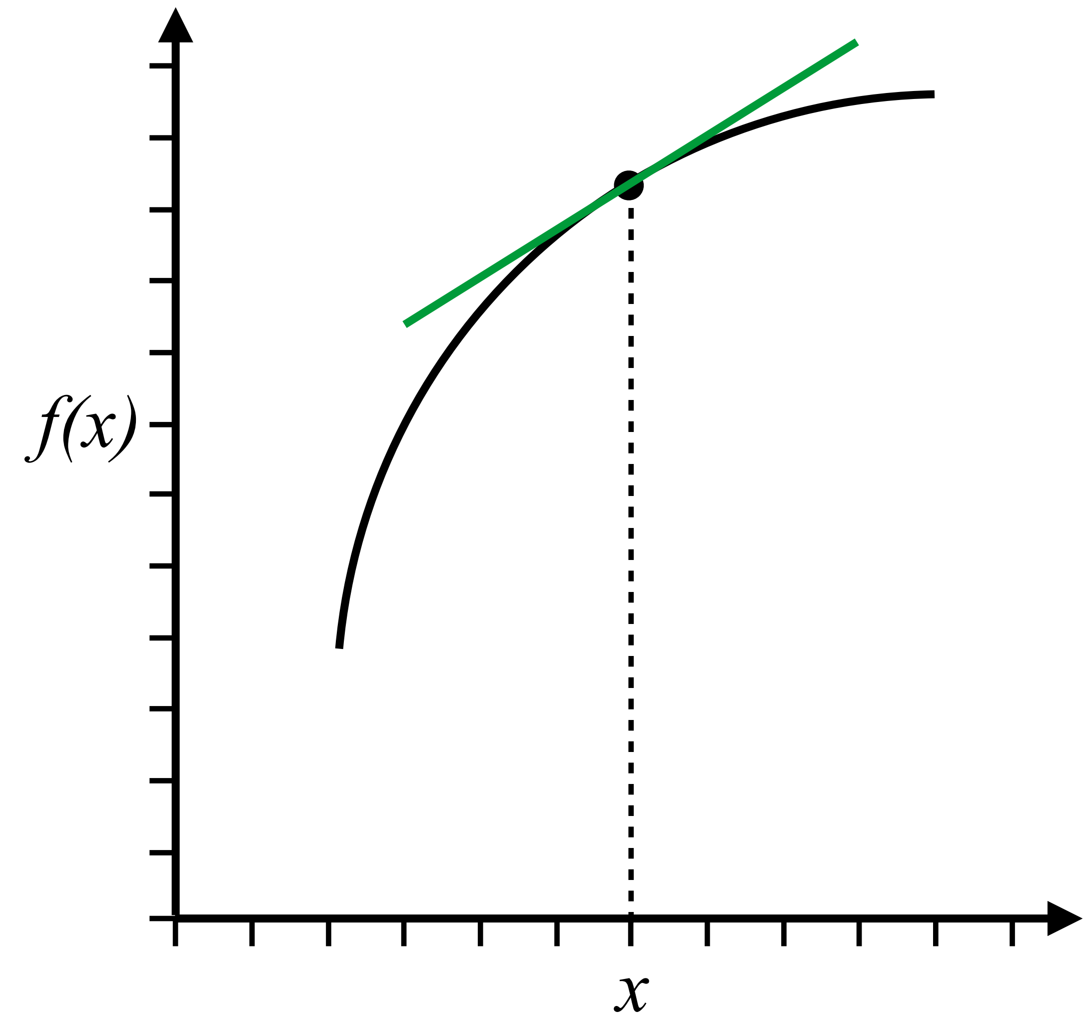
Key concept: multi dimensional integration

A multi dimensional integral can be performed as nested sum over the variables.

Derivatives

Derivative: $$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- we wish to find the derivative of a function numerically

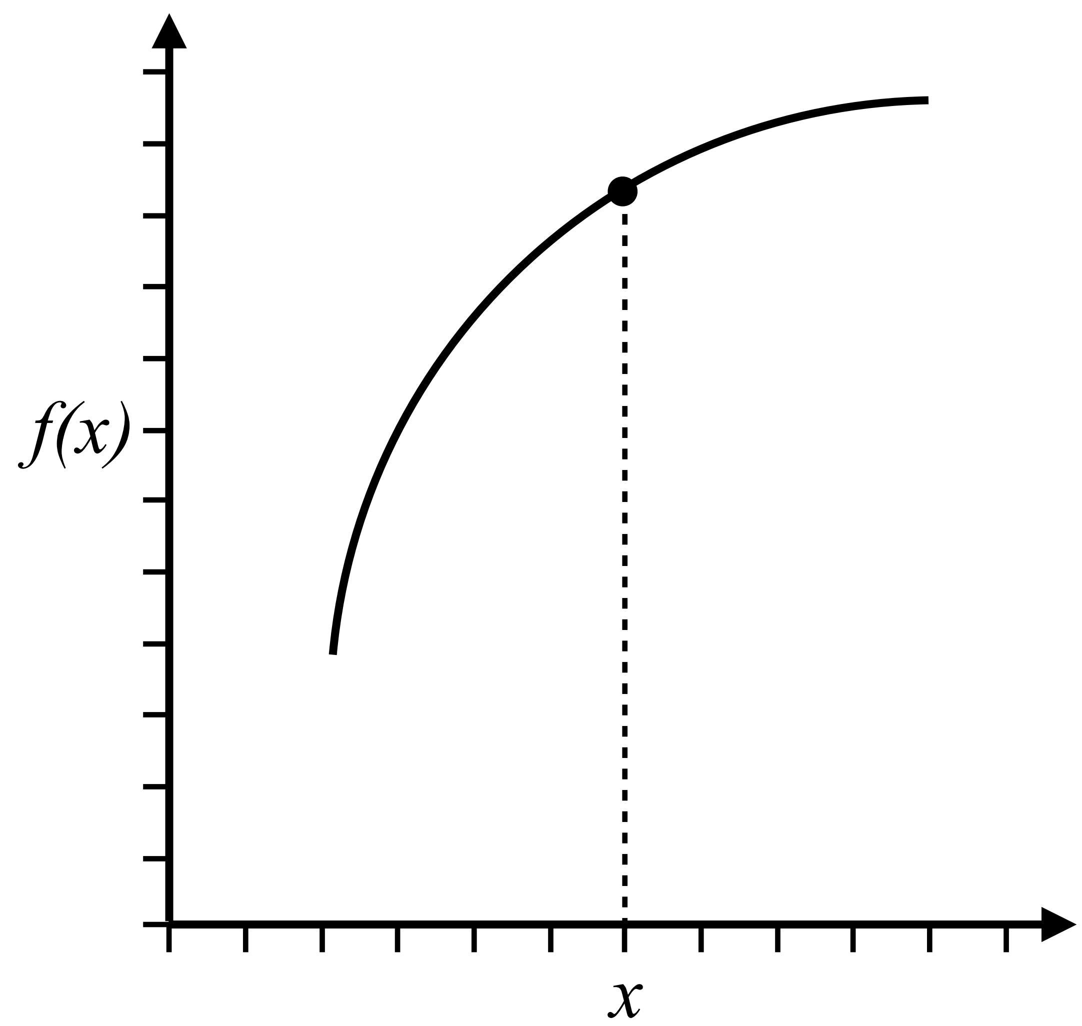


Derivatives

Derivative: $$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- in practice we cannot take the limit *h->0* numerically
- but we can make h very small:

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h}$$



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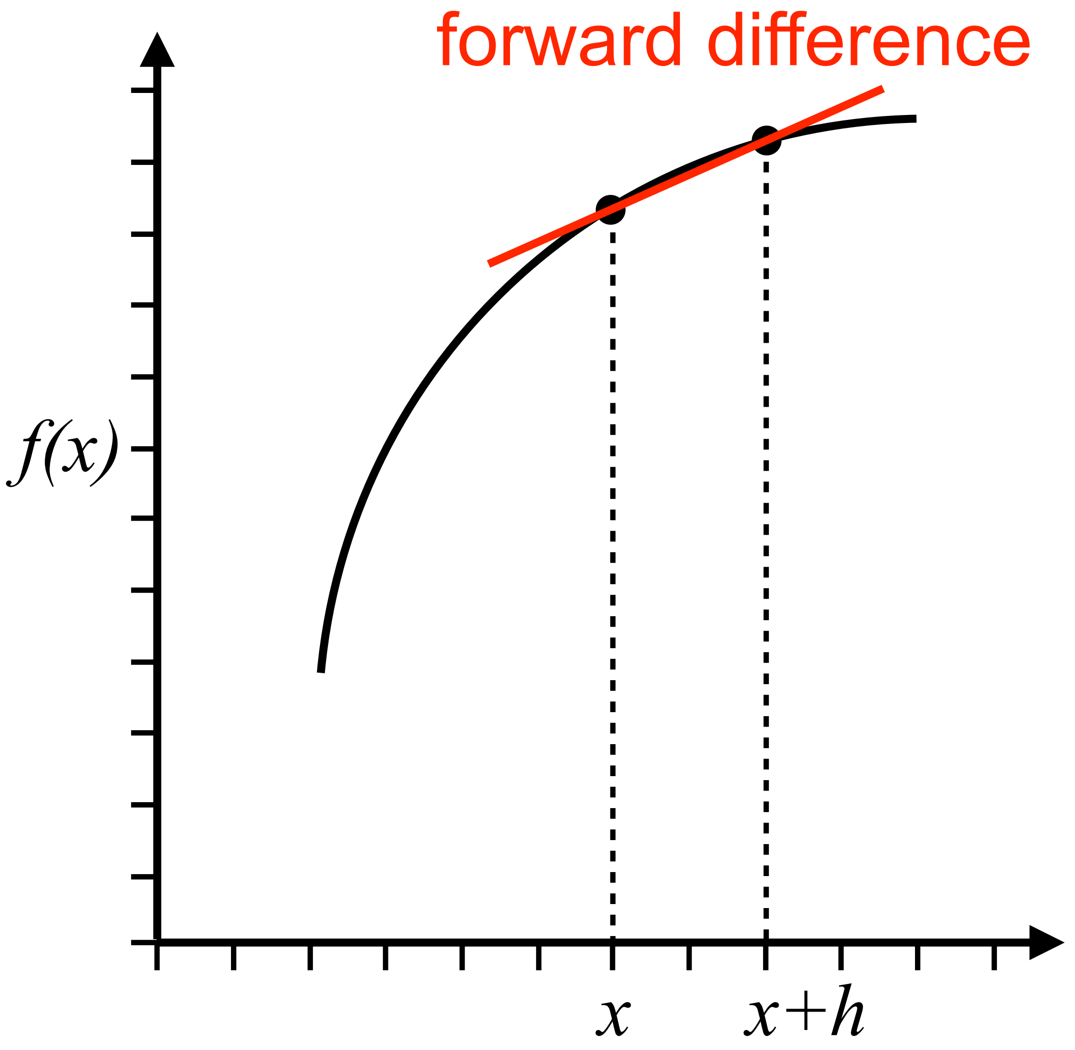
forward difference



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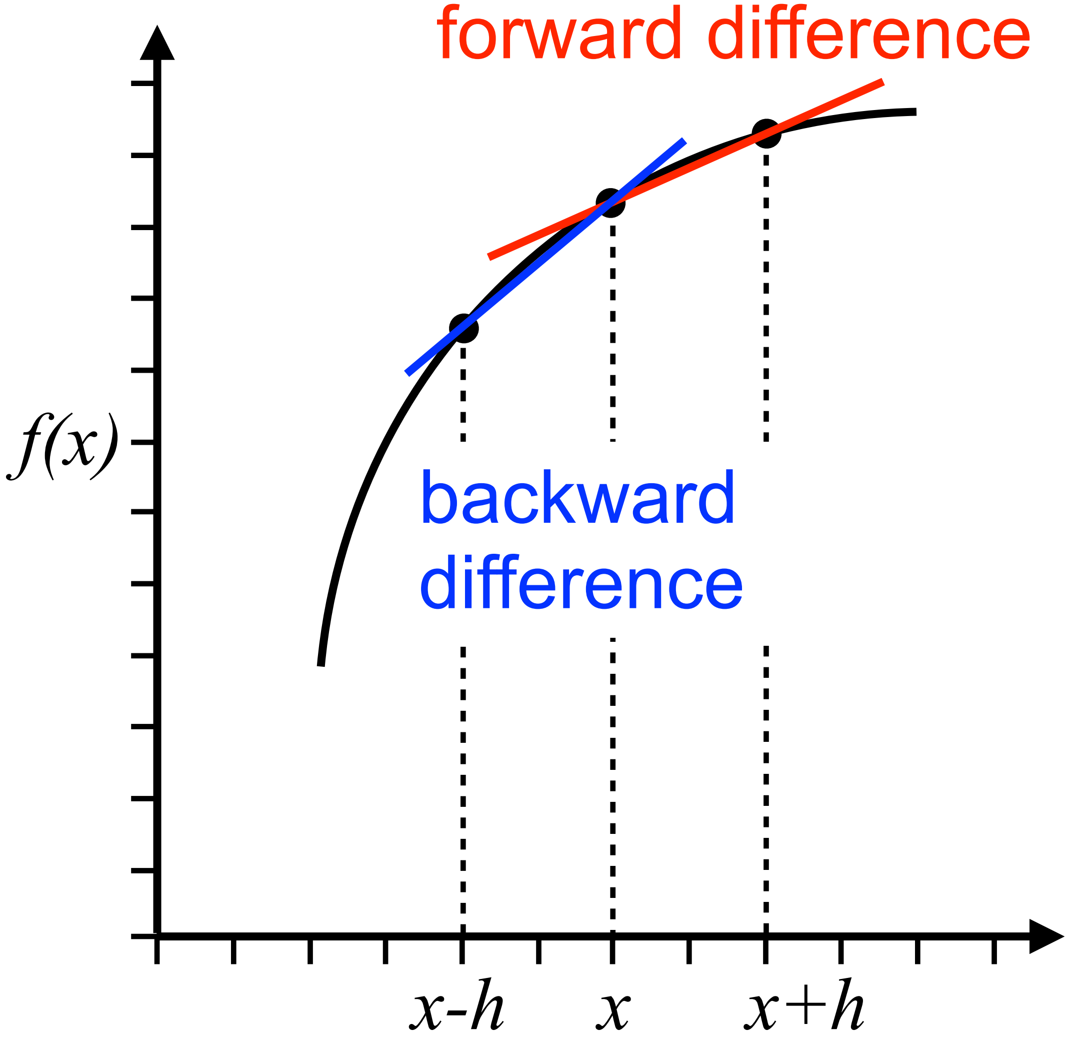
$$\frac{df}{dx} \approx \frac{f(x) - f(x-h)}{h}$$

backward difference



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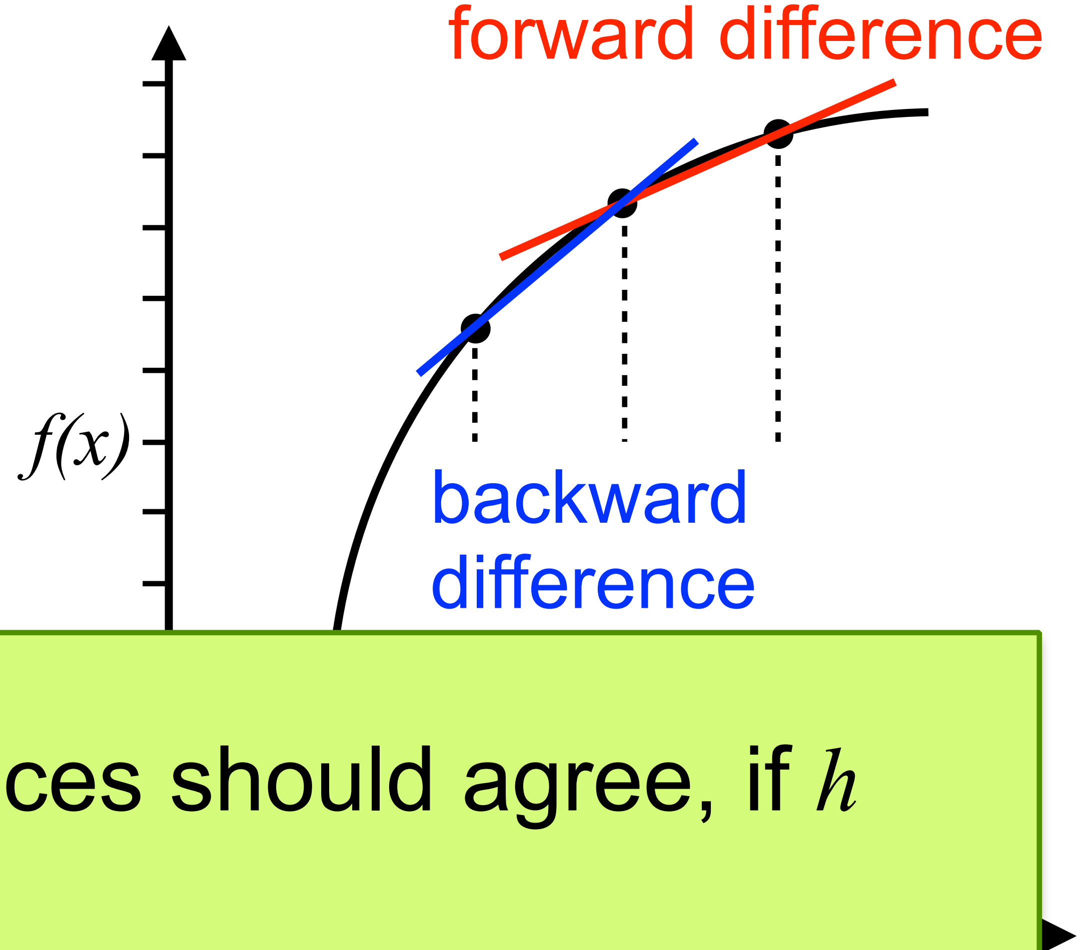


Forward and backward differences should agree, if h is small enough.

Derivatives - Exercise 3

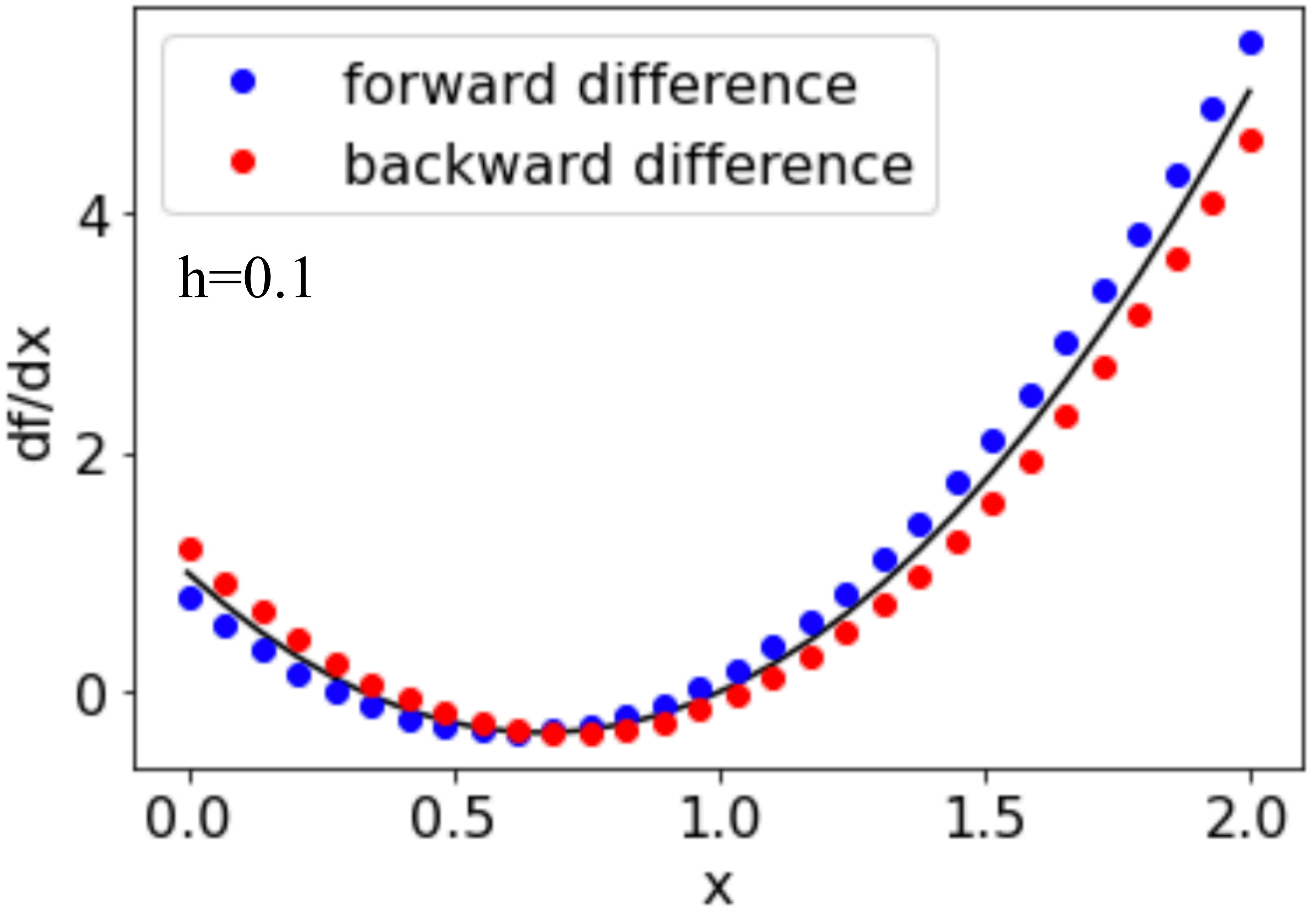
Differentiate: $f(x) = x^3 - 2x^2 + x - 1$

1. Use the forward and backward difference rule to calculate $f'(x)$ for $h=0.1$ and $h=0.01$.
2. Plot the analytic and your numeric derivatives.
3. Plot the difference between the two.

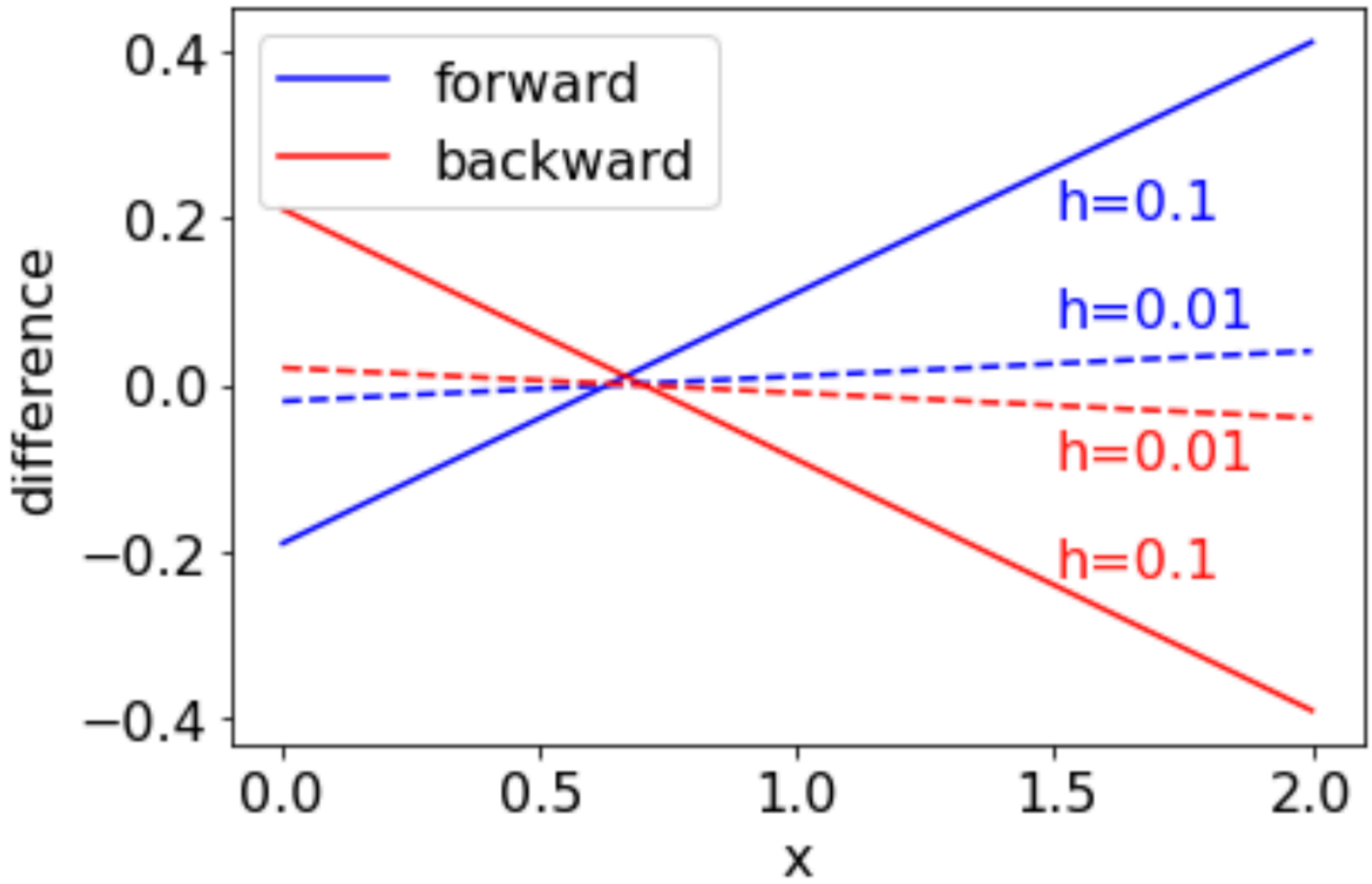
Talking points:

1. **What do you observe?**
2. **How does the error in the numeric derivatives behave with x and h?**
3. **How can we do better?**

Derivatives - forward and backward difference



Derivatives - forward and backward difference



Derivatives - Error analysis

- Forward and backward differences are usually not too accurate.
- To understand this, we Taylor expand $f(x)$ around x:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \ldots$$

Derivatives - Error analysis

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- To understand this, we Taylor expand *f(x)* around x:

$$f(x+h) = f(x) + hf'(x) + \frac{1}{2}h^2 f''(x) + \ldots$$

- Rearranging gives us:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2}hf''(x) + \ldots$$

forward difference

This and higher order terms we omit. They contribute to the error!

Derivatives - Error analysis

Error is proportional to 2nd derivative of the function.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2} h f''(x) + \ldots$$

forward difference

This and higher order terms we omit. They contribute to the error!

Derivatives - Error analysis

- In our example: $$f(x) = x^3 - 2x^2 + x - 1$$ $$f''(x) = 6x - 4$$

Now we understand, why the numeric deviation was linear.

Error is proportional to 2nd derivative of the function.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2} h f''(x) + \ldots$$

forward difference

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Derivatives - Error analysis

Proportional to h; the smaller h, the smaller the error.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2} h f''(x) + \dots$$

forward difference

This and higher order terms we omit. They contribute to the error!

Derivatives - Error analysis

But we are bound by machine precision, C, in the difference!

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forward difference

This and higher order terms we omit. They contribute to the error!

Derivatives - Error analysis

f(x+h) and *f(x)* are close, so their rounding error is: $2C|f(x)|$

But we are bound by machine precision, C, in the difference!

Proportional to h; the smaller h, the smaller the error.

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2} h f''(x) + \ldots$$

forward difference

This and higher order terms we omit. They contribute to the error!

Derivatives - Error analysis

- Our total error is thus:

$$\epsilon = \frac{2C|f(x)|}{h} + \frac{1}{2}h|f''(x)|$$

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- We seek the h that minimises ϵ. So we differentiate ϵ and set the result to 0.

$$-\frac{2C|f(x)|}{h^2} + \frac{1}{2}|f''(x)| = 0 \quad \text{or equivalently} \quad h_{\text{min}} = \sqrt{4C\left|\frac{f(x)}{f''(x)}\right|}$$

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- Substituting h_{min} into ϵ gives us the minimum error:

$$\epsilon_{\text{min}} = \sqrt{4C|f(x)f''(x)}$$

Derivatives - Error analysis

Minimum error of forward and backward difference.

$$\epsilon_{\min} = \sqrt{4C|f(x)f''(x)|}$$

Assuming $f(x)$ and $f''(x)$ are of order 1 and $C \approx 10^{-16}$ we get: $\epsilon_{min} \approx 10^{-8}$

Derivatives - Error analysis

Minimum error of forward and backward difference.

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Assuming $f(x)$ and $f''(x)$ are of order 1 and $C \approx 10^{-16}$ we get: $\epsilon_{min} \approx 10^{-8}$

Key concept: error analysis

Using analytic considerations, we can estimate the expected error of a numeric method. This helps us in our judgment of a method.

Derivatives - Error analysis

Minimum error of forward and backward difference.

$$\epsilon_{\min} = \sqrt{4C|f(x)f''(x)|}$$

Assuming $f(x)$ and $f''(x)$ are of order 1 and $C \approx 10^{-16}$ we get: $\epsilon_{min} \approx 10^{-8}$

- An error of 10^{-8} is usually sufficient, but we can do better!

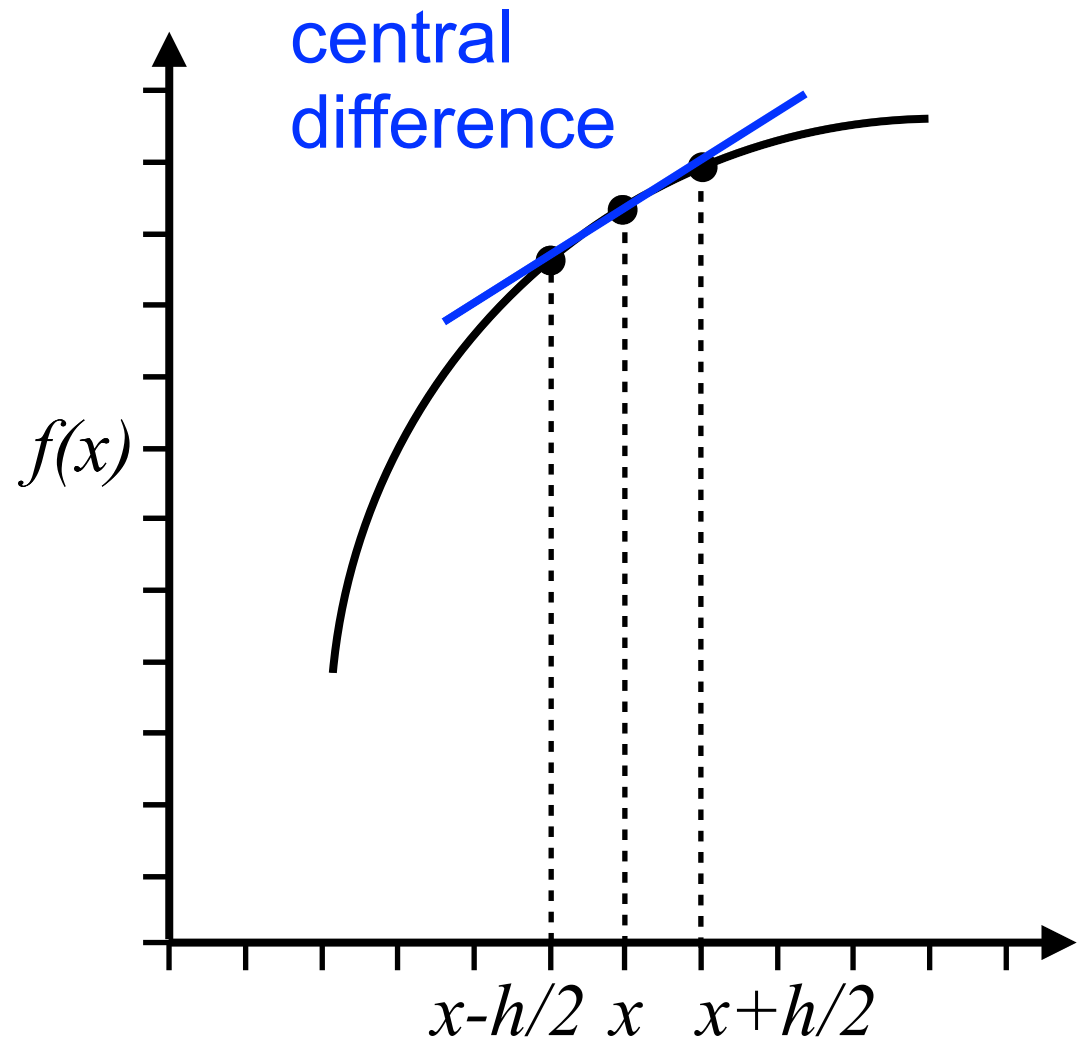
Derivatives - Central differences

Derivative: $$\frac{df}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- take a symmetric difference:

$$\frac{df}{dx} \approx \frac{f((x+h/2) - f(x-h/2)}{h}$$

central difference



Derivatives - Exercise 4

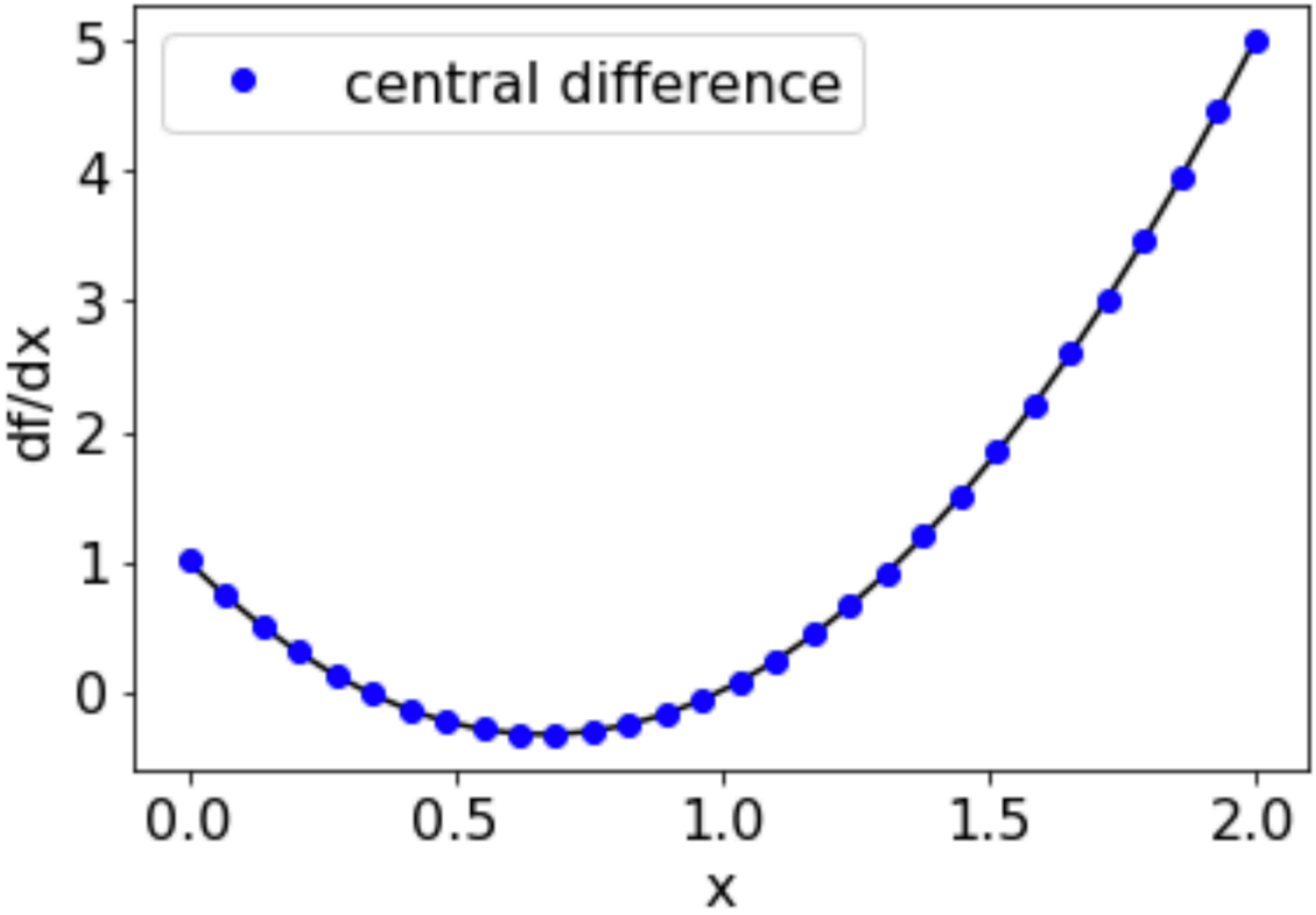
Differentiate: $f(x) = x^3 - 2x^2 + x - 1$

1. Use the central difference rule to calculate $f'(x)$ for $h=0.1$ and $h=0.01$.
2. Plot the analytic and your numeric derivatives.
3. Plot the difference between the two.

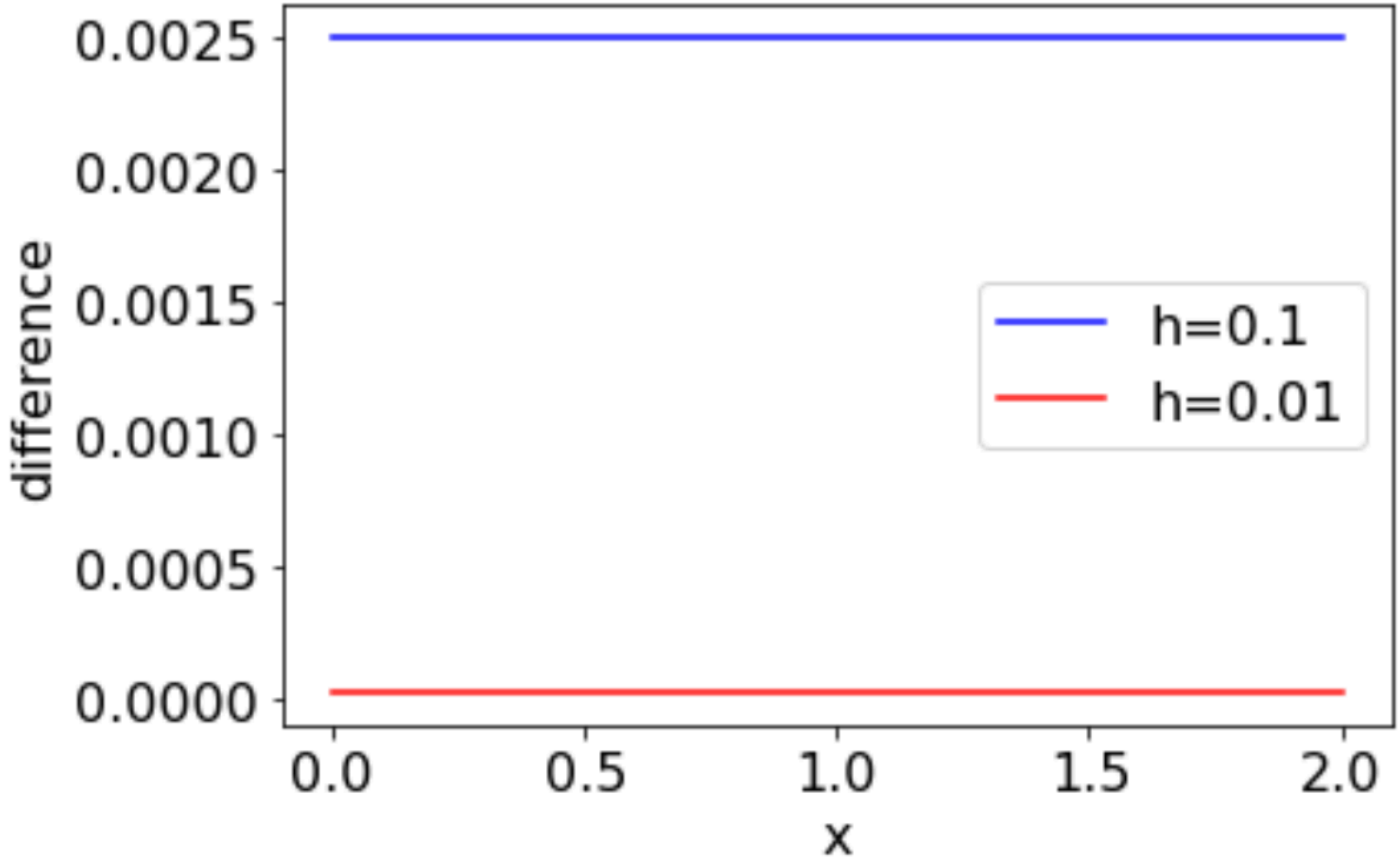
Talking points:

1. **What do you observe?**
2. **How does the error in the numeric derivatives now behave with x and h?**

Derivatives - Central difference



Derivatives - Central difference



Derivatives - Central difference error analysis

- We once again Taylor expand:

$$f(x+h/2) = f(x) + \frac{1}{2}hf'(x) + \frac{1}{8}h^2 f''(x) + \frac{1}{48}h^3 f'''(x) + \dots$$

$$f(x-h/2) = f(x) - \frac{1}{2}hf'(x) + \frac{1}{8}h^2 f''(x) - \frac{1}{48}h^3 f'''(x) + \dots$$

Derivatives - Central difference error analysis

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- and take the difference of the two expansions divided by h:

$$f'(x) = \frac{f((x+h/2) - f(x-h/2)}{h} - \frac{1}{24}h^2 f'''(x) + \ldots$$

Derivatives - Central difference error analysis

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- and take the difference of the two expansions divided by h:

$$f'(x) = \frac{f((x+h/2) - f(x-h/2)}{h} - \frac{1}{24}h^2 f'''(x) + \dots$$

central difference

now of order h^2 and not h
and proportional to $f'''(x)$

Derivatives - Central difference error analysis

- Our total error for the central difference is thus:

$$\epsilon = \frac{2C|f(x)|}{h} + \frac{1}{24}h^2|f'''(x)|$$

Derivatives - Central difference error analysis

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- We agin seek the h that minimises ϵ. So we differentiate ϵ and set the result to 0. We find for the minimising h:

$$h_{\text{min}} = \left(24C\left|\frac{f(x)}{f'''(x)}\right|\right)^{\frac{1}{3}}$$

Derivatives - Central difference error analysis

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- We agin seek the h that minimises ϵ. So we differentiate ϵ and set the result to 0. We find for the minimising h:

$$h_{\mathrm{min}} = \left(24C\left|\frac{f(x)}{f'''(x)}\right|\right)^{\frac{1}{3}}$$

- Substituting h_{min} into ϵ gives us the minimum error:

$$\epsilon_{\mathrm{min}} = \left(\frac{9}{8}C^2[f(x)]^2|f'''(x)|\right)^{\frac{1}{3}}$$

Derivatives - Error summary

- forward/backward difference:

$$h_{\min} \approx C^{\frac{1}{2}} \approx 10^{-8}$$

$$\epsilon_{\min} \approx C^{\frac{1}{2}} \approx 10^{-8}$$

- central difference:

$$h_{\min} \approx C^{\frac{1}{3}} \approx 10^{-5}$$

$$\epsilon_{\min} \approx C^{\frac{2}{3}} \approx 10^{-10}$$

Key concept: numeric differentiation

Using finite differences, derivatives of functions can be calculated numerically.

Derivatives - Second derivatives

2nd derivative: $$\frac{d^2 f}{dx^2} = \lim_{h \to 0} \frac{f'(x+h) - f'(x)}{h}$$

Question:

Now that we successfully solved 1st derivatives, can we also compute 2nd derivatives?

Derivatives - Second derivatives

2nd derivative: $$\frac{d^2 f}{dx^2} = \lim_{h \to 0} \frac{f'(x+h) - f'(x)}{h}$$

- The solution lies in the above formula. We need the central difference of the central difference:

$$f''(x) \approx \frac{f'(x+h/2) - f'(x-h/2)}{h}$$

- We already know how to deal with the 1st derivatives:

$$f'(x+h/2) \approx \frac{f(x+h) - f(x)}{h} \quad \text{and} \quad f'(x-h/2) \approx \frac{f(x) - f(x-h)}{h}$$

Derivatives - Second derivatives

2nd derivative: $$\frac{d^2 f}{dx^2} = \lim_{h \to 0} \frac{f'(x+h) - f'(x)}{h}$$

- This gives:

$$\begin{aligned} f''(x) &\approx \frac{f'(x+h/2) - f'(x-h/2)}{h} \\ &= \frac{(f(x+h) - f(x)) - (f(x) - f(x-h))}{h^2} \\ &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \end{aligned}$$

Derivatives - Second derivative error estimate

- We can again estimate the error by Taylor expanding around $f(x+h)$ and $f(x-h)$. This gives:

$$\epsilon = \frac{4Cf(x)}{h^2} + \frac{1}{12}h^2|f''''(x)|$$

Derivatives - Second derivative error estimate

- We can again estimate the error by Taylor expanding around *f(x+h)* and *f(x-h)*. This gives:

$$\epsilon = \frac{4Cf(x)}{h^2} + \frac{1}{12}h^2|f''''(x)|$$

- The minimal error is then:

$$h_{\text{min}} = \left(48C\left|\frac{f(x)}{f''''(x)}\right|\right)^{\frac{1}{4}} \quad \text{and} \quad \epsilon_{\text{min}} = (\frac{4}{3}C|f(x)f''''(x))^{\frac{1}{2}}$$

$\sim C^{1/2} \approx 10^{-8}$

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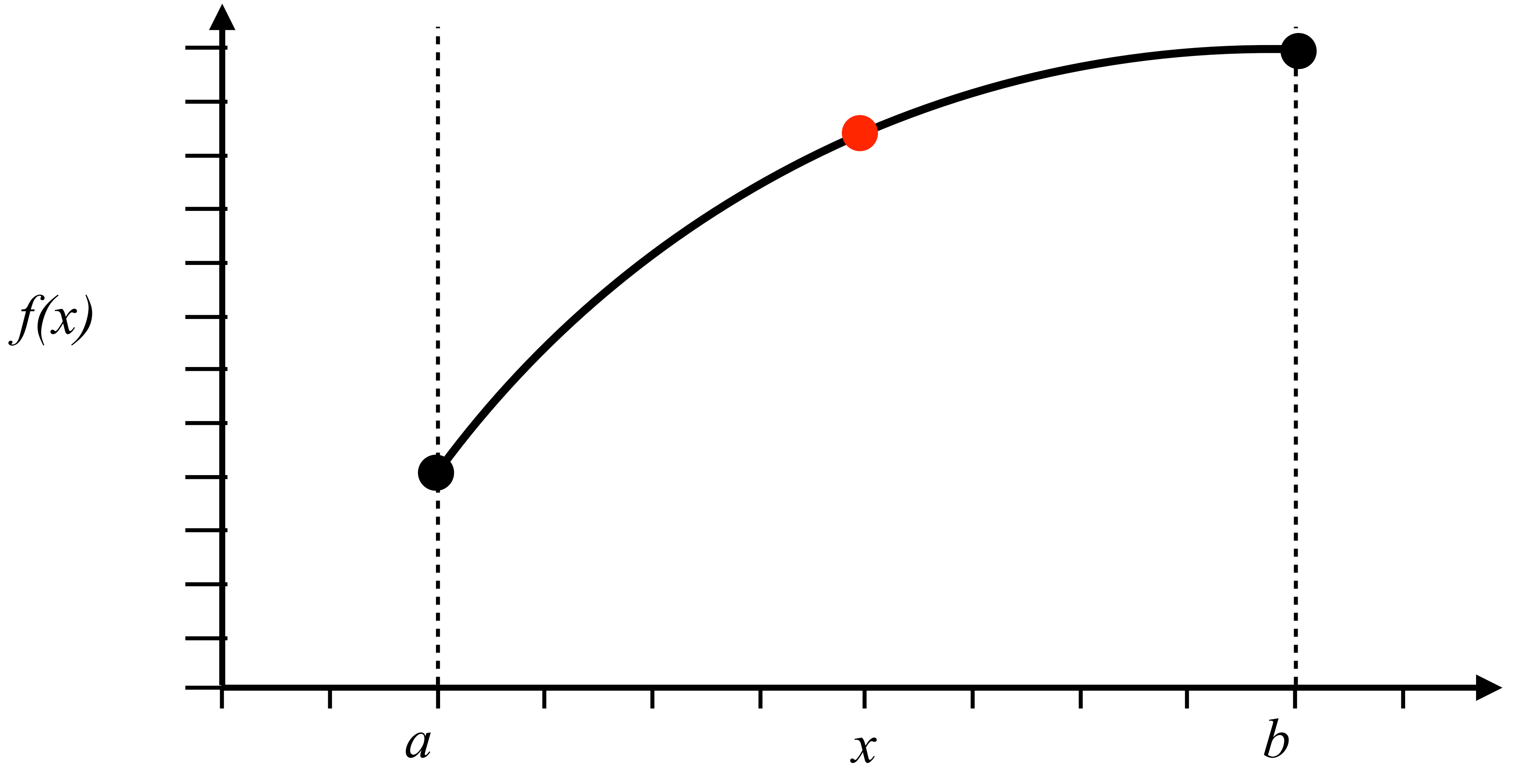
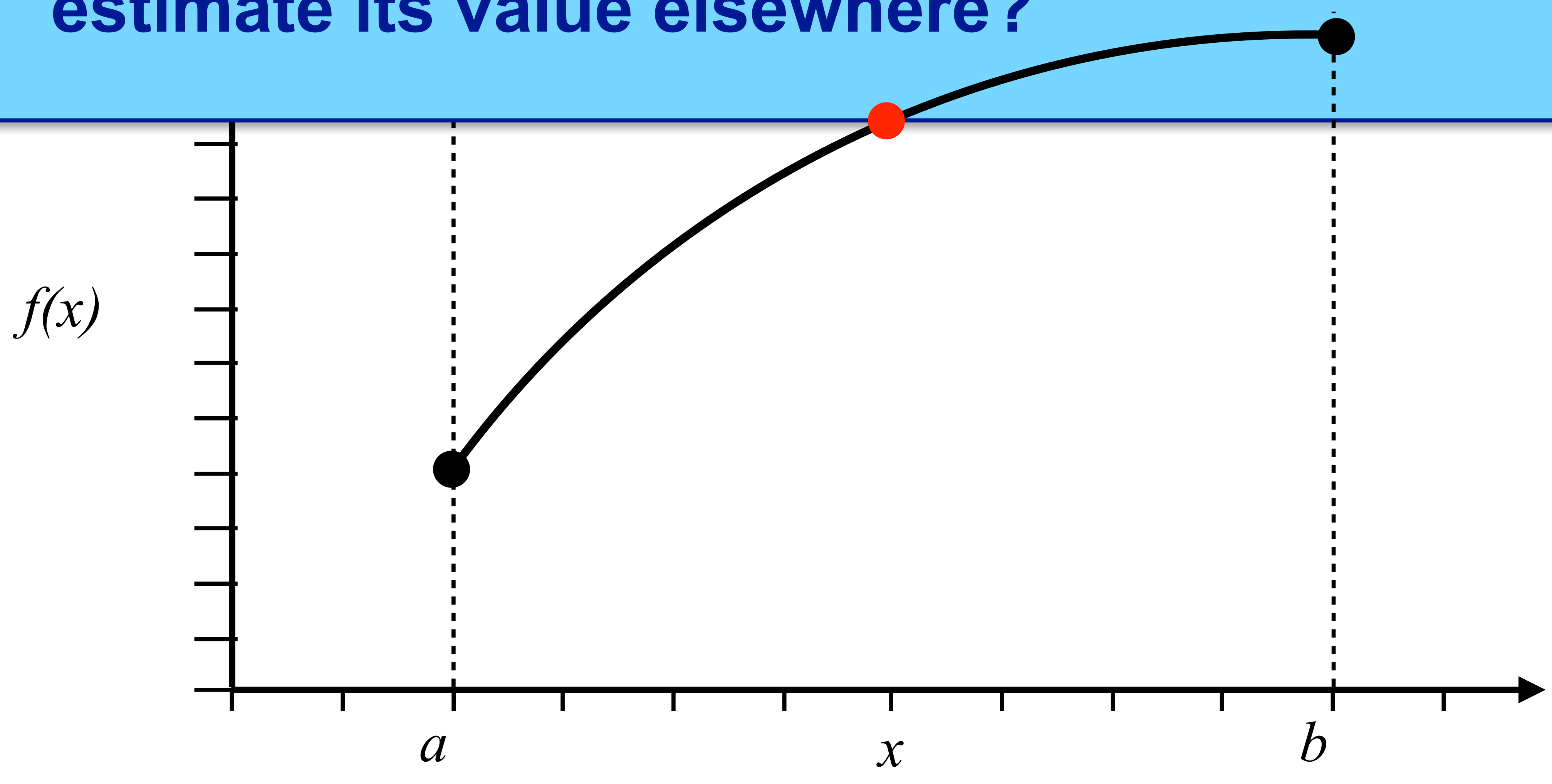
Interpolation



Interpolation

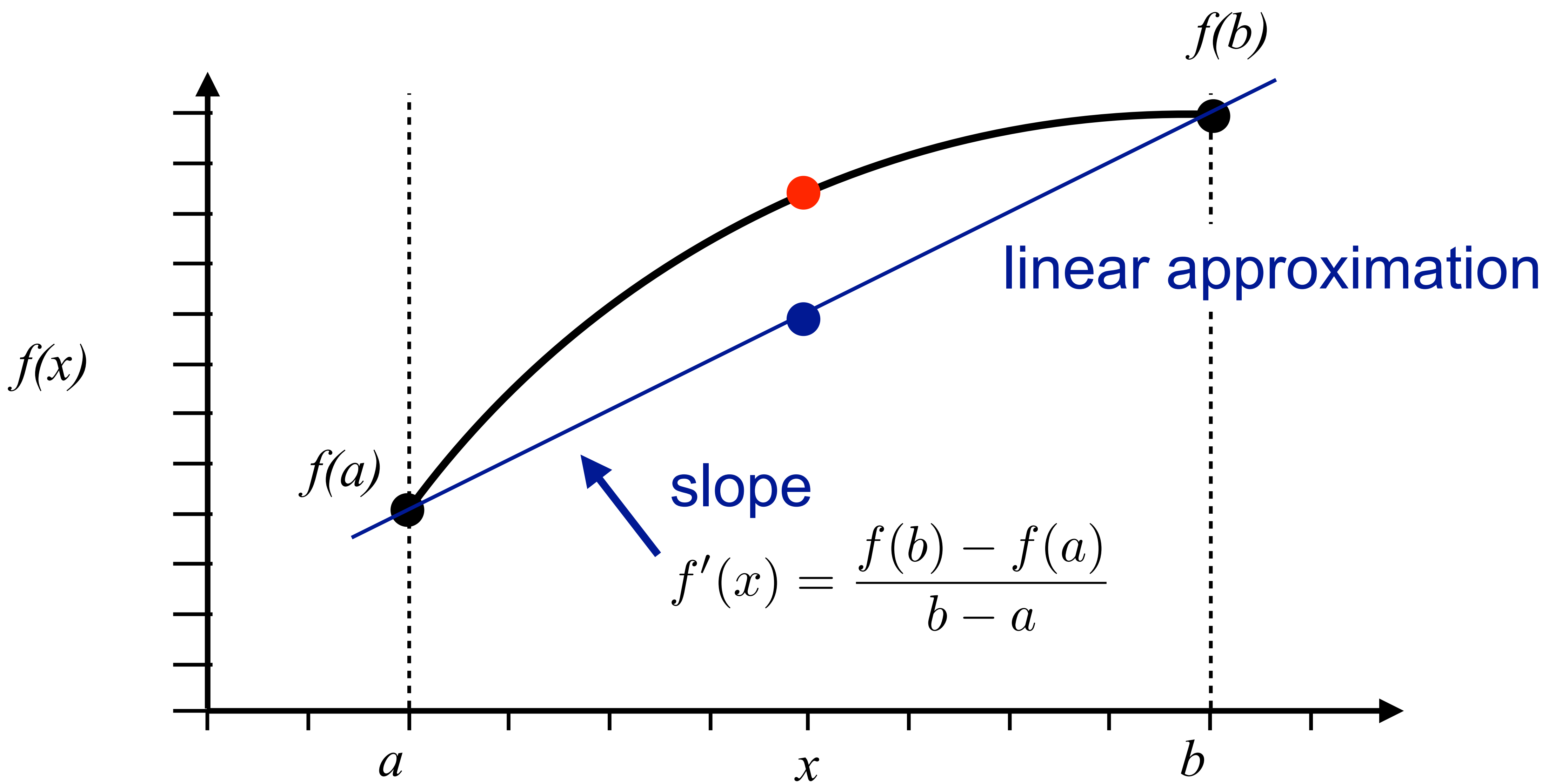
Question:

If we know a function at two points, can we estimate its value elsewhere?



Interpolation

- interpolation: $f(x) \approx \dfrac{f(b) - f(a)}{b - a}(x - a) + f(a)$



Interpolation

- interpolation: $$f(x) \approx \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$$
$$= \frac{(b - x)f(a) + (x - a)f(b)}{b - a}$$

Interpolation

- interpolation: $$f(x) \approx \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$$
$$= \frac{(b - x)f(a) + (x - a)f(b)}{b - a}$$

- to estimate the error we once more Taylor expand:

$$f(a) = f(x) + (a - x)f'(x) + \frac{1}{2}(a - x)^2 f''(x) + \dots$$
$$f(b) = f(x) + (b - x)f'(x) + \frac{1}{2}(b - x)^2 f''(x) + \dots$$

Interpolation

- interpolation: $$f(x) \approx \frac{f(b)-f(a)}{b-a}(x-a)+f(a)$$ $$= \frac{(b-x)f(a)+(x-a)f(b)}{b-a}$$

- to estimate the error we once more Taylor expand:

$$f(a) = f(x) + (a-x)f'(x) + \frac{1}{2}(a-x)^2 f''(x) + \ldots$$
$$f(b) = f(x) + (b-x)f'(x) + \frac{1}{2}(b-x)^2 f''(x) + \ldots$$

- substituting into the above equation and rearranging:

$$f(x) = \frac{(b-x)f(a)+(x-a)f(b)}{b-a} + (a-x)(b-x)f''(x) + \ldots$$

Interpolation

This term becomes largest in the middle of the [a,b] interval:

$$x - a = b - x = \frac{1}{2}h$$

$$f(x) = \frac{(b-x)f(a) + (x-a)f(b)}{b-a} + (a-x)(b-x)f''(x) + \ldots$$

Interpolation

- the interpolation error is quadratic in h:

$$\epsilon = \frac{1}{4}h^2|f''(x)|$$

This term becomes largest in the middle of the [a,b] interval:

$$x - a = b - x = \frac{1}{2}h$$

$$f(x) = \frac{(b-x)f(a) + (x-a)f(b)}{b-a} + (a-x)(b-x)f''(x) + \dots$$

Interpolation

- linear interpolation: $f(x) \approx \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$

Key concept: linear interpolation

By calculating first derivatives numerically, we can linearly interpolate functions.

- The accuracy of linear interpolation is determined by the available point density (i.e. the value of h).

Interpolation

- linear interpolation: $f(x) \approx \frac{f(b) - f(a)}{b - a}(x - a) + f(a)$

Key concept: linear interpolation

By calculating first derivatives numerically, we can linearly interpolate functions.

- The accuracy of linear interpolation is determined by the available point density (i.e. the value of h).
- Going beyond linear interpolation is not trivial and we will not cover this in this lecture.