So how would I use calculus on an interpolant?

$f(x_i) = \tilde{f}(x_i) \quad i=1 \ldots n$

Have: interpolant $\hat{f}(x) = \alpha_1 \varphi_1(x) + \cdots + \alpha_n \varphi_n(x)$

Want: derivative

$$\vec{\alpha} = V^{-1} \vec{f}$$

$$\tilde{f}'(x) = \alpha_1 \varphi_1'(x) + \cdots + \alpha_n \varphi_n'(x)$$

$\tilde{f}'(x_i)$

$$V' = \begin{pmatrix} \varphi_1'(x_1) & & \varphi_n'(x_1) \\ & \ddots & \\ \varphi_1'(x_n) & & \varphi_n'(x_n) \end{pmatrix}$$

$$\vec{\tilde{f}'} = \underbrace{V' V^{-1}}_{} \vec{f}$$

Differentiation Matrix

So how would I use calculus on an interpolant? (cont'd)

Give a matrix that takes two derivatives.

$$D^2$$

$$V'V^{-1}\underbrace{V'V^{-1}}_{D}\vec{f}$$

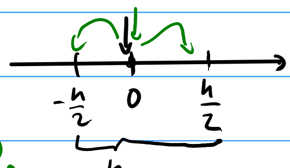
What is the observed behavior of the error when taking a derivative?

$$|f'(x) - \hat{f}'(x)| \le C \cdot h^n \quad \leftarrow \text{deriv}$$

$$|f(x) - \hat{f}(x)| \le C \cdot h^{n+1} \quad \leftarrow \text{intp.}$$

$$|\textstyle\int f - \int \tilde{f}| \le C \cdot h^{n+2} \quad \text{integ.}$$

What do the entries of the differentiation matrix mean?



do not care

$$D = V'V^{-1} = \begin{pmatrix} \boxed{\quad} \\ d_{21} \quad d_{22} \quad d_{23} \\ \boxed{\quad} \end{pmatrix} = \begin{pmatrix} \boxed{\quad} \\ -\frac{1}{h} \quad 0 \quad \frac{1}{h} \\ \boxed{\quad} \end{pmatrix}$$

$$V'V^{-1}\begin{pmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \end{pmatrix} = \begin{pmatrix} \boxed{\quad} \\ d_{21}f_0 + d_{22}f_1 + d_{23}f_2 \\ \boxed{\quad} \end{pmatrix}$$

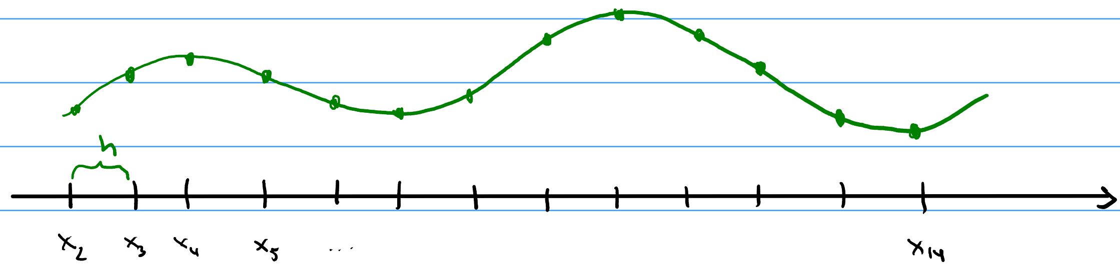
$f(x_0) = f_0$, $f(x_2) = f_2$

$$= -\frac{1}{h} \cdot f_0 + \frac{1}{h} \cdot f_2$$

$$f'(x_1) \approx \frac{f(x_2) - f(x_0)}{h}$$

"Second-order" centered finite difference

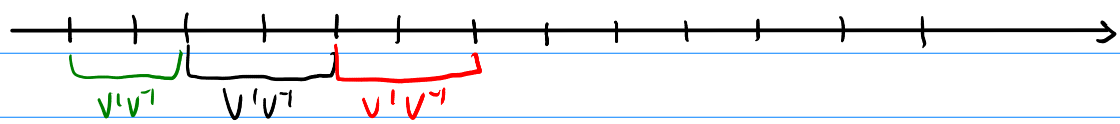
Can we simplify the proccess for equispaced x-coordinates?

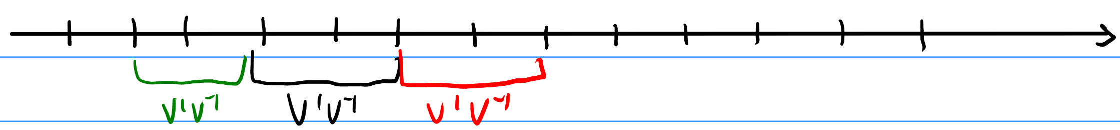


(1) Form group

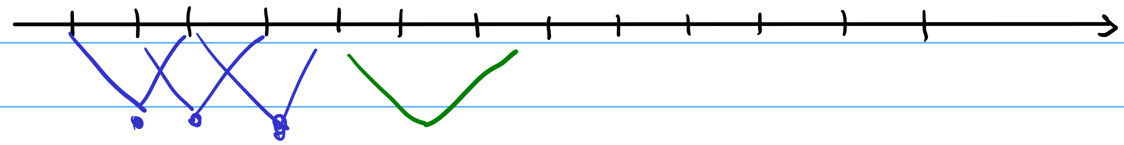
(2) Compute interp.

(3) Find deriv.



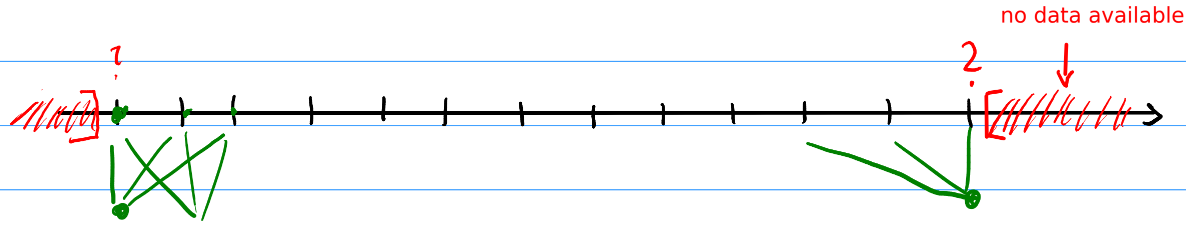


How would we use translation invariance with centered differences?



$$\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix} \begin{pmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \end{pmatrix} = \begin{pmatrix} f'(x_1) \\ f'(x_2) \\ f'(x_3) \end{pmatrix}$$

What do we do at the edges?

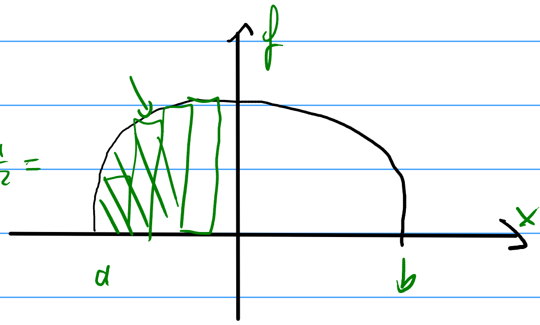


How accurate are finite difference formulas?

Can anything else go wrong when we numerically compute derivatives?

Can we use a similar process to compute (approximate) integrals?

$\frac{\pi}{2} = \frac{22}{7} \cdot \frac{1}{2} =$



$\rightarrow \overbrace{\text{Quadrature}}^{\text{Brick}}$

= numerical integration

Have $\quad \tilde{f}(x) = \alpha_1 \varphi_1(x) + \dots + \alpha_n \varphi_n(x)$

Want: $\quad \underline{\int_a^b \tilde{f}(x)\,dx} = \alpha_1 \underbrace{\int_a^b \varphi_1(x)\,dx}_{d_1} + \dots + \alpha_n \underbrace{\int_a^b \varphi_n(x)\,dx}_{d_n}$

$= \vec{\alpha} \cdot \vec{d} = (V^{-1}\vec{f}) \cdot \vec{d} = (V^{-1}\vec{f})^T \vec{d} \qquad \vec{d} = \begin{pmatrix} d_1 \\ \vdots \\ d_n \end{pmatrix}$

$x \cdot y = x^T y$

$= \vec{f}^T \underbrace{V^{-T}\vec{d}}_{\vec{w}} = \vec{f} \cdot \vec{w}$

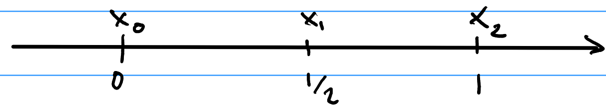
$(Ax)^T = x^T A^T$

$\vec{w} \leftarrow$ Quadrature weights

$= w_1 f(x_1) + \dots + w_n f(x_n)$

So, once I know my nodes and my weights, what does quadrature look like?

Can you do a full example?



$f(x_0) = 2 \qquad f(x_1) = 0 \qquad f(x_2) = 3$

1. Find coefficients $\qquad \vec{\alpha} = V^{-1}\begin{pmatrix}2\\0\\3\end{pmatrix}$

2. Compute integrals

$$\int_0^1 1 \, dx = 1$$
$$\int_0^1 x \, dx = 1/2$$
$$\int_0^1 x^2 \, dx = 1/3$$

$$\vec{d} = \begin{pmatrix}1\\1/2\\1/3\end{pmatrix}$$

3. Combine it all together

$$\int \approx \underbrace{\vec{d}\cdot V^{-1}}_{\text{weights}}\begin{pmatrix}2\\0\\3\end{pmatrix}$$

$$\int e^{-x^2}$$

"Simpson's rule"

$$\int_0^1 \tilde{f}(x)\,dx = \frac{1}{6}\cdot f(0) + \frac{4}{6}\cdot f\left(\tfrac{1}{2}\right) + \frac{1}{6}\cdot f(1)$$

What does Simpson's Rule look like on [0, 1/2]?

What does Simpson's Rule look like on [5, 6]?

How accurate is Simpson's rule?

5 points

$\downarrow$

$n=4$

$$\partial 3 = E(h) = C \cdot h^{n+2}$$

$$E\left(\frac{h}{10}\right) = C \cdot \left(\frac{h}{10}\right)^{n+2} = \underbrace{C \cdot h^{n+2}}_{E(h)} \cdot \left(\frac{1}{10}\right)^{\overset{6}{n+2}}$$

$$\int_{-1}^{1} 1 \, dx = 2$$

$$\int_{-1}^{1} x \, dx = 0$$

$$\int_{-1}^{1} x^2 = \frac{2}{3}$$

d

(11) **Solving nonlinear equations**

Have: $f : \mathbb{R} \to \mathbb{R}$ function

Want: x such that $f(x) = y$

Rewrite the problem so that we only need $g(x) = 0$. (i.e. no explicit right-hand side)

What if we know that f is continuous and $f(a) \cdot f(b) < 0$?

Can we use this "bracket" to track down the zero?

Convergence Rates of Iterative Procedures

Consider the "error" in the bisection method in the kth step:

$$e_k =$$

What's the error in the next step, relative to e_k ?

$$e_{k+1} =$$

Generally, error behavior like this is called "linear convergence" ("order 1"):

$$e_{k+1} \leq$$

Generally, error behavior like this is called "quadratic convergence" ("order 2"):

$$e_{k+1} \leq$$

Generally, error behavior like this is called "cubic convergence" ("order 3"):

$$e_{k+1} \leq$$

(... and so on) Which of these is fastest?

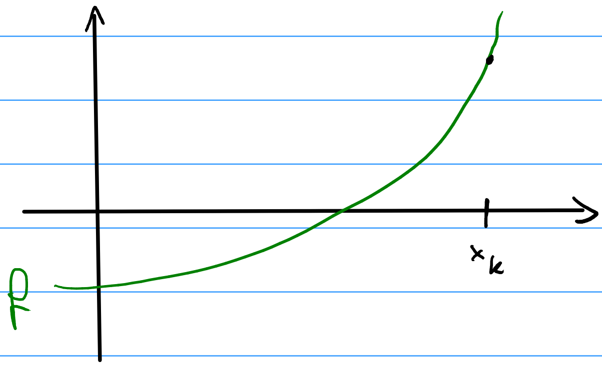
Rewrite this so that the constant stands on its own, for a general order q :

$$C \approx$$

Do not confuse this with "q-th order" convergence for a mesh width h!

Newton's method

Suppose x_k is our current guess of the zero.



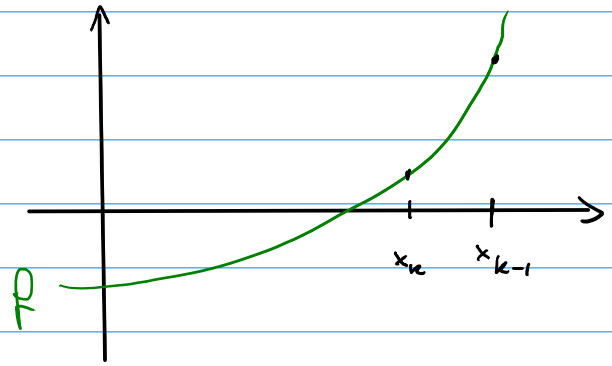
Idea: Build a solvable approximate version of f using $f(x_k)$ and $f'(x_k)$

Find the zero of the approximate version.

Name some downsides of Newton's method.

Secant Method

How else could we find a line approximating a function?



Estimate the slope of the approximating line:

Now use this estimate in Newton's method:

Solving systems of nonlinear equations

Want to solve $\vec{f}(\vec{x}) = \vec{0}$. $\quad f: \mathbb{R}^n \to \mathbb{R}^n$! why?

Let's try to carry over our 1-dimensional ideas.

Let's first get an idea of what behavior can occur.

Based on the demo: Does bisection stand a chance?

Let's try Newton's method then. What's the linear approximation of f ?

OK, now solve that for h.

Let's do an example of that:

$$f(x,y) = \begin{pmatrix} x + 2y - 2 \\ x^2 + 4y^2 - 4 \end{pmatrix}$$

What are the downsides of this method?

So how about (an n-dimensional analog of) the secant method?

So carrying over the secant method to n dimensions is not easy.

It's possible, but beyond the scope of our class.

Here are two starting points to search:

- Broyden's method
- Secant updating methods

Here's one more idea: If we could figure out where the linear approximation in Newton is 'trustworthy', would that buy us anything?