



NUMERICAL ANALYSIS

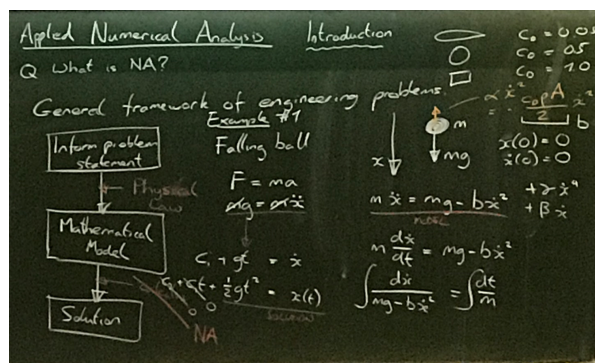
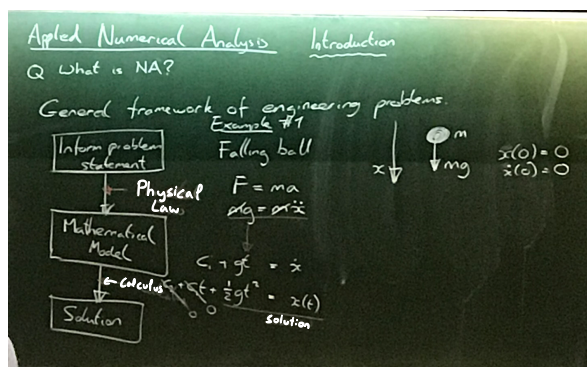


Applied Numerical Analysis

Introduction

What is Numerical Analysis?

General framework of engineering problems



NA is a solution method (method $\rightarrow$ solution) using only operations (that a computer can perform) $+$, $-$, $\times$, $\div$, etc.

Example:

$$\dot{x} = f(x)$$

we can approx

$$x(\Delta t n) \approx \hat{x}_n = \hat{x}_{n+1} + \Delta t f(\hat{x}_n)$$

n indicates that it is a numerical solution

Module 5

Modules:

Problem Statement.

1. Find x s.t. $f(x) = 0$ such that Root-finding.

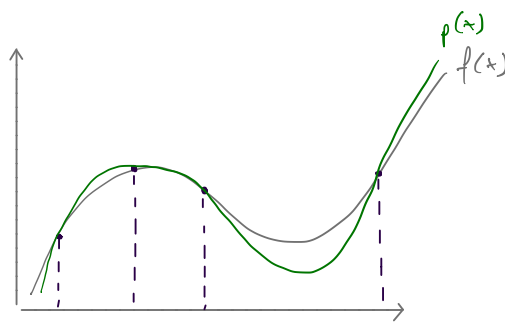
2. Find $p(x)$, s.t. $p(x_i) = f(x_i)$ for all i . Interpolation

3. Find $p(x, y)$ s.t. $p(x_i, y_i) = f(x_i, y_i) \forall i$. Multidimensional interpolation Advanced interpolation.

4. Approximate $f' \approx \frac{df}{dx}$ and $\hat{F} \approx \int_a^b f dx$ Numerical Calculus Differentiation + integration.

5. Find $u(x)$ s.t. $u' = f(u)$, $u(0) = u_0$ Numerical ODEs

6. Find $x \in [a, b]$ s.t. $f(x)$ is a minimum. Optimization.

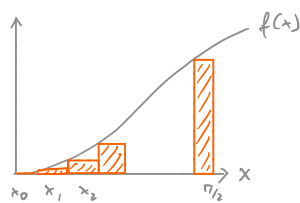


Example Statement & analysis of a numerical method.

Module 4 $I(t) = \int_0^{\pi/2} f(x) dx$ $f(x) = x \sin x$

Analytic solution $I[f] = 1$

Numerically

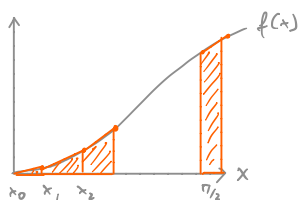


$$h = \frac{\pi/2 - 0}{N} = \frac{\pi}{2N}$$

$$I(f) \approx \sum_{i=0}^{N-1} h f(x_i)$$

Piecewise Constant Rule

$$f_i = f(x_i)$$



$$I(f) = \sum_{i=0}^{N-1} h \frac{f(x_i) + f(x_{i+1})}{2}$$

Trapezoidal Rule

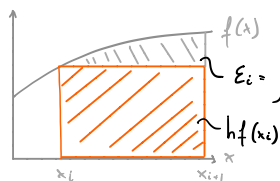
Error $\varepsilon := |Q(f) - I(f)|$

Convergence rate Is the rate at which $\varepsilon \rightarrow 0$, as $h \rightarrow 0$ (or $h \rightarrow \infty$) **Important**

Eg. If $\varepsilon \sim h^\alpha$ then we say the method is α -order accurate.

Consistency NM is consistent if $\varepsilon \rightarrow 0$ as $h \rightarrow 0$

Conv. of P.C rule Q:



$$f(x) = f(x_i) + \theta f'(x_i) + \frac{\theta^2}{2} f''(x_i) + \dots$$

$\theta = x - x_i$

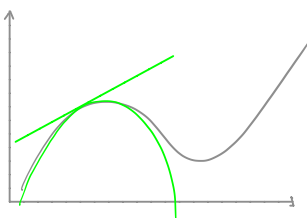
$$\begin{aligned} \varepsilon_i &= \int_{x_i}^{x_{i+1}} f(x) - f_i dx = \int_0^h \theta f'(x_i) d\theta + \int_0^{\frac{\theta^2}{2}} \frac{1}{2} f''(x_i) d\theta + \dots \\ &= \left[\frac{1}{2} \theta^2 f'_i \right]_0^h + \left[\frac{1}{6} \theta^3 f''_i \right]_0^h + \dots \\ &= O(h^2) + O(h^3) + \dots \end{aligned}$$

Order notation
Constants do not matter. All we are trying to prove is that $\varepsilon \propto h^2$
Bigger order h do not matter either since h is small.

Taylor approximation **MAJOR**

Assume $f(x) \in C^{N+1}([a, b]) \rightarrow$ then $\rightarrow$

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2} f''(x_0)(x - x_0)^2 + \sum_{j=3}^N \frac{1}{j!} f^{(j)}(x_0)(x - x_0)^j + O(x - x_0)^{N+1}$$



$$\varepsilon = \sum_{i=0}^{N-1} \varepsilon_i = \sum_{i=0}^{N-1} O(h^2) = O(Nh^2) = O\left(\frac{1}{h} h^2\right) = O(h)$$

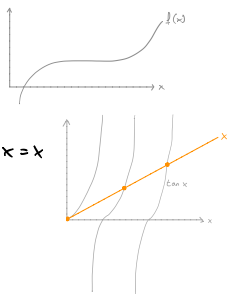
$$h = \frac{b-a}{N} \quad h \propto \frac{1}{N}$$

Module 1- Root finding

Problem statement: Find $\tilde{x} \in \mathbb{R}$ s.t. $f(\tilde{x})=0$

Examples Polynomials
 $ax^2+bx+c=0$
 $ax^5+bx^4+\dots+f=0$

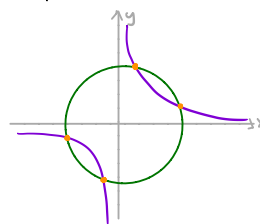
Structural analysis $\tan x = x$



More generally

Find $\tilde{x} \in \mathbb{R}^m$ s.t. $f(\tilde{x})=0$ where $f: \mathbb{R}^m \rightarrow \mathbb{R}^m$

Ex. - $Ax=b$
 $-(x^2+y^2=1)$
 $xy=\frac{1}{4}$

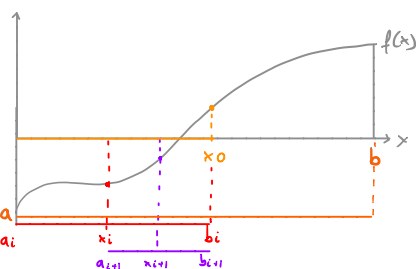


Does the solution exist?
Is it unique?

We are going to discuss three algorithms

Algorithm *1. Recursive bisection.

Assume $f \in C^0([a,b])$ and $f(a)<0$, $f(b)>0$



Given $[a_i, b_i]$

if $f(x_i)>0$: $a_{i+1}=a_i$
 $b_{i+1}=x_i$

if $f(x_i)<0$: $a_{i+1}=x_i$
 $b_{i+1}=b_i$

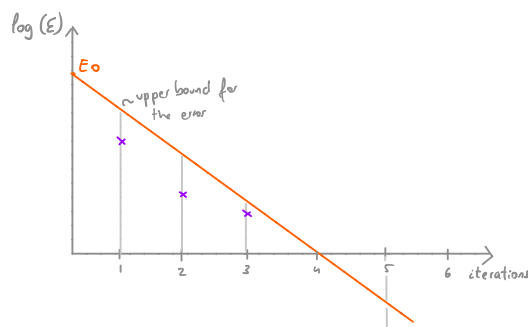
Error $\varepsilon_i = |x_i - \tilde{x}|$

It is guaranteed that $\tilde{x} \in [a_i, b_i]$, $\varepsilon \leq$

Iteration $\varepsilon_0 \leq \frac{|b_0 - a_0|}{2} = E_0$ $\varepsilon_{i+1} = \frac{\varepsilon_i}{2}$

$\varepsilon_i \leq \varepsilon_0 = \frac{\varepsilon_0}{2^i} = \dots = \frac{\varepsilon_0}{2^i}$

$\frac{|b_i - a_i|}{2} \leftarrow$ upper bound for the error.



Method *2. Fixed-Point Iteration (FPI)

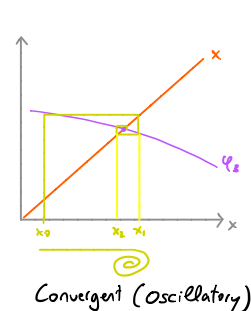
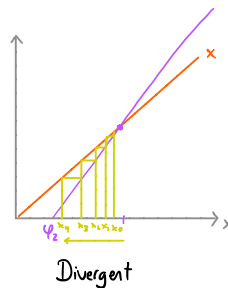
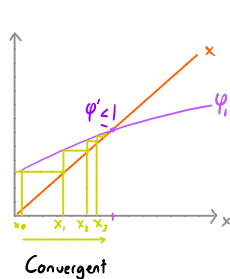
Rewrite $f(x)=0$ as $\varphi(x)=x$

Iteration $x_{i+1}=\varphi(x_i)$

Example $f(x) = x^3 + 2 = 0$ $\varphi(x) = x^3 + 2 + x$
 $\varphi(x) = \frac{-2}{x^2}$
 etc.

Observe that if $f(\tilde{x})=0 \Leftrightarrow \tilde{x}=\varphi(\tilde{x})$

Observe that if $x_i=\tilde{x} \Rightarrow x_{i+1}=\tilde{x}$



Error $\varepsilon_i = x_i - \tilde{x}$

The goal is to relate ε_{i+1} to ε_i

$$\varepsilon_{i+1} = x_{i+1} - \tilde{x} = \varphi(x_i) - \varphi(\tilde{x}) \rightarrow \frac{\varphi(x_i) - \varphi(\tilde{x})}{(x_i - \tilde{x})} (x_i - \tilde{x}) = \varphi'(\xi) \varepsilon_i$$

We make a trick and divide and multiply by $(x_i - \tilde{x})$
 Fine as long as $x_i \neq \tilde{x}$

$\varphi'(\xi)$ $\xi \in [x_i, \tilde{x}]$

Mean Value Theorem MVT

$\varphi(x) \in C'([a,b])$

$\varphi'(\xi) \frac{\varphi(b) - \varphi(a)}{b-a} \exists \xi \in [a,b]$

Assume $|\varphi'(x)| < k \quad \forall x \in [a,b]$

$$|\varepsilon_{i+1}| \leq k |\varepsilon_i| \leq k^2 |\varepsilon_{i-1}| \leq \dots \leq k^i |\varepsilon_0|$$

If $k < 1 \Rightarrow$ convergence

$k > 1 \Rightarrow$ divergence

Method #3 Newton

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

$$x_{i+1} = \varphi(x_i)$$

$$\text{FPI } |\varphi'(\xi)| < 1 \quad \xi \in [x_i, \tilde{x}]$$

$$\varphi' = \frac{ff''}{f'^2} \quad [f' \neq 0] \rightarrow \text{function can not touch the axis of the root.}$$

Error behaviour:

$$\varepsilon_{i+1} = x_{i+1} - \tilde{x}$$

$$x_{i+1} = \varphi(x_i) = \varphi(\tilde{x} + \varepsilon_i)$$

taylor expansion: nonlinear operator acting on $(a+b)$ when b is small.

$$x_{i+1} = \underbrace{\varphi(\tilde{x})}_{\tilde{x}} + \varphi'(\tilde{x})\varepsilon_i + \frac{1}{2}\varphi''(\tilde{x})\varepsilon_i^2 + [\mathcal{O}(\varepsilon_i^3)] \rightarrow \text{negligible because } \varepsilon_i \text{ small}$$

$$\varepsilon_{i+1} = \underbrace{\varphi'(\tilde{x})\varepsilon_i}_{\text{at root this is } 0} + \frac{1}{2}\varphi''(\tilde{x})\varepsilon_i^2$$

Quadratic convergence

$$\boxed{\varepsilon_{i+1} \propto \varepsilon_i^2}$$

EXAMPLE:

$$f(x) = \cos(x) - 2x$$

Fixed point iteration $\varphi(x) = \frac{\cos x}{2}$ because needs to converge $\varphi'(x) = -\frac{\sin(x)}{2} \rightarrow$ varies between $-\frac{1}{2}$ and $\frac{1}{2}$

$$\text{FPI: } \varepsilon_{i+1} = \varphi'(\xi)\varepsilon_i \rightarrow |\varphi'(\xi)| < \frac{1}{2} \quad \forall \xi \in \mathbb{R} \rightarrow \text{error will reduce by } \frac{1}{2} \text{ or more!}$$

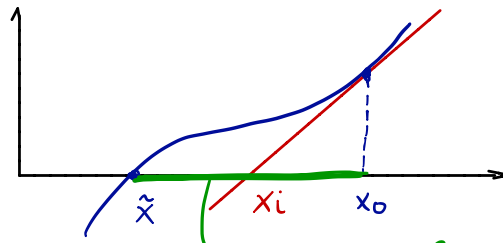
EXAMPLE:

MULTI-DIMENSIONAL ROOT-FINDING

$$\text{Find } \tilde{x} \text{ s.t. } f(\tilde{x}) = 0 \quad \underline{x} \in \mathbb{R}^n$$

$$\text{Taylor } f(x) = f(x_0) + \underbrace{f'(x_0)}_{\text{JACOBIAN MATRIX}}(x - x_0) = 0 \rightarrow f = \begin{bmatrix} f_1(x,y) \\ f_2(x,y) \end{bmatrix} \quad \frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix}$$

$$\underline{x} = x_0 - \frac{f(x_0)}{f'(x_0)} \rightarrow \underline{x} = x_0 - (f'(x_0))^{-1} \cdot f(x_0)$$



Taylor Approximation

continuous function if we differentiate

Theorem: let $f \in C^{n+1}([x, x_0])$ then

$$f(x) = f(x_0) + f'(x_0) \cdot (x - x_0) + \frac{1}{2!} f''(x_0) \cdot (x - x_0)^2 + \dots + \frac{1}{n!} f^{(n)}(x_0) \cdot (x - x_0)^n + O(x - x_0)^{n+1}$$

$$f(x) = \sum_{n=0}^n \frac{1}{n!} f^{(n)}(x_0) (x - x_0)^n + O(x - x_0)^{n+1}$$

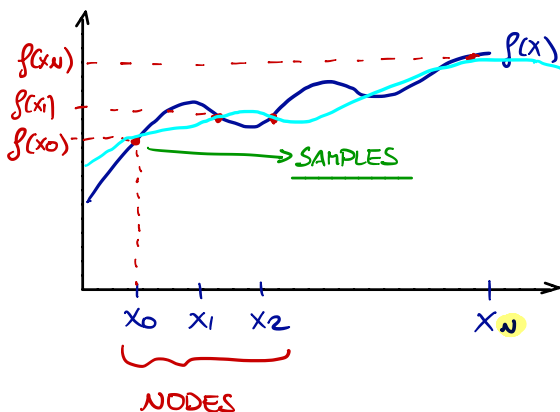
must be small in order to be useful.

$$\text{Explicit form of } O(x - x_0)^{n+1} = \frac{1}{(n+1)!} f^{(n+1)}(\xi) (x - x_0)^{n+1} \quad \xi \in [x, x_0]$$

this is hard to find, so that's why $(x - x_0)$ must be small.

Module #2 INTERPOLATION

Find a function $p(x)$ s.t. $f(x_i) = p(x_i)$ for $x_i \in [a, b] \subset \mathbb{R}$ $i = 0, 1, \dots, n$



Find another function of $p(x)$ that passes through the samples similar to EXCEL:

Interpolation means, find $p(x)$ and worry later.

Usually polynomial functions.

$$p(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n = \sum_{i=0}^n a_i x^i$$

SOME MATHEMATICAL NOTATIONS

$\forall$ for all $\Rightarrow$ implies

$\exists$ there exist s.t. such that

$G(h)$ order h $C^n(\mathbb{R})$ n times continuous differentiable function on $\mathbb{R}$

$f \in C^n$ f in C^0 $A \subset B$ A subset of B

P^n Polynomial of degree n

INTERPOLATION CONDITIONS

$$p(x_i) = f(x_i) \quad \forall i \in \{0, \dots, n\}$$

writing out.

$$\left. \begin{array}{l} 1. a_0 + a_1 x_0 + a_2 x_0^2 + \dots + a_n x_0^n = f(x_0) \quad i=0 \\ 2. a_0 + a_1 x_n + a_2 x_n^2 + \dots + a_n x_n^n = f(x_n) \quad i=n \end{array} \right\} \text{LINEAR IN COEFFICIENTS}$$

$$\begin{bmatrix} 1 & x_0 & \dots & x_0^n \\ 1 & x_1 & \dots & x_1^n \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & \dots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}$$

Vandermonde matrix V

Properties of interpolation:

1. $p(x)$ to exist - Existence

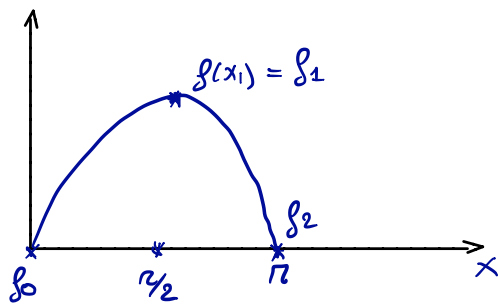
2. $p(x)$ is unique - Uniqueness

When do we have this? If V is invertible

$$\det(V) = \prod_{0 \leq i < j \leq n} (x_j - x_i)$$

• Implies $x_i \neq x_j \quad \forall i \neq j$

EXAMPLE $f(x) = \sin(x)$ on $[0, \pi]$



$$\underline{x} = (0, \frac{\pi}{2}, \pi)$$

$$\underline{f} = (0, 1, 0)$$

$$V \underline{a} = \underline{f}$$

$$V = \begin{bmatrix} 1 & 0 & 0 \\ 1 & \pi/2 & \pi^2/4 \\ 1 & \pi & \pi^2 \end{bmatrix}$$

Solve for a_i

$$p(x) = a_0 + a_1 x + a_2 x^2$$

$$\left. \begin{array}{l} a_0 = 0 \\ a_1 = 4/\pi \\ a_2 = -4/\pi^2 \end{array} \right\}$$

$$\underline{p(x) = \frac{4}{\pi} x - \frac{4}{\pi^2} x^2} \rightarrow \text{satisfies goes through the points.}$$

NIQUIST SAMPLE THEOREM: IN an oscillating signal you need at least two samples per wavelength.

MORE GENERALLY:

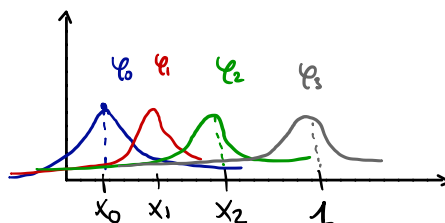
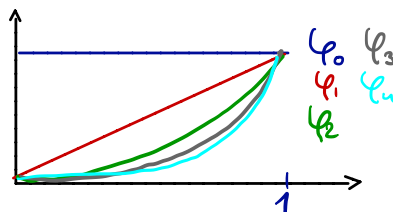
$$\text{Interpolate } \phi(x) = \sum_{i=0}^n a_i \varphi_i(x)$$

$\varphi_i \rightarrow$ "basis functions"

e.g. $\varphi_i(x) = x^i$ monomial basis

$$\varphi_i(x) = \sin\left(\frac{2\pi i x}{\lambda}\right)$$

$$\varphi_i(x) = \exp[-(x-x_i)^2]$$



INTERP. CONDITIONS:

$$\left. \begin{aligned} a_0 \cdot \varphi_0(x_0) + a_1 \varphi_1(x_0) + \dots + a_n \varphi_n(x_0) &= f(x_0) \\ a_0 \cdot \varphi_0(x_n) + a_1 \varphi_1(x_n) + \dots + a_n \varphi_n(x_n) &= f(x_n) \end{aligned} \right\} [n+1]$$

MATRIX EQUATION:

$$\begin{bmatrix} \varphi_0(x_0) & \varphi_1(x_0) & \dots & \varphi_n(x_0) \\ \varphi_0(x_n) & \varphi_1(x_n) & \dots & \varphi_n(x_n) \end{bmatrix} \begin{bmatrix} a_0 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f_0 \\ f_n \end{bmatrix} \quad \text{non singular}$$

Polynomial case: comparison to linear algebra:

$\varphi_i(x) = x^i$

1. $p = a_0 \underline{e}_0 + a_1 \underline{e}_1$
 2. $p = b_0 \underline{d}_0 + b_1 \underline{d}_1$

$\{e_0, e_1\}$ and $\{d_0, d_1\}$ span $\mathbb{R}^2$

$\mathbb{R}^2$

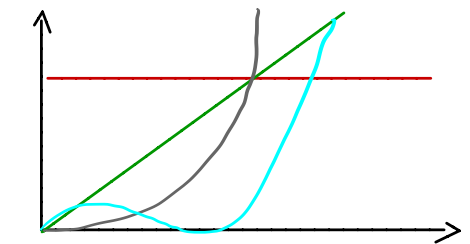
Basis

Similarly for polynomials:
 Assuming $x_i, i=0, \dots, n$ forms a basis for $\mathbb{P}^n$
 For any $p \in \mathbb{P}^n$ $p = \sum_{i=0}^n a_i x^i$

Newton Basis:

Def: $n_0(x) = 1$
 $n_1(x) = x - x_0$
 $n_2(x) = (x - x_0)(x - x_1)$

$n_k(x) = \prod_{j=0}^k (x - x_j)$



Property: $n_k(x_j) = 0, j < k$

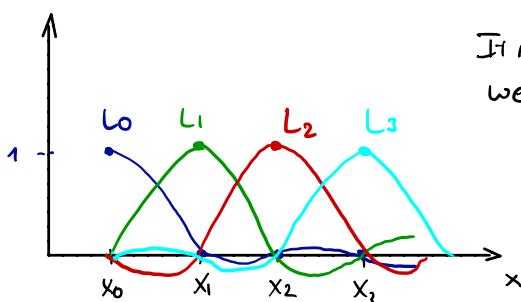
$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & x-x_0 & 0 & 0 & 0 \\ 1 & x-x_0 & (x-x_1) & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \end{bmatrix}$$

lower triangular.

- Invertible
- Find coefficients easily!

LAGRANGE BASIS:

Can we obtain $A=I$? Done with $L_i(x_j) = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$



It needs to be a cubic because we have three roots.

Directly:

$\hat{p}_0(x) = (x-x_1)(x-x_2)(x-x_3)$ three roots and 0 at locations
 $\hat{p}_0(x_0) = 1 = (x_0-x_1)(x_0-x_2)(x_0-x_3) \neq 0 \rightarrow p_0(x) = \frac{\hat{p}_0(x)}{\hat{p}_0(x_0)}$
 $l_k(x) = \prod_{j=0, j \neq k}^n \frac{(x-x_j)}{(x_k-x_j)} \quad p(x) = \sum_{i=0}^n f_i l_i(x)$

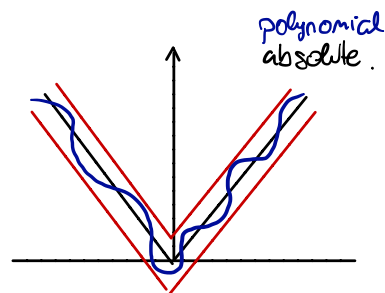
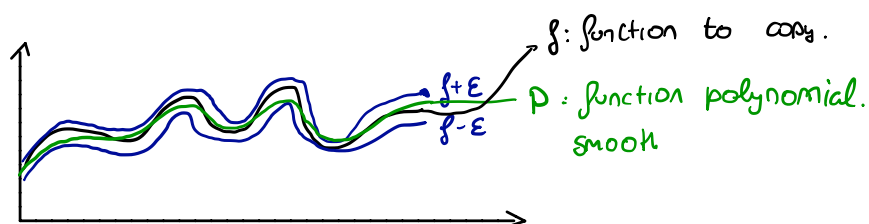
Why do we use polynomials:

- smooth.
- easy to differentiate and integrate.
- unique interpolation.

Weierstrass Theorem:

$\exists p \in P^N$, the same N , st for any $\varepsilon > 0$ for any $f \in C^0$

$$\max_x |f(x) - p(x)| < \varepsilon$$



Interpolation Error:

Let $f \in C^{N+1}([a, b])$, $p(x_i) = f(x_i) \forall i$

$$E = f(x) - p(x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} \cdot w_{N+1}(x) \longrightarrow w_{N+1} = \prod_{i=0}^N (x - x_i) - \text{nodal poly}$$

Proof 1.

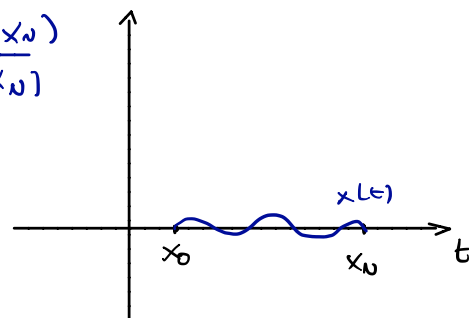
$$1. x = x_0 \quad f(x_i) - p(x_i) = 0 \quad w(x_i) = 0$$

$$2. x \neq x_i \quad g(t) = f(t) - p(t) - [f(x) - p(x)] \frac{(t - x_0) \dots (t - x_N)}{(x - x_0) \dots (x - x_N)}$$

Properties of g , Roots of g ? $t = x_0 \rightarrow g = 0$

On $[a, b]$ g has $N+2$ roots. $t = x \rightarrow g = 0$

g is $N+1$ times differentiable.



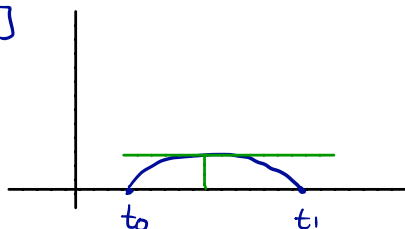
$$0 = g^{(N+1)}(\xi) = f^{(N+1)}(\xi) - p^{(N+1)}(\xi) - (f(x) - p(x)) \frac{N!}{w(x)}$$

$$\Rightarrow f(x) - p(x) = \frac{f^{(N+1)}(\xi)}{(N+1)!} w(x)$$

Rolle's Theorem $g \in [a, b]$

$$g(t_i) = 0 \quad i = 0, 1$$

$$g \in C^1 \rightarrow g'(\xi) = 0$$



GENERALIZED:

$$N: g(t_i) = 0 \quad i = 0, \dots, N$$

$$g \in C^{N+1} \rightarrow g^{(N+1)}(\xi) = 0$$

Then (Control of ω)

Of all polynomials P^n with leading coefficient 1.

the best minimum absolute value of $[-1, 1]$ is

$$\frac{T_N(x)}{2^{N+1}} \xrightarrow{\text{Chebyshev}} x = \cos \theta$$

$$\text{Def: } T_n(\cos \theta) = \cos(n\theta) \longleftrightarrow T_n(x) = \cos(n \cos^{-1}(x))$$

Possible $\cos(n\theta) = p(\cos \theta)$

$N=0$	$\cos \theta = 1$	$T_0 = 1$
1	$\cos \theta = \cos \theta$	$T_1 = x$
2	$\cos 2\theta = 2\cos^2 \theta - 1$	$T_2 = 2x^2 - 1$

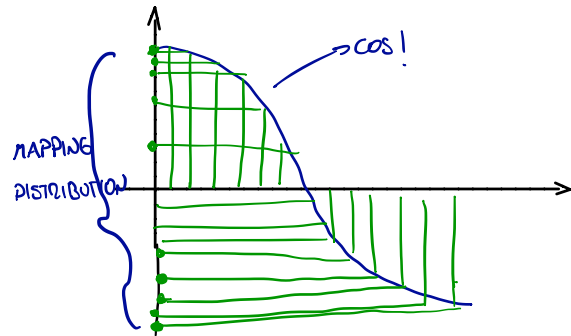
$$\text{Property: } \max_x |T_N(x)| = 1$$

$$\max_{\xi} \left| \frac{T_N(\xi)}{2^{N-1}} \right| = \frac{1}{2^{N-1}}$$

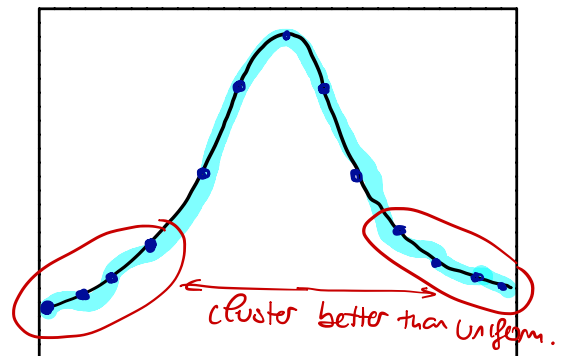
$$|f(x) - p(x)| \leq \frac{f^{(N+1)}(\xi)}{(N+1)!} \cdot \frac{1}{2^{N+1}} \quad \text{bound of error}$$

WHAT ARE THE T_N 's

1. $T_N(x) = \cos(N \arccos(x))$
2. $T_N(\cos(x)) = \cos(Nx)$
3. Degree N polynomial with roots $\eta_i = \cos\left(\frac{2i-1}{2N}\pi\right)$ $i = 1, \dots, N$



EXAMPLE



PROBLEMS:

For large numbers of N . Oscillations on the sides may occur that is why we use piecewise polynomial interpolation.

MODULE 3

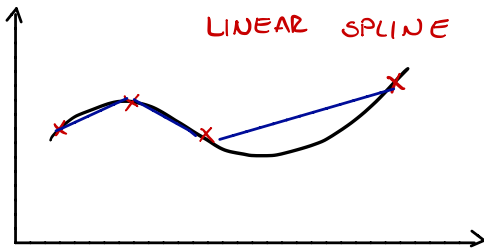
SPLINES, MULTI-DIMENSIONS AND RADIAL BASES

Spline of degree S : (datapoints $a = x_0 < x_1 < x_2 < \dots < x_N = b$)

S is a spline of degree D if:

1. S is a polynomial of degree $\leq d$ on $[x_i, x_{i+1}]$
2. $S, S', S'', \dots, S^{(d-1)}$ continuous on the entire interval.

polynomial in each subinterval, but not in total.



$$S = \begin{cases} s_0(x) & x \in [x_0, x_1] \\ s_1(x) & x \in [x_1, x_2] \\ \vdots & \\ s_{N-1}(x) & x \in [x_{N-1}, x_N] \end{cases}$$

Cubic splines are more used because derivative is not immediately a constant.

$$s_i(x) = \frac{f_{i+1} - f_i}{x_{i+1} - x_i} \cdot (x - x_i) + f_i \quad \text{for } x \in [x_i, x_{i+1}]$$

CUBIC SPLINES:

$[a, b]$

1. $s \in C^2[a, b]$

$i = 0, 1, 2, 3, \dots, N-1 \rightarrow \text{D.O.F} = \boxed{4 \cdot N}$
 $4(a_i + b_i + c_i + d_i)$

2. $[x_i, x_{i+1}] \quad s_i(x) = a_i(x - x_i)^3 + b_i(x - x_i)^2 + c_i(x - x_i) + d_i$

$$s_i'(x_i) = 3a_i(x - x_i)^2 + 2b_i(x - x_i) + c_i$$

$$s_i''(x_i) = 6a_i(x - x_i) + 2b_i \rightarrow \text{pretend we know this. } s_i''(x_i) = m_i$$

$$s_i''(x_{i+1}) = m_{i+1} \rightarrow 6a_i(x_{i+1} - x_i) + m_i = m_{i+1}$$

$\underbrace{\hspace{1cm}}_{\ell_i \rightarrow \text{spacing}}$

$$2b_i = m_i$$

$$\boxed{b_i = \frac{m_i}{2}}$$

$$\boxed{a_i = \frac{m_{i+1} - m_i}{6\ell_i}}$$

$$s_i(x) = \frac{m_{i+1} - m_i}{6\ell_i} (x - x_i)^3 + \frac{m_i}{2} (x - x_i)^2 + c_i (x - x_i) + d_i \rightarrow \text{need more constraints}$$

$s_i(x_i) = f_i$ continuity of function.

$\rightarrow \boxed{d_i = f_i}$

$s_i(x_{i+1}) = f_{i+1}$

$$\frac{m_{i+1}}{6\ell_i} \ell_i^3 + \frac{m_i}{2} \ell_i^2 + c_i \ell_i + f_i = f_{i+1}$$

$$c_i = \frac{f_{i+1} - f_i}{\ell_i} - \frac{\ell_i}{3} m_i - \frac{\ell_i}{6} m_{i+1}$$

$$S_i(x) = \frac{M_{i+1} - M_i}{6l_i} \cdot (x - x_i)^3 + \frac{M_i}{2} (x - x_i)^2 + \left(\frac{f_{i+1} - f_i}{l_i} - \frac{l_i}{3} M_i - \frac{l_i}{6} M_{i+1} \right) (x - x_i) + f_i$$

still to determine

First derivative

$$S_i'(x) = \frac{M_{i+1} - M_i}{2l_i} (x - x_i)^2 + \frac{M_i}{l_i} (x - x_i) + \left(\frac{f_{i+1} - f_i}{l_i} - \frac{l_i}{3} M_i - \frac{l_i}{6} M_{i+1} \right)$$

$$S_i'(x_i) = S_{i-1}'(x_i) \rightarrow \text{continuity.}$$

$$S_i'(x_i) = \left(\frac{f_{i+1} - f_i}{l_i} - \frac{l_i}{3} M_i - \frac{l_i}{6} M_{i+1} \right)$$

$$S_{i-1}'(x) = \frac{M_i - M_{i-1}}{2l_{i-1}} (x - x_{i-1})^2 + \frac{M_{i-1}}{l_{i-1}} (x - x_{i-1}) + \left(\frac{f_i - f_{i-1}}{l_{i-1}} - \frac{l_{i-1}}{3} M_{i-1} - \frac{l_{i-1}}{6} M_i \right)$$

$$S_{i-1}'(x_i) = \frac{M_i - M_{i-1}}{2l_{i-1}} (l_{i-1})^2 + \frac{M_{i-1}}{l_{i-1}} (l_{i-1}) + \left(\frac{f_i - f_{i-1}}{l_{i-1}} - \frac{l_{i-1}}{3} M_{i-1} - \frac{l_{i-1}}{6} M_i \right)$$

$$= \frac{l_{i-1}}{6} M_{i-1} + \frac{l_{i-1}}{3} M_i + \frac{f_i - f_{i-1}}{l_{i-1}}$$

$$\frac{l_{i-1}}{6} M_{i-1} + \frac{l_{i-1} + l_i}{3} M_i + \frac{l_i}{6} M_{i+1} = \frac{f_i - f_{i-1}}{l_i} - \frac{f_i - f_{i-1}}{l_{i-1}} \quad \text{for } i = 1, 2, 3, \dots, N-1$$

first derivative continuous.

We have $N+1$ unknowns, and we have less constraints.

USE: NATURAL CUBIC SPLINE $N+1$ unknowns $N-1$ constraints.

$$M_0 = 0 \quad M_N = 0$$

$$\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \frac{l_0}{6} & \frac{l_0+l_1}{6} & \frac{l_1}{6} & \dots & 0 \\ 0 & \frac{l_1}{6} & \frac{l_1+l_2}{6} & \frac{l_2}{6} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \frac{l_{N-2}}{6} & \frac{l_{N-2}+l_{N-1}}{6} & \frac{l_{N-1}}{6} \\ 0 & 0 & 0 & \dots & \dots & 1 \end{bmatrix} \begin{bmatrix} M_0 \\ M_1 \\ M_2 \\ \vdots \\ M_{N-1} \\ M_N \end{bmatrix} = \begin{bmatrix} \frac{f_1 - f_0}{l_1} - \frac{f_1 - f_0}{l_0} \\ \frac{f_2 - f_1}{l_2} - \frac{f_2 - f_1}{l_1} \\ \vdots \\ \frac{f_N - f_{N-1}}{l_{N-1}} - \frac{f_N - f_{N-1}}{l_{N-2}} \end{bmatrix}$$

tridiagonal matrix

FORMALIZED SOLUTION

$$A \cdot M = f \quad A \text{ is tridiagonal} \quad M = A^{-1} \cdot f$$

if $|a_{ii}| > \sum_{j \neq i} |a_{ij}| \rightarrow A$: strictly diagonally dominant. $\rightarrow \det(A) \neq 0$ then we can invert.

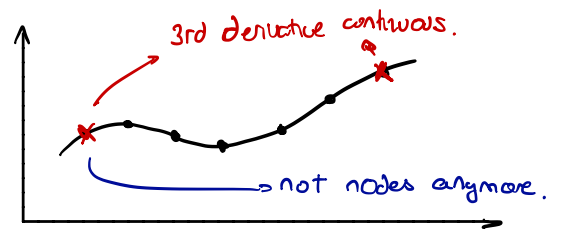
$$\underbrace{\left| \frac{l_{i-1} + l_i}{3} \right|}_{\text{general}} > \left| \frac{l_{i-1}}{6} \right| + \left| \frac{l_i}{6} \right| \rightarrow \text{true? yes always true}$$

TRUE

OTHER OPTIONS

$$S_0''(x_0) = M_0 = f''(x_0) \quad \text{instead of } M_0 = 0$$

not-a-knot spline



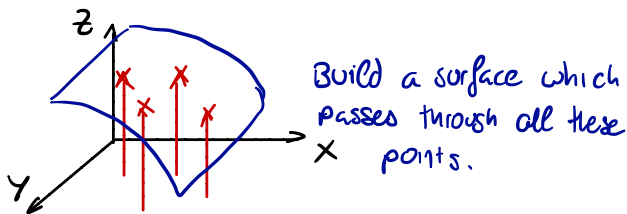
BIVARIATE INTERPOLATION

Set of data points:

$$\left. \begin{aligned} \{x: i=0, 1, \dots, n\} &\in D \subset \mathbb{R}^2 \\ \{f: i=0, 1, \dots, n\} \end{aligned} \right\}$$

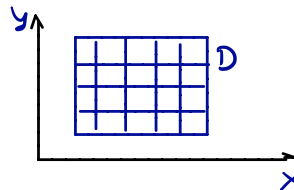
find a function that interpolates these data points.

$$p(x_i) = f_i \quad i=0, 1, \dots, n$$

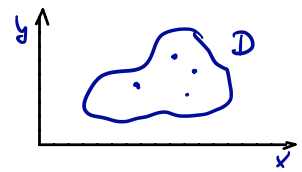


Build a surface which passes through all these points.

STRUCTURED GRID



UNSTRUCTURED GRID



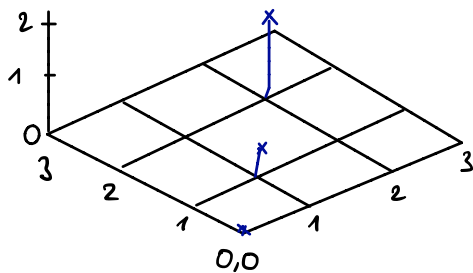
$$p(x, y) = \sum_{h=0}^n c_h \cdot b_h(x, y) \rightarrow p(x_i) = f_i \rightarrow \sum_{h=0}^n c_h b_h(x_i) = f_i$$

$$A \cdot c = f \quad c = A^{-1} \cdot f$$

$$A_{ij} = b_j(x_i) \quad \det(A) \neq 0$$

EXAMPLE

$$p(x, y) = a_0 + a_1 x + a_2 y$$



$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 2 \end{bmatrix}$$

A

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ -1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

$$a_0 = 0$$

$$a_1 + a_2 = 1$$

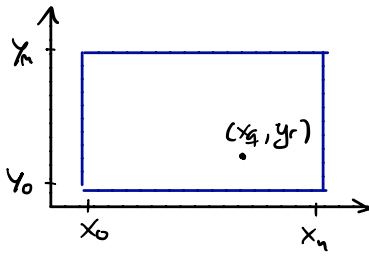
$$\det(A) = 0$$

$p(x, y) = a_1 x + (1 - a_1) y$ is a solution, no unique solution.

TENSOR - PRODUCT INTERPOLATION

$$\{(x_i, y_j)\}$$

split between functions depending only on x and only on y .



$$b_{ij}(x, y) = p_i(x) \cdot \psi_j(y)$$

$$p(x, y) = \sum_{i=0}^n \sum_{j=0}^m p_i(x) \cdot \psi_j(y) \cdot C_{ji}$$

$$p_i(x) = \alpha_i^{(x)}(x) = \prod_{\substack{h=0 \\ h \neq i}}^n \frac{(x - x_h)}{(x_i - x_h)}$$

$$\psi_j(y) = \alpha_j^{(y)}(y) = \prod_{\substack{h=0 \\ h \neq j}}^m \frac{(y - y_h)}{(y_j - y_h)}$$

Basis function $b_{ij}(x_q, y_r)$?

$$\alpha_i^{(x)}(x_q) \cdot \alpha_j^{(y)}(y_r) = \begin{cases} 1 & q=i \text{ and } r=j \\ 0 & \text{otherwise} \end{cases}$$

$$p(x_q, y_r) = \sum_{i=0}^n \sum_{j=0}^m b_{ij}(x_q, y_r) \cdot C_{ij} = C_{qr} \text{ is the only term that "survives" because the rest go to 0. } \rightarrow = \boxed{C_{qr}} \rightarrow \boxed{C_{ij} = f_{ij}}$$

$$p(x, y) = \sum_{i=0}^n \sum_{j=0}^m f_{ij} \cdot \alpha_i^{(x)}(x) \cdot \alpha_j^{(y)}(y)$$

due to the fact of using the Lagrange basis.

EXAMPLE:

find the bilinear polynomial $p(x, y)$ from the data.

$$f(0,0)=1 \quad f(1,0)=f(0,1)=f(1,1)=0$$

$$\begin{aligned} \alpha_0(x) &= \frac{x-1}{0-1} = 1-x & \alpha_0(y) &= \frac{y-1}{0-1} = 1-y \\ \alpha_1(x) &= \frac{x-0}{1-0} = x & \alpha_1(y) &= \frac{y-0}{1-0} = y \end{aligned}$$

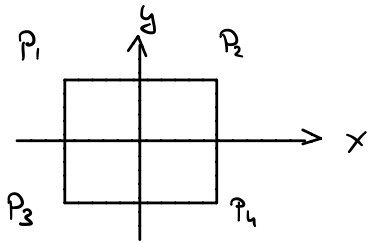
$$p(x, y) = f_{00} \alpha_0(x) \cdot \alpha_0(y) + \cancel{f_{10} \alpha_1(x) \cdot \alpha_0(y)} + \cancel{f_{01} \alpha_0(x) \cdot \alpha_1(y)} + \cancel{f_{11} \alpha_1(x) \cdot \alpha_1(y)}$$

$$p(x, y) = (1-x)(1-y) = \boxed{p\left(\frac{1}{2}, \frac{1}{2}\right) = \left(\frac{1}{4}\right)}$$

When n and m are increased a lot the grunge phenomenon on the edges does not work.

PATCH INTERPOLATION RECTANGULAR

- In 1D, to avoid oscillations of the interpolant we use splines.
- In 2D, we can use patch interpolation
- Perform the interpolation in rectangular or triangular pieces.



$$\begin{aligned} P_1 (-1, 1) &\rightarrow f_1 \\ P_2 (1, 1) &\rightarrow f_2 \\ P_3 (-1, -1) &\rightarrow f_3 \\ P_4 (1, -1) &\rightarrow f_4 \end{aligned}$$

$$P(x, y) = a_0 + a_1 x + a_2 y + a_3 xy$$

$$\begin{bmatrix} 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix}$$

$A \qquad a \qquad f$

$$a^T = [a_0, a_1, a_2, a_3]$$

$$b^T(x, y) = [1, x, y, xy]$$

$$P(x, y) = b^T(x, y) \cdot a = \underbrace{b^T(x, y) \cdot A^{-1}}_{\text{shape function } S(x, y)} \cdot f$$

→ different notation.

$$S(x, y) = [1, x, y, xy] \cdot \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 \end{bmatrix}$$

$$S(x, y) = \frac{1}{4} \cdot \begin{bmatrix} 1-x+y & -xy \\ 1+x-y & -xy \\ 1-x-y & +xy \\ 1+x-y & -xy \end{bmatrix} = \frac{1}{4} \begin{bmatrix} (1-x)(1+y) \\ (1+x)(1+y) \\ (1-x)(1-y) \\ (1+x)(1-y) \end{bmatrix}$$

$$P(x, y) = S(x, y) \cdot f = \sum_{i=1}^4 S_i(x, y) \cdot f_i$$

Not always a rectangle, so we should map into a rectangle whatever the surface.

EXAMPLE: 1

find $p(x, y)$ of $f(0, 0, 1, 2)$, on the unit rectangle

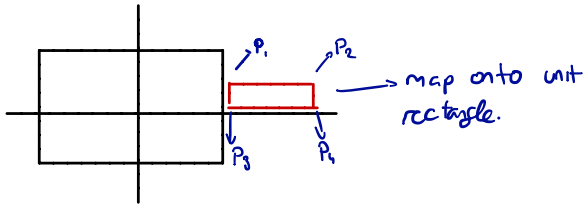
determine $p(0, 0)$

$$p(x, y) = \frac{f_1}{4} (1-x)(1+y) + \frac{0}{4} (1+x)(1+y) + \frac{1}{4} (1-x)(1-y) + \frac{2}{4} (1+x)(1-y)$$

$$\boxed{p(0, 0) = \frac{3}{4}}$$

EXAMPLE 2

$$\left. \begin{array}{l} P_1 = (1, 1/2) \quad P_2 = (2, 1/2) \quad P_3 = (1, 1/5) \quad P_4 = (2, 1/5) \\ f_1 = 1 \quad f_2 = 2 \quad f_3 = 3 \quad f_4 = 4 \end{array} \right\} P = (3/2, 1/4) ?$$

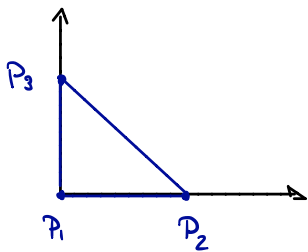


$$x \in [a_x, b_x] \rightarrow \xi_x \in [-1, 1]$$

$$\xi_{xp} = 2 \frac{x_p - a_x}{b_x - a_x} - 1 = 2 \frac{x_p - 1}{2 - 1} - 1 = 2x - 3$$

$$\xi_y = 2 \frac{y - a_y}{b_y - a_y} - 1 = 2 \frac{y - 1/5}{1/2 - 1/5} - 1 = -\frac{2}{3}$$

PATCH INTERPOLATION: TRIANGULAR PATCH



$$P_1 = (0,0) \rightarrow f_1$$

$$P_2 = (1,0) \rightarrow f_2$$

$$P_3 = (0,1) \rightarrow f_3$$

$$P(x,y) = a_0 + a_1 x + a_2 y \quad 3 \text{ DOF} - 3 \text{ points}$$

INTERPOLATION CONDITION

$$P(x_i) = f_i \quad i=1,2,3$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

$A \qquad \qquad a \qquad \qquad f$

$$P(x,y) = b^T(x,y) \cdot a \quad b^T(x,y) = [1, x, y]$$

$$P(x,y) = \underbrace{b^T(x,y) \cdot A^{-1}}_{S(x,y)} \cdot f$$

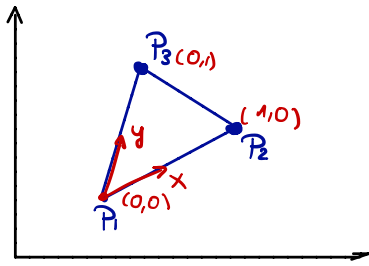
$$\det(A) = 1$$

$$A^* = \begin{bmatrix} 1 & -1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad A^{-1} = \frac{1}{\det(A)} \cdot A^{*T} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$S(x,y) = [1, x, y] \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 - x - y \\ x \\ y \end{bmatrix}$$

$$P(x,y) = \sum_{i=1}^3 S_i(x,y) \cdot f_i = (1-x-y)f_1 + xf_2 + yf_3$$

How do we map triangles into unit triangles?



$P_i = (u_i, v_i)$ To make the transformation from $(x, y) \rightarrow (u, v)$

$$\begin{cases} u = u_1 + (u_2 - u_1)x + (u_3 - u_1)y \\ v = v_1 + (v_2 - v_1)x + (v_3 - v_1)y \end{cases} \quad \left. \begin{array}{l} \text{we want to do the} \\ \text{opposite} \end{array} \right\}$$

along equations $\longrightarrow$

$$x = x(u, v)$$

$$y = y(u, v)$$

$$S(x, y) = S(x(u, v), y(u, v)) \Rightarrow S^*(u, v)$$

$$P(x, y) = P(u, v) = \sum_{i=1}^3 S_i^*(u, v) \cdot f_i$$

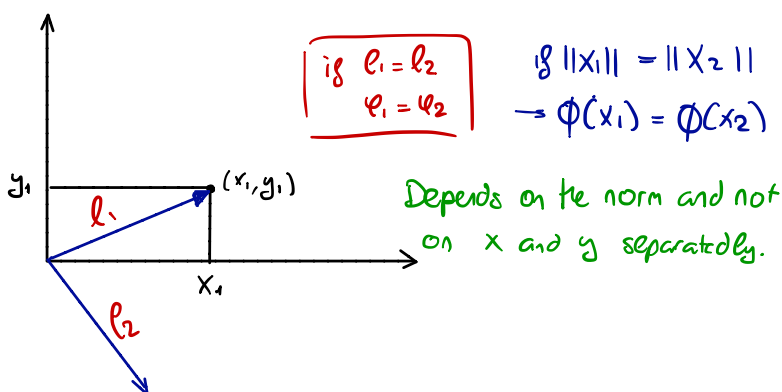
RADIAL BASIS FUNCTIONS

Scattered grid instead of regular, to get continuous and smooth approximation, same as in 2D.

Guarantees uniqueness and existence of bivariate interpolation for arbitrary distinct data points.

$\phi: \mathbb{R}^2 \rightarrow \mathbb{R}$ is a radial function if a function $\varphi: [0, +\infty) \rightarrow \mathbb{R}$ exists such that $(x, y) \rightarrow \text{real number}$

$$\phi(x) = \varphi(r) \quad r = \|x\| = \sqrt{x^2 + y^2}$$



$$\{x_i : i = 0, 1, \dots, n\}$$

$$\{f_i : i = 0, 1, \dots, n\}$$

RBF interpolant:

$$S(x) = \sum_{j=0}^n a_j \cdot \phi(\|x - x_j\|)$$

$$S(x_i) = f_i \quad i = 0, 1, \dots, n$$

$$\sum_{j=0}^n a_j \cdot \phi(\|x_i - x_j\|) = f_i$$

$$A \cdot a = f \quad A_{ij} = \phi(\|x_i - x_j\|)$$

$$A = \begin{bmatrix} \phi(\|x_0 - x_0\|) & \phi(\|x_0 - x_1\|) & \dots & \phi(\|x_0 - x_n\|) \\ \phi(\|x_1 - x_0\|) & \phi(\|x_1 - x_1\|) & \dots & \phi(\|x_1 - x_n\|) \\ \vdots & \vdots & \ddots & \vdots \\ \phi(\|x_n - x_0\|) & \phi(\|x_n - x_1\|) & \dots & \phi(\|x_n - x_n\|) \end{bmatrix}$$

$$A_{ii} = \phi(0) \rightarrow$$

$$A_{ij} = A_{ji} \iff \|x_i - x_j\| = \|x_j - x_i\|$$

RADIAL FUNCTION INTERPOLATION

- Gaussian $\phi(r) = \exp[-(\gamma \cdot r)^2]$
- Inverse quadratic $\phi(r) = \frac{1}{1 + (\gamma \cdot r)^2}$
- Inverse multiquadratic $\frac{1}{\sqrt{1 + (\gamma \cdot r)^2}}$
- Linear $\phi(r) = r$

EXAMPLE:

$\phi(r) = \exp[-(\gamma \cdot r)^2]$ used to interpolate $x = \{1, 3, 7\}$ $f = \{1, 1, 1\}$

$$x_0 - x_0 = 0 \rightarrow \phi(0) = e^{-(\gamma \cdot 0)^2} = 1$$

$$x_1 - x_0 = 2 \rightarrow \phi(2) = e^{-4\gamma^2}$$

$$x_2 - x_0 = 6 \rightarrow \phi(6) = e^{-36\gamma^2}$$

$$x_2 - x_1 = 4 \rightarrow \phi(4) = e^{-16\gamma^2}$$

Try $\gamma = 10$

$$\begin{bmatrix} 1 & \exp(-400) & \exp(-3600) \\ \exp(-400) & 1 & \exp(-1600) \\ \exp(-3600) & \exp(-1600) & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}$$

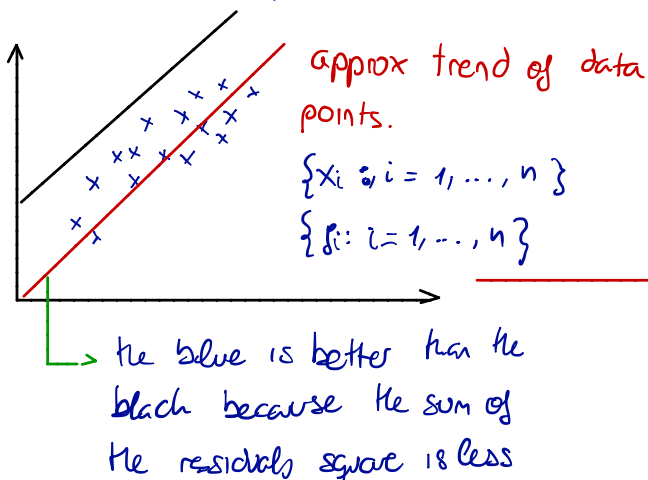
NOT good approximation!

Sure the solution exists, but maybe is not a good solution!

If $\gamma = 1 \rightarrow$ better
If $\gamma = 0.1 \rightarrow$ perfect. } in the order of separation of datapoints.

LEAST SQUARE REGRESSION

Approximate the values of the data points instead of finding a function that passes through the data points.



$$\phi(x) = \sum_{i=1}^m c_i \phi_i(x) \quad m \leq n$$

it does not care about order, more DOF.

HOW WE DETERMINE COEFFICIENTS?

$$R = \sum_{i=1}^n (f_i - a_0 - a_1 x_i)^2 \rightarrow \frac{\partial R}{\partial a_0} = -2 \sum_{i=1}^n (f_i - a_0 - a_1 x_i) = 0$$

$$\sum_{i=1}^n a_0 + \sum_{i=1}^n x_i a_1 = \sum_{i=1}^n f_i \rightarrow n a_0 + \sum_{i=1}^n x_i a_1 = \sum_{i=1}^n f_i$$

$$R = \sum_{i=1}^n r_i^2 \quad | \quad r_i = f_i - \phi(x_i) \quad i = 1, \dots, n$$

$$\frac{\partial R}{\partial a_1} = 0 \quad \sum x_i a_0 + \sum x_i^2 a_1 = \sum x_i f_i$$

$$\phi(x) = a_0 + a_1 x \quad r_i = f_i - a_0 - a_1 x$$

$$\left. \begin{aligned} n a_0 + \sum_{i=1}^n x_i a_i &= \sum_{i=1}^n f_i \\ \sum x_i a_0 + \sum x_i^2 a_i &= \sum x_i f_i \end{aligned} \right\} \text{Linear system of 2 eq w 2 unk}$$

$$\begin{bmatrix} n & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \sum f_i \\ \sum x_i f_i \end{bmatrix}$$

$$f(x), g(x) \rightarrow \text{scalar product of } \langle f, g \rangle = \sum_{i=1}^n f(x_i) \cdot g(x_i)$$

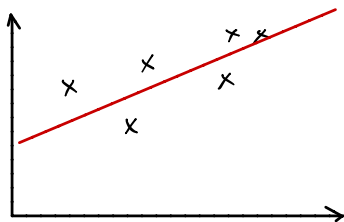
$$\begin{bmatrix} \langle 1, 1 \rangle & \langle 1, x \rangle \\ \langle 1, x \rangle & \langle x, x \rangle \end{bmatrix} = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \langle 1, f \rangle \\ \langle x, f \rangle \end{bmatrix}$$

$$\phi(x) = \sum_{j=1}^m a_j \varphi_j(x) \quad m \leq n \quad r_i = f_i - \phi(x_i) = f_i - \sum_{j=1}^m a_j \varphi_j(x_i)$$

$$R = \sum_{i=1}^n r_i^2 = \sum_{i=1}^n \left[f_i - \sum_{j=1}^m a_j \varphi_j(x_i) \right]^2 \quad \frac{\partial R}{\partial a_j} = 0 \quad j = 1, \dots, m$$

$$\begin{bmatrix} \langle \varphi_1, \varphi_1 \rangle & \langle \varphi_1, \varphi_2 \rangle & \dots & \langle \varphi_1, \varphi_n \rangle \\ \langle \varphi_2, \varphi_1 \rangle & & & \\ \vdots & & & \\ \langle \varphi_m, \varphi_1 \rangle & \dots & \dots & \langle \varphi_m, \varphi_n \rangle \end{bmatrix} \cdot \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \langle f, \varphi_1 \rangle \\ \langle f, \varphi_2 \rangle \\ \vdots \\ \langle f, \varphi_n \rangle \end{bmatrix}$$

$$\langle \varphi_2, \varphi_1 \rangle = \sum_{i=1}^n \varphi_2(x_i) \cdot \varphi_1(x_i)$$

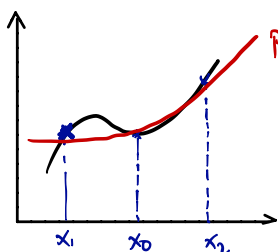


$$\text{ROOT MEAN SQUARED ERROR} \quad \sigma_{RMS} = \sqrt{\frac{\langle r, r \rangle}{n}}$$

How well the trend of the data points its approx by our approximant

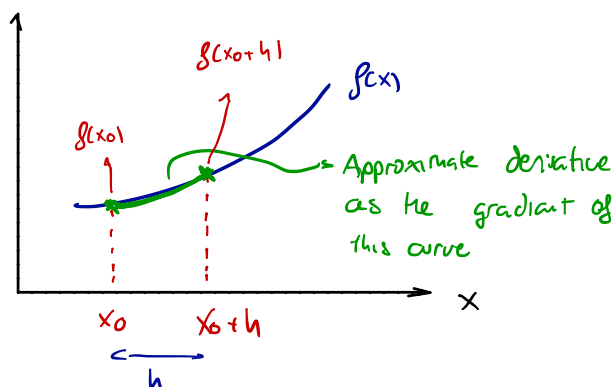
NUMERICAL DIFFERENTIATION

Approximate $f'(x) \approx \sum_{j=0}^m a_j f(x_j) \rightarrow$ solve root finding faster.
 $\hookrightarrow$ derivative



$p(x) \rightarrow$ evaluate derivative $\rightarrow$ and it will be an approximation. If we make the points closer will be a good approximation.

METHOD 1: FORWARD DIFFERENCES



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

D_f

Error?

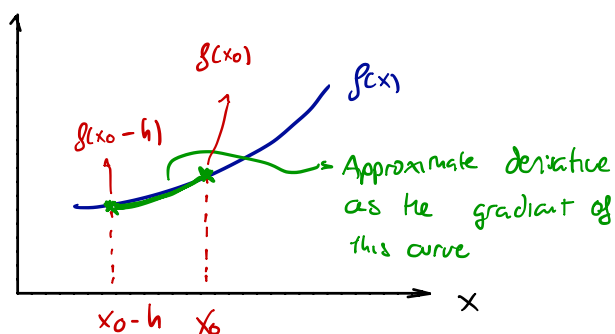
$$\epsilon = D_F(f) - f'(x_0)$$

Apply Taylor series to $f(x_0+h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + O(h^3)$

Substitute

$$\frac{f(x_0+h) - f(x_0)}{h} = \underbrace{f'(x_0)}_{\text{approx of } f'(x)} + \underbrace{\frac{1}{2}f''(x_0)h + O(h^2)}_{\text{Truncation error}}$$

METHOD 2: BACKWARD DIFFERENCES



$$f'(x_0) \approx \frac{f(x_0) - f(x_0-h)}{h} \quad D_B$$

Error

$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{1}{2}f''(x_0)h^2 + O(h^3)$$

$$\frac{f(x_0) - f(x_0-h)}{h} = f'(x_0) - \frac{1}{2}f''(x_0)h + O(h^2)$$

Which one is better? both are the same.

METHOD 3: CENTRAL DIFFERENCES

Adding both methods together

$$f'(x_0) \approx \frac{1}{2}(D_F(f) + D_B(f)) \approx \frac{1}{2} \left[\frac{f(x_0+h) - f(x_0)}{h} + \frac{f(x_0) - f(x_0-h)}{h} \right]$$

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$

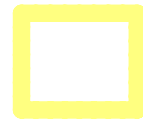
Error?

$$\left. \begin{array}{l} \text{Taylor } f(x_0+h) = f + hf' + \frac{1}{2}h^2f'' + \frac{1}{3!}h^3f''' + O(h^4) \\ \text{Taylor } f(x_0-h) = f - hf' + \frac{1}{2}h^2f'' - \frac{1}{3!}h^3f''' + O(h^4) \end{array} \right\} \quad \cancel{2hf'} = \cancel{2hf'} + \frac{1}{3!}h^2f''' + O(h^4) \text{ error}$$

GENERALIZED DIFFERENCE RULES

$$D[f] = \sum_{i=0}^n a_i f(x_0 + ih) \rightarrow \text{solve for coefficients} \quad f'(x_0) = D[f] + O(h^n)$$

find rules for highest possible orders $n=3$



4×4 invertible

$n=3$ Taylor of	a_0 $f(x_0)$	a_1 $f(x_0+h)$	a_2 $f(x_0+2h)$	a_3 $f(x_0+3h)$
$f(x_0)$	1	1	1	1
$hf'(x_0)$	0	1	2	3
$\frac{1}{2!} h^2 f''$	0	1	4	9
$\frac{1}{3!} h^3 f'''$	0	1	8	27
$\frac{1}{4!} h^4 f^{(4)}$	0	1	16	81

$$\begin{bmatrix} 1 \\ 3 \\ 9 \\ 27 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0 \\ h \\ 0 \\ 0 \end{bmatrix}$$

$$a = \frac{1}{6} (-11, 18, -9, 2) \rightarrow \text{build difference rule}$$

is it invertible?

$$f'(x_0) = \frac{1}{6} (-11 \cdot f(x_0) + 18 \cdot f(x_0+h) - 9 \cdot f(x_0+2h) + 2 \cdot f(x_0+3h))$$

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ x_0 & x_1 & x_2 & x_3 \\ x_0^2 & x_1^2 & x_2^2 & x_3^2 \\ x_0^3 & x_1^3 & x_2^3 & x_3^3 \end{bmatrix}$$

BALANCING TRUNCATION ERROR + ROUNDING ERROR

$$\text{FD} \quad f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \underbrace{\frac{1}{2} h f''(x_0)}_{\text{truncation error}} + O(h^2)$$

Assume rounding error in $f(x)$ of $\epsilon(x)$ we are evaluating

$|\epsilon(x)| < E$, constant E , true for $\forall x$

$$\frac{F(x_0+h) - F(x_0)}{h} = \frac{f(x_0+h) - f(x_0)}{h} + \frac{\epsilon(x_0+h) - \epsilon(x_0)}{h}$$

$$\text{Error: } \left| f' - \frac{f(x_0+h) - f(x_0)}{h} \right| = \left| \frac{\epsilon(x_0+h) - \epsilon(x_0)}{h} - \frac{1}{2} h f''(x_0) + O(h^2) \right|$$

$$\leq \left| \frac{\epsilon(x_0+h)}{h} \right| + \left| \frac{\epsilon(x_0)}{h} \right| + \left| \frac{1}{2} h f'' \right| + O(h^2)$$

$$\left| \frac{f(x+h)}{h} \right| + \left| \frac{f(x)}{h} \right| + \left| \frac{1}{2} h f'' \right| + O(h^2) \leq \underbrace{\frac{2E}{h}}_{\text{rounding}} + \underbrace{\frac{1}{2} h M + O(h^2)}_{\text{truncation}} \} e(h)$$

Assume $f'' < M, \forall x$

At 64 bit FP $\rightarrow E_{\text{mach}} = 10^{-16}$ $E = 10^{-16}$ $M = 1$ → not massive independent of h

Choose h such that h s.t. upper bound is minimum

$$\frac{de}{dh} = 0 = -\frac{2E}{h^2} + \frac{M}{2} \quad h^2 \rightarrow \frac{4E}{M} = \boxed{h = \frac{2\sqrt{E}}{\sqrt{M}}} \rightarrow \text{optimum } h \text{ to minimize error.}$$

$\frac{2 \cdot 10^{-8}}{1}$

RICHARDSON EXTRAPOLATION

General technique for increasing the order of the truncation method.

Rule $D_h(f)$ with step h , with order N α, β are constants, unknown

$$D_h(f) = f' + \alpha \cdot h^N + \beta h^{N+1} + O(h^{N+2})$$

Compare: $D_h(f) = f' + \alpha h^N + \beta h^{N+1} + O(h^{N+2})$

$$D_{h/2}(f) = f' + \alpha \frac{h^N}{2^N} + \beta \frac{h^{N+1}}{2^{N+1}} + O(h^{N+2})$$

$$2^N D_{h/2}(f) - D_h(f) = (2^N - 1) \cdot f' + \gamma h^{N+1} + O(h^{N+2})$$

$$\frac{2^N D_{h/2}(f) - D_h(f)}{2^N - 1} = f' + \underbrace{\gamma h^{N+1}}_{\text{truncation}} + O(h^{N+2})$$

EXAMPLE: FD

$$D_h(f) = \frac{f(x+h) - f(x)}{h} + O(h) \quad \boxed{N=1}$$

$$D_{h/2}(f) = \frac{f(x+h/2) - f(x)}{(h/2)} + O(h)$$

Using (*)

$$D'(f) = \frac{2 D_{h/2} - D_h}{2^1 - 1} = \frac{4 \cdot f(x+h/2) - 3 \cdot f(x) - f(x+h)}{h} = f' + O(h^2)$$

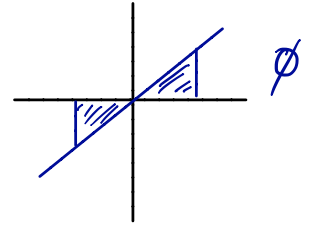
MODULE 4 NUMERICAL INTEGRATION

$$I[f] = \int_a^b f(x) dx = \sum_{i=0}^n w_i f(x_i) = Q[f]$$

Degree of Precision (DoP)

Defn $Q[f]$ has DoP d :

- if $Q[p] = I[p] \quad \forall p \in \mathbb{P}^d$
- and $Q[q] \neq I[q] \quad \exists q \in \mathbb{P}^{d+1}$



Equivalent Q is exact $\forall ax^d + ax^{d-1} + \dots + a_0$
and Q is not exact for x^{d+1}

Linearity: $I[ap + bq] = aI[p] + bI[q]$
 $Q[ap + bq] = aQ[p] + bQ[q]$

INTEGRATION CONDITIONS:

- Q is exact for $x^0, \dots, x^d$

Linear system:

Vandermonde $\rightarrow$ invertible

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_0 & x_1 & \dots & x_n \\ x_0^2 & x_1^2 & \dots & x_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ x_0^d & x_1^d & \dots & x_n^d \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} b-a \\ \frac{b^2-a^2}{2} \\ \frac{b^3-a^3}{3} \\ \vdots \\ \frac{b^{d+1}-a^{d+1}}{d+1} \end{bmatrix}$$

$$I[p] = Q[p]$$

$$p=1 \quad (b-a) = \int_a^b 1 dx = \sum_{i=0}^n w_i$$

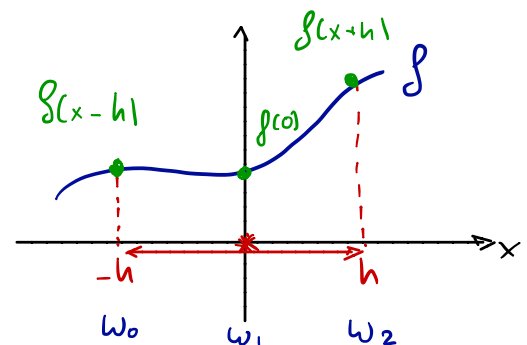
$$p=x \quad \frac{b^2-a^2}{2} = \int_a^b x dx = \sum_{i=0}^n w_i x_i$$

$$p=x^2 \quad \frac{b^3-a^3}{3} = \int_a^b x^2 dx = \sum_{i=0}^n w_i x_i^2$$

SIMPSON'S RULE

Am for DoP 2.

$$Q[f] = w_0 f(-h) + w_1 f(0) + w_2 f(h)$$



From below:

$$Q[f] = \frac{h}{3} f(-h) + \frac{4h}{3} f(0) + \frac{h}{3} f(h)$$

$$\begin{matrix} p=1 \\ p=x \\ p=x^2 \end{matrix} \begin{bmatrix} 1 & 1 & 1 \\ -h & 0 & h \\ h^2 & 0 & h^2 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 2h \\ 0 \\ \frac{2h^3}{3} \end{bmatrix}$$

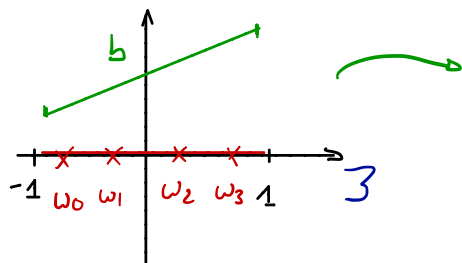
$$\rightarrow \omega_0 = \omega_2 \quad (\text{from } p=x)$$

$$(p=x^2) \Rightarrow h^2 \omega_0 + h^2 \omega_2 = \frac{2h^3}{3} \quad \omega_0 = \omega_2 = \frac{h}{3}$$

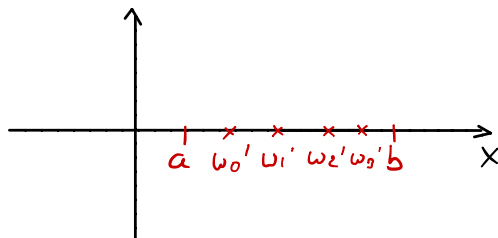
$$(p=1) \Rightarrow \omega_1 = \frac{4h}{3}$$

Interval Transformation

Unit-space:



Physical space:



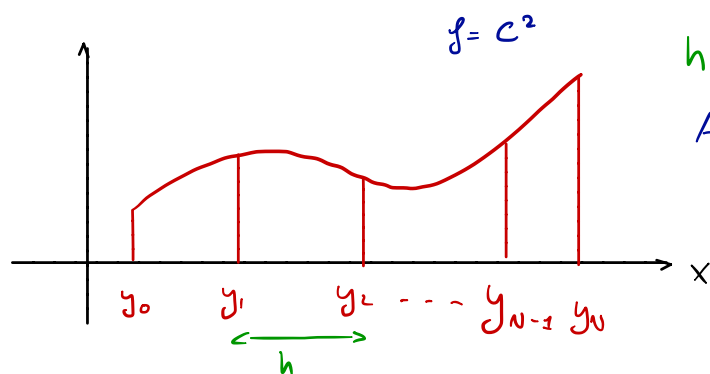
$$x = \left(\frac{a+b}{2} \right) + \left(\frac{b-a}{2} \right) \zeta$$

$$\frac{dx}{d\zeta} = \frac{b-a}{2}$$

$$x_i = \left(\quad \right) + \left(\quad \right) \zeta$$

$$I[f] = \int_a^b f(x) dx = \int_{-1}^1 f(x(\zeta)) \frac{dx}{d\zeta} d\zeta \approx \left(\frac{b-a}{2} \right) \sum_{i=0}^3 \omega_i f(x_i) = \sum_{i=0}^3 \underbrace{\left(\frac{b-a}{2} \omega_i \right)}_{\boxed{\omega_i'}} f(x_i)$$

Composite Rules



$$h = y_{i+1} - y_i$$

Add up all the approximations of each interval.

divide into subinterval.

REDUCE Error: by increasing d . Oscillation can be a problem. so better not

$$I[f] = \int_a^b f(x) dx = \sum_{i=0}^{N-1} \int_{y_i}^{y_{i+1}} f(x) dx \approx \sum_{i=0}^N \underbrace{Q[f; y_i, y_{i+1}]}_{\text{Composite rule}}$$

Composite rule $\rightarrow$ do not go to high degrees of polynomials.

ERROR BEHAVIOUR WITH $h \rightarrow 0$

- Degree of $Q = d$
- Define $g_i(x) = f(y_i + x)$

TAYLOR'S EXPANSION
small, so "h".

$$\int_0^h g_i(x) dx = \int_0^h \left(g(0) + g'(0)x + \frac{1}{2}g''(0)x^2 + \dots + \frac{1}{d!}g^{(d)}(0)x^d \right) dx$$

$$+ \underbrace{\int_0^h \frac{1}{(d+1)!}g^{(d+1)}(g(x))x^{d+1} dx}_{\text{error term.}}$$

Error $E_i \leq A \int_0^h x^{d+1} dx = \frac{A}{d+2} h^{d+2} \sim O(h^{d+2})$

Total error $E = \sum_{i=0}^n E_i \leq \frac{MA}{d+2} h^{d+2} + O(h^{d+1}) \quad M \propto \frac{1}{h}$

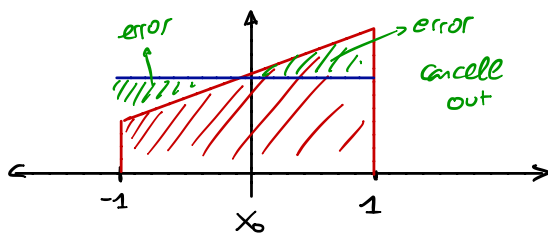
straight line.

TRAPEZOIDAL RULE
DoP: 1 Error: h^2

GAUSS - LEGENDRE QUADRATURE

Allow free choice of x_i , as well as w_i . DoF $\rightarrow 2(N+1)$

Solve DoP $2(N+1) - 1 = \boxed{2N+1}$



DO THE SAME WITH DIFFERENT POINTS.

$$Q(1) = I(1)$$

$$Q(x) = I(x)$$

$$Q[f] = 2f(0)$$

QUADRATURE RULE 1

$$w_0 = 2$$

$$w_0 \cdot x_0 = 0 \quad \checkmark \quad \boxed{x_0 = 0}$$

Exact $\int_{-1}^1 a x + b dx = b \cdot 2$

$N=0$

$N=1$

(1) $Q[1] = I[1]$ (3) $Q[x^2] = I[x^2]$

(2) $Q[x] = I[x]$ (4) $Q[x^3] = I[x^3]$

(1) $w_0 f(x_0) + w_1 f(x_1) = 2 \quad \checkmark$

(2) $w_0 x_0 + w_1 x_1 = 0 \quad \checkmark$

(3) $w_0 x_0^2 + w_1 x_1^2 = 2/3 \quad \checkmark$

(4) $w_0 x_0^3 + w_1 x_1^3 = 0 \quad \checkmark$

NON LINEAR
NO STANDARD ALGEBRAIC
TECHNIQUES.
USE NEWTON'S METHOD
4 unknowns 4 equations.

Assume symmetry:

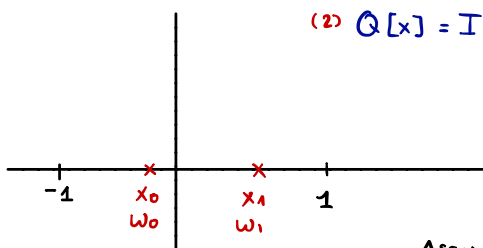
$$w_0 = w_1 = 1 \quad (3) \quad x_0^2 + x_1^2 = 2/3 = \frac{1}{\sqrt{3}} = x_0$$

$$x_0 = -x_1$$

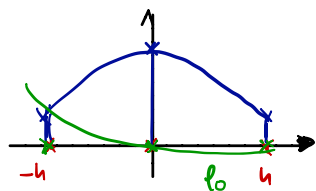
QUADRATURE RULE 2

$$Q[f] = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Symmetry assumption result.



IDEA: POLYNOMIAL INTERPOLATION + INTEGRATE THE INTERPOLANT



$$Q[f] = \int_{-h}^h p(x) dx$$

Simpson's Rule:

$$\text{Lagrange: } p(x) = \sum_{i=0}^2 f_i l_i(x)$$

$$Q[f] = \sum_{i=0}^2 f_i \underbrace{\int_{-h}^h l_i(x) dx}_{\text{weight of node. } w_i}$$

$$l_0(x) = \frac{(x)(x-h)}{2h^2}$$

$$w_0 = \int_{-h}^h l_0(x) dx = \frac{1}{2h} \left[\frac{1}{3}x^3 - \frac{h}{2}x^2 \right]_{-h}^h = \left[\frac{h}{3} \right] \rightarrow \boxed{w_0 = w_2} \text{ same.}$$

MODULE 5: Numerical Solutions of ODEs

PROBLEM STATEMENT

Find $\underline{u}(t)$ satisfying $\frac{d\underline{u}}{dt} = \underline{f}(\underline{u})$ and $\underline{u}(0) = \underline{u}_0$ → takes some space $\underline{u}$ and maps it on to the derivative of $\underline{u}$.

$\underline{u}$ is a function $\underline{u}: \mathbb{R} \rightarrow \mathbb{R}^n$
 $\underline{f}: \mathbb{R}^n \rightarrow \mathbb{R}^n$

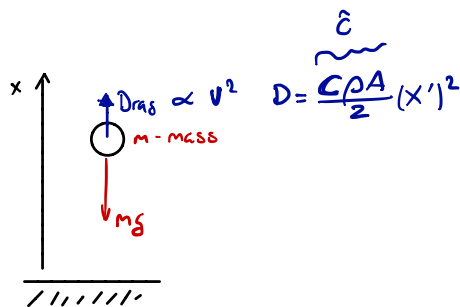
$$\frac{d\underline{u}}{dt} = \underline{u}'$$

1-D case: $u' = f(u)$ $u: \mathbb{R} \rightarrow \mathbb{R}$ $f: \mathbb{R} \rightarrow \mathbb{R}$

Initial value problem, we know to and we want to know the end. Not boundary value.

• $S(u(0), u(T)) = \emptyset$ } NOT COVERED

EXAMPLE Body accelerating under gravity.



No Air

$$m x'' = -mg$$

$$\underline{u} = \begin{pmatrix} x \\ x' \end{pmatrix} = \begin{pmatrix} u_0 \\ u_1 \end{pmatrix}$$

$$m u_1' = -mg$$

$$u_0' = u_1$$

$$\underline{u}' = \begin{pmatrix} u_1 \\ -g \end{pmatrix}$$

$$\underline{u}' = \underline{f}(\underline{u})$$

Air

$$m x' = -mg + \hat{c}(x')^2$$

$$\underline{u} = \begin{pmatrix} x \\ x' \end{pmatrix}$$

$$m u_1' = -mg + \hat{c} \cdot u_1^2$$

$$u_0' = u_1$$

$$\underline{u}' = \begin{pmatrix} u_1 \\ -g + \frac{\hat{c}}{m} u_1^2 \end{pmatrix}$$

$$\underline{u}' = \underline{f}(\underline{u})$$

→ transform to $\frac{d\underline{u}}{dt} = \underline{u}'$
 we need x and x'

EXAMPLE AEROSPACE

STRUCTURAL EQUATIONS:

$$mh'' + S_0 \cdot \theta'' + k_h \cdot h = -L(h', \theta)$$

$$S_0 h'' + I_0 \theta'' + k_\theta \cdot \theta = M(h', \theta)$$

S_0 = static mass moment

I_0 = mass moment of inertia

m = mass.

$$u = \begin{bmatrix} h \\ h' \\ \theta \\ \theta' \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

consider just h' and θ' $u_0' = u_1$ $\theta_0' = \theta_1$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & m & 0 & S_0 \\ 0 & 0 & 1 & 0 \\ 0 & S_0 & 0 & I_0 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{bmatrix}' + \begin{bmatrix} 0 & 1 & 0 & 0 \\ k_h & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & k_\theta & 0 \end{bmatrix} \bar{u} = \begin{bmatrix} 0 \\ -L \\ 0 \\ M \end{bmatrix}$$

$$u' = f(u)$$

NON AUTONOMOUS ODES

(scalar) $u' = f(u, t)$ → rewrite it without a t , we can always do it.
↪ explicit dependence on time.

Trick: fake variable;

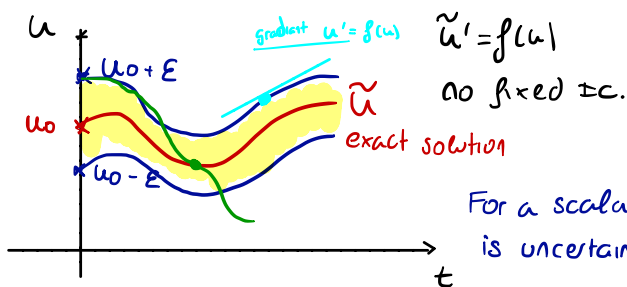
$$\underline{u} = \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \begin{pmatrix} u \\ t \end{pmatrix}$$

$$u_0' = f(u_0, t) \rightarrow u_0' = f(u_0, u_1)$$

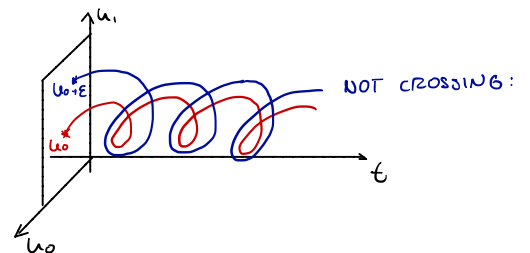
$$u_1' = 1 = t$$

no dependence on t .

GRAPHICALLY

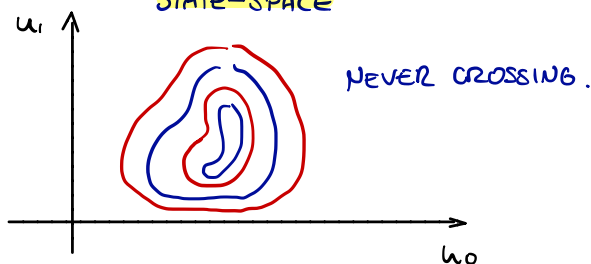


$$u: \mathbb{R} \rightarrow \mathbb{R}^2$$



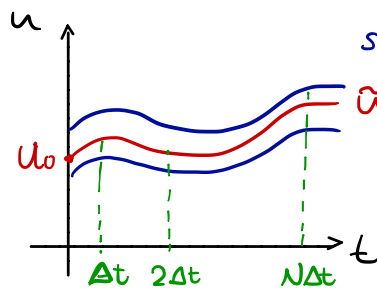
For a scalar equation, this lines should never cross if they do the future is uncertain •

STATE-SPACE



DISCRETIZATION OF $u(t)$

$u: \mathbb{R}^+ \rightarrow \mathbb{R}^n \rightarrow$



SCALAR SYSTEM

$\tilde{u} = f(\tilde{u}) \quad (1)$

Discretize solution:

$\tilde{u} = \begin{bmatrix} \tilde{u}(0) \\ \tilde{u}(\Delta t) \\ \vdots \\ \tilde{u}(N\Delta t) \end{bmatrix} \in \mathbb{R}^{N+1} \quad (\text{b/c } u: \mathbb{R} \rightarrow \mathbb{R})$

$\downarrow$
solution at time instant.

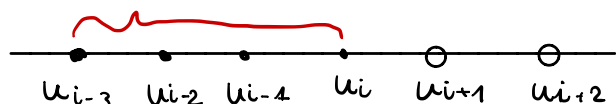
If $u: \mathbb{R} \rightarrow \mathbb{R}^m \quad \tilde{u} \in \mathbb{R}^{(m+1)N}$

Reduced an infinite dimension $u \rightarrow$ finite-dimension vector.

NUMERICAL METHOD TO FIND u_i

- Aiming to approximate $\tilde{u}(i\Delta t) \approx u_i$
- Assume past is known but future is unknown $u_0, u_1, \dots, u_i$ known
 $u_{i+1}, \dots, u_N$ UNKNOWN

predict the future using this

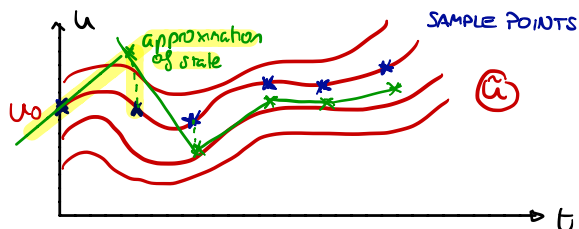


Find u_{i+1} in terms of $u_i, u_{i-1} \dots$

$u'(t_i) \approx \frac{u_{i+1} - u_i}{\Delta t}$

$\rightarrow f(u_i)$ from Equation (1)

$u_{i+1} = u_i + \Delta t \cdot f(u_i)$ FORWARD EULER



$\tilde{u} = f(\tilde{u})$

F-Euler approximation of $\tilde{u}$

DOES NOT GOOD VERY GOOD. } decrease Δt to improve

ERROR IN F-E

Taylor expansion:

(+) $u'(t_i) = \frac{u_{i+1} - u_i}{\Delta t} + \epsilon = \frac{u(t_i + \Delta t) - u(t_i)}{\Delta t} + \epsilon$

$\rightarrow$ Taylor.

(#) $u(t_i + \Delta t) = u(t_i) + u'(t_i) \Delta t + \frac{1}{2} u''(\xi) \cdot \Delta t^2 \quad \xi \in [t_i, t_{i+1}]$

$\epsilon = -\frac{1}{2} u''(\xi) \cdot \Delta t$ Rearrange (#) $\rightarrow$ (+)

Next step

$u_i' = f(u_i) \quad \frac{u_{i+1} - u_i}{\Delta t} + \epsilon = f(u_i)$

$u_{i+1} = u_i + \Delta t f(u_i) - \Delta t \cdot \epsilon$

error at each time step

$\rightarrow$ Proportional to $O(\Delta t^2)$

Error in u_n at $t=T$

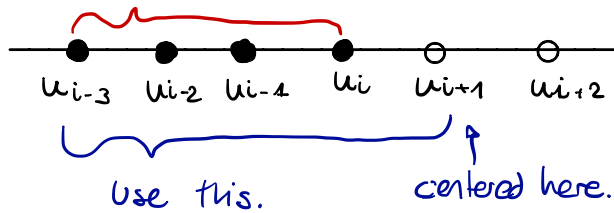
Take N steps, each step error $\sim O(\Delta t^2)$

$$E_T \sim N \cdot O(\Delta t^2) \quad N \text{ depends on } \Delta t \rightarrow N \propto \frac{1}{\Delta t}$$

$\sim O(\Delta t) \rightarrow$ F-E is a first order accurate method.

BACKWARD EULER

predict the future using this



$$f(u_{i+1}) u'_{i+1} = \frac{u_{i+1} - u_i}{\Delta t} + O(\Delta t)$$

Rearrange:

BACKWARD EULER

$$u_{i+1} = u_i + \Delta t f(u_{i+1})$$

HOW TO USE METHOD:

- Assume f linear: $f(u) = Au + B$

$$u_{i+1} = u_i + \Delta t \cdot [Au_{i+1} + B] \quad \underbrace{[I - \Delta t \cdot A]}_{J} u_{i+1} = u_i + \Delta t B$$

If J invertible

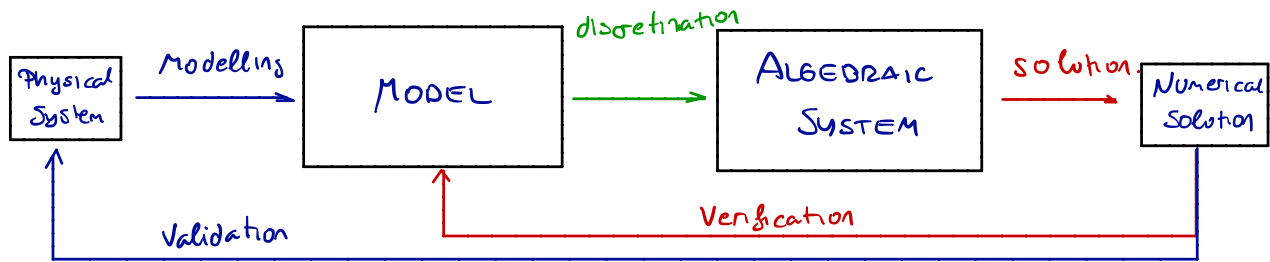
$$u_{i+1} = \dots$$

- Use root-finding at each time-step.
- linearize f

$$f(u_{i+1}) = f(u_i + \Delta u) = f(u_i) + \underbrace{f'(u_i)}_{\text{Jacobian}} \Delta u + \cancel{O(\Delta u^2)} \quad \text{error } O \text{ to linearize}$$

COMPUTATIONAL MODELLING

Process



MODELLING

UNCERTAINTIES

Epistemic: Due to unrecognized or unanticipated behaviour.

Aleatory: Impractical to measure.

MODEL ERRORS

Due to the use of simplified equations, linearization and sub-models for difficult to compute phenomena.

DISCRETIZATION

Take a continuous function and make it discrete. Solve for discrete function it is easier for computers.

DISCRETIZATION ERROR

$$\text{Taylor: } u_{i+1} = u_i + \Delta x \left. \frac{du}{dx} \right| + \underbrace{\frac{\Delta x^2}{2} \left. \frac{d^2u}{dx^2} \right|}_{\text{discretization error}} + \dots$$

SOLUTION

Iteration and Round-off errors.

LINEAR ITERATION ERROR: error due to halting of the iterative procedure for the solution of a linear algebraic system. ($< \text{tol}_2$)

NON-LINEAR ITERATION ERROR: error due to halting of the iterative solution of the non-linear problem ($< \text{tol}_1$)

VERIFICATION

TYPE 1 Establishes consistency with the PDE + BCs done using exact solution.

TYPE 2 Provides error estimate, done with grid study.

VALIDATION

Establishes the magnitude of model errors and uncertainties.

REQUIREMENTS

CONVERGENT: If when running the code if I increase the nodes, I get more close to the solution.

- Consistency: When substituting an exact solution into the discrete equations the only terms that remain are those that tend to 0.
- Stability: Numerical solution is unique. Small changes to the input produce only small changes to the numerical solution.

It is possible to have a consistent algorithm which is not stable.

ACCURACY: It is possible to design methods with a certain order of accuracy.

AFFORDABILITY: Some solution methods are much faster than others.

Computers are not better but methods are.

PARTIAL DIFFERENTIAL EQUATIONS

HEAT EQUATION

$$\frac{du}{dt} = \nu \cdot \frac{\partial^2 u}{\partial x^2}$$

CONVECTION EQUATION

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0$$

• Unattenuated

•

ADVECTION-DIFFUSION EQUATION

$$\frac{du}{dt} + c \frac{\partial u}{\partial x} = \nu \cdot \frac{\partial^2 u}{\partial x^2}$$

• Combination of two previous

•

SECOND ORDER WAVE EQUATION

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad \bullet$$