NTNU

Norwegian University of Science and Technology

TMA4130 Matematikk 4N

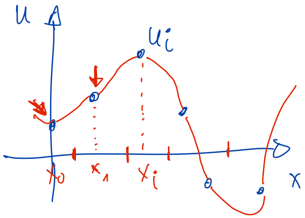
Week 35:
Interpolation and numerical integration

Douglas R. Q. Pacheco

Department of Mathematical Sciences, NTNU.

Autumn semester, 2022

Remember: finite different solution



$p(x)$

Interpolation

– Given data points (x_i, y_i), $i = 1, \ldots, n$, we want to find a function $p(x)$ within a certain function space, such that $\boxed{p(x_i) = y_i}$.

x_i	y_i
0	-1
0.5	2
1	3
1.1	4.5

$p(0) = -1$

$p(0.5) = 2$

$\vdots$

Polynomial interpolation: if I have n distinct points, the minimum degree I need is $n-1$

Example

x_i	y_i
0	0
$1/2$	$1/4$
1	0

$n=3 \Rightarrow$ 2nd degree : $p_2(x) = a_2 x^2 + a_1 x + a_0$; $p(x_i) = y_i$, $i = 1,2,3$

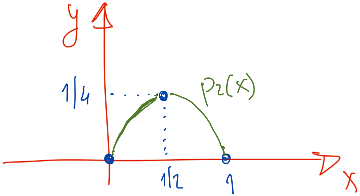
$* \; p(0) = 0 \Rightarrow a_2 0^2 + a_1 0 + a_0 = 0 \Rightarrow a_0 = 0$

$* \; p(1/2) = 1/4 \Rightarrow a_2 \left(\frac{1}{2}\right)^2 + a_1 \left(\frac{1}{2}\right) = 1/4 \Rightarrow a_2 + 2a_1 = 1$

$* \; p(1) = 0 \Rightarrow a_2 (1)^2 + a_1 (1) = 0 \Rightarrow a_2 + a_1 = 0$

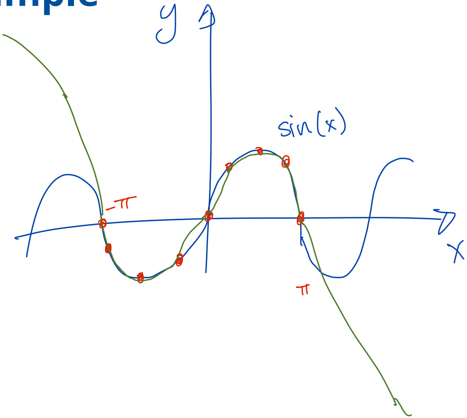
$\Rightarrow \; a_1 = 1$, $\; a_2 = -1$

$P_2(x) = -x^2 + x$



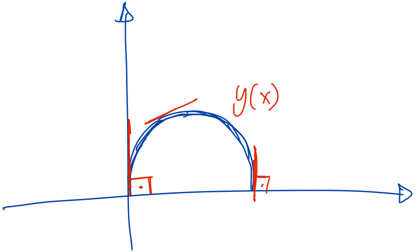
NTNU

Example



Let's say we have a polynomial $P_n(x)$ interpolating $\sin(x)$ within $x \in [-\pi, \pi]$

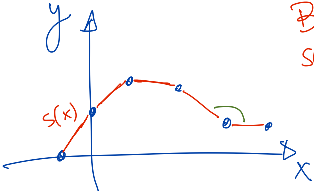
$$(x-x_0)^2+(y-y_0)^2=R^2$$



Splines

Splines are piecewise polynomial functions that are often used as interpolators.

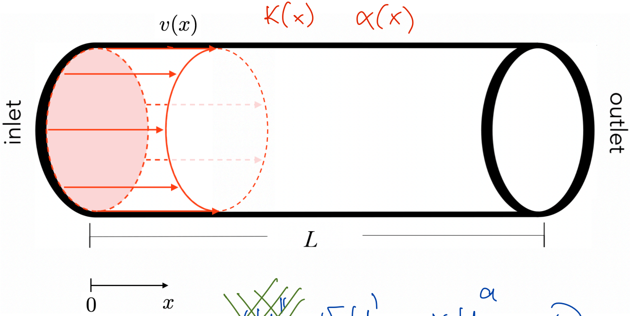
Ex.: first-degree splines



Between two points x_i and x_{i+1}, $S(x)$ is a first-degree polyn.

Ex.: cubic splines are continuous and have continuous first and second derivatives

Remember: simplified reactor model



$u = [A]$

$$\cancel{\alpha u''} - v u' - K u^a = 0$$

diffusion   convection   reaction

$a \in \mathbb{N}$

Reaction: aA → bB + cC

if $v(x)$ is high, we can neglect diffusion $\Rightarrow$ $\begin{cases} u'(x) = -\frac{K}{v} u^a \\ u(0) = u_0 \end{cases}$

Remember: simplified reactor model

$a = 1$: $u(x) = u_0 \exp\left[-\int_0^x \frac{k}{v}\, dx\right]$

$a = 2$: $u(x) = \dfrac{u_0}{1 + u_0 \int_0^x \frac{k}{v}\, dx}$

⋮

if $v(x) = \ln(x+1)$

↳ I have to compute $\int_0^x \frac{1}{\ln(x+1)}\, dx = F(x)$

if $v(x) = e^{x^2}$

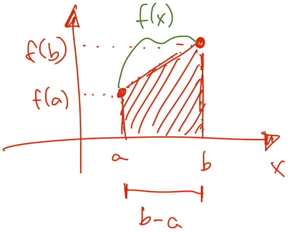
↳ $\int_0^x e^{-x^2}\, dx$ → no analytical representation!

→ Motivation for numerical integration!

NTNU

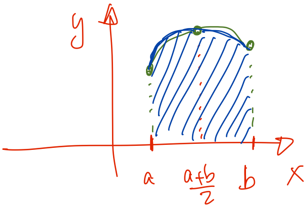
Revision: numerical integration

* Trapezoidal rule



$$\int_a^b f(x)\,dx \approx (b-a)\frac{f(a)+f(b)}{2}$$

* Simpson's rule



With 3 points, I can define a parabola that interpolates f(x)

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]$$

c or m

Quadrature rules

$$\int_a^b f(x)\,dx \approx \mathcal{I} = \sum_{j=1}^{n} w_j f(x_j)$$

quadrature points

weights

Let's say we have a quadrature formula for $\int_{-1}^{1} f(x)\,dx$. Can we transfer this to a general interval $[a,b]$?

$$\rightarrow \int_a^b f(x)\,dx = \int_{-1}^{1} f(x(\varphi))\, J \, d\varphi$$

Jacobian

$$x(-1) = \left(\frac{b-a}{2}\right)(-1) + \left(\frac{b+a}{2}\right) = a$$

What if we have $\boxed{x(\varphi) = \left(\frac{b-a}{2}\right)\varphi + \frac{b+a}{2}}$

$$\rightarrow x(+1) = \left(\frac{b-a}{2}\right)(1) + \frac{b+a}{2} = b$$

Quadrature rules

$$\boxed{x(\varphi) = \left(\frac{b-a}{2}\right)\varphi + \left(\frac{b+a}{2}\right)} \Rightarrow \frac{dx}{d\varphi} = \frac{b-a}{2} \Rightarrow dx = \overbrace{\left(\frac{b-a}{2}\right)}^{J} d\varphi$$

$$\Rightarrow \int_a^b f(x)dx = \int_{-1}^{1} f(x(\varphi))\, J\, d\varphi = \frac{b-a}{2}\int_{-1}^{1} f(x(\varphi))d\varphi$$

→ we can use any quadrature rule defined for $[-1,1]$

Ex.: Simpson's rule revisited

Given: $\int_{-1}^{1} f(\varphi)d\varphi \approx \frac{1}{3}\left[f(\underbrace{-1}_{\varphi_1}) + 4f(\underbrace{0}_{\varphi_2}) + f(\underbrace{1}_{\varphi_3})\right]$. How about $\int_a^b f(x)dx$?

$$\int_a^b f(x)dx = \frac{b-a}{2}\int_{-1}^{1} f(x(\varphi))d\varphi\,;$$

$\varphi = -1 \Rightarrow x = a$ ✓

$\varphi = 0 \Rightarrow x = (a+b)/2 = c$

$\varphi = 1 \Rightarrow x = b$ ✓

$$\int_a^b f(x)dx \approx \left(\frac{b-a}{2}\right)\frac{1}{3}\left[f(a) + 4f(c) + f(b)\right]$$

Trapezoidal rule!

Quadrature rules

Ex.:

x_i	φ_i	w_i
$1-\sqrt{3/5}$	$-\sqrt{3/5}$	$5/9$
1	0	$8/9$
$1+\sqrt{3/5}$	$+\sqrt{3/5}$	$5/9$

$a = 0$

$b = 2$

$f(x) = \sin(x)$

$$x(\varphi) = \left(\frac{b-a}{2}\right)\varphi + \left(\frac{b+a}{2}\right) = \varphi + 1$$

$$\int_0^2 \sin(x)\,dx = \underbrace{\left(\frac{b-a}{2}\right)}_{1} \int_{-1}^{1} f(x(\varphi))\,d\varphi = 1 \cdot \sum_{i=1}^{3} w_i f(x_i) = \frac{5}{9}\sin\left(1-\sqrt{\frac{3}{5}}\right) + \frac{8}{9}\sin(1) + \frac{5}{9}\sin\left(1+\sqrt{\frac{3}{5}}\right)$$

Composite integration rules

Remember our motivation

$a = 2$:

$$\boxed{u(x) = \frac{u_0}{1 + F(x)}}, \quad \text{with} \quad F(x) = \int_0^x \frac{k u_0}{v(x)}\,\mathrm{d}x = ???$$

Composite integration rules

Remember our motivation

$$u(x) = \frac{u_0}{1 + F(x)}, \quad \text{with} \quad F(x) = \int_0^x \overbrace{\frac{ku_0}{v(x)}}^{f(x)} \mathrm{d}x = ???$$

$$F(x_i) = \int_0^{x_i} f(x) = \int_0^{x_{i-1}} f(x)\,dx + \underbrace{\int_{x_{i-1}}^{x_i} f(x)\,dx}_{I_i} \approx I_i + \underbrace{\sum_{j=1}^{i-1} I_j}_{\text{accumulated}}$$

$\leftarrow$ quadrature rules