Short overview quadrature

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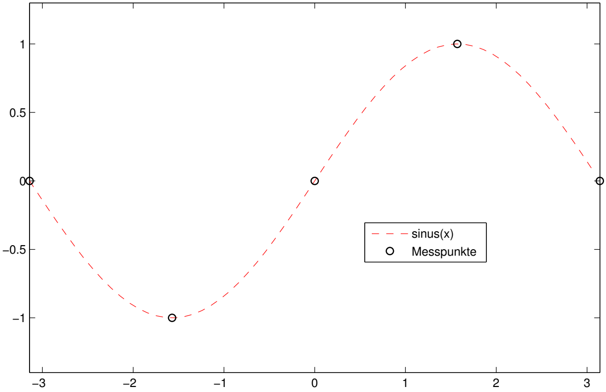
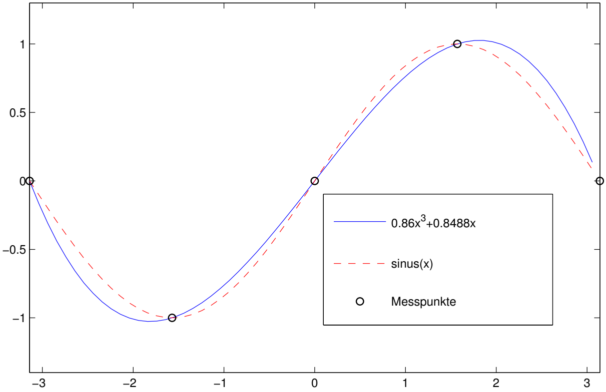
Motivation

$$\int_{-\pi}^{\pi} sin(x)dx? \tag{1}$$

Motivation



Motivation



Problem setting

Given:

- points $x_0 < x_1 < \cdots < x_n$
- associated measurements $y_0, y_1, \ldots, y_n$

Goal:
Find a function f with:

$$f(x_i) = y_i \quad i \in \{0, 1, \ldots, n\} \tag{2}$$

Questions

- Does such a polynomial exist ?
- If yes, is it unique?
- How well is $p(x)$ approximating original function $f(x)$?

Polynomial Interpolation

Given:

- points $x_0 < x_1 < \cdots < x_n$
- associated measurements $y_0, y_1, \ldots, y_n$

Goal:
Find a polynomial p of grade n

$$p(x_i) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_1 x + a_0 \tag{3}$$

with:

$$p(x_i) = y_i \quad i \in \{0, 1, \ldots, n\} \tag{4}$$

Example

Given:

- $(x_0, y_0) = (-1, -3)$
- $(x_1, y_1) = (0, -1)$
- $(x_2, y_2) = (1, 5)$

Goal:
Find a polynomial $p(x) = a_2x^2 + a_1x + a_0$ with:

- $p(-1) = -3$
- $p(0) = -1$
- $p(1) = 5$

Example

School:
Find a polynomial $p(x) = a_2 x^2 + a_1 x + a_0$ with:

$$p(-1) = a_2(-1)^2 + a_1(-1) + a_0 = -3 \tag{5}$$

$$p(0) = a_2 \cdot (0)^2 + a_1 0 + a_0 = -1 \tag{6}$$

$$p(1) = a_2 \cdot (1)^2 + a_1 \cdot 1 + a_0 = 5 \tag{7}$$

Example

Solve the system of linear equations:

$$p(-1) = a_2 - a_1 + a_0 = -3 \tag{8}$$

$$p(0) = a_0 = -1 \tag{9}$$

$$p(1) = a_2 + a_1 + a_0 = 5 \tag{10}$$

Example

Solve the system of linear equations:

$$\begin{bmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} -3 \\ -1 \\ 5 \end{bmatrix} \tag{11}$$

Example

Solve the system of linear equations:

$$\begin{bmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} -3 \\ -1 \\ 5 \end{bmatrix} \tag{12}$$

$$\rightarrow \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ -1 \end{bmatrix} \tag{13}$$

Example

Solve the system of linear equations:

$$\begin{bmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} -3 \\ -1 \\ 5 \end{bmatrix} \tag{12}$$

$$\rightarrow \begin{bmatrix} a_2 \\ a_1 \\ a_0 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ -1 \end{bmatrix} \tag{13}$$

$$\rightarrow p(x) = 2x^2 + 4x - 1 \tag{14}$$

More general

Solve the system of linear equations:
Find a polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$ with:

$$\begin{aligned} p(x_0) &= a_n(x_0)^n + \cdots + a_1 x_0 + a_0 = y_0 \\ p(x_1) &= a_n(x_1)^n + \cdots + a_1 x_1 + a_1 = y_1 \\ &\vdots \\ p(x_n) &= a_n(x_n)^n + \cdots + a_1 x_n + a_n = y_n \end{aligned}$$

More general

Solve the system of linear equations:
Find a polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$ with:

$$\begin{bmatrix} (x_0)^n & \dots & x_0 & 1 \\ (x_1)^n & \dots & x_1 & 1 \\ \vdots & \dots & \vdots & 1 \\ (x_n)^n & \dots & x_n & 1 \end{bmatrix} \begin{bmatrix} a_n \\ a_{n-1} \\ \vdots \\ a_0 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix} \tag{15}$$

More general

Solve the system of linear equations:
Find a polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$ with:

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$\rightarrow$ Gauss-Approach

Linear Algebra

Vector space

$$\mathbf{R}_{\leq n}[x] \in \mathbf{R}^{n+1} \tag{16}$$

Kanonical Basis

$$B = \{1, x, x^2, x^3, \ldots, x^n\} \tag{17}$$

Element

$$P_n(x) = \sum_{i=0}^{n} a_i x^i \tag{18}$$

Linear Algebra

Vector space

$$\mathbf{R}_{\leq n}[x] \in \mathbf{R}^{n+1} \tag{19}$$

Lagrange Basis

Given:

$$x_0 < x_1 < \cdots < x_n \tag{20}$$

$$L = \{l_0(x), l_1(x), \ldots, l_n(x)\} \tag{21}$$

with

$$l_i(x) := \prod_{\substack{k=0,\\ i \neq k}}^{n} \frac{x - x_k}{x_i - x_k} \tag{22}$$

Element

$$P_n(x) = \sum_{i=0}^{n} b_i l_i(x) \tag{23}$$

Example

Given:

- $x_0 = -1$
- $x_1 = 0$
- $x_2 = 1$

$$
\begin{aligned}
l_0(x) &= \frac{x-0}{-1-0} \cdot \frac{x-1}{-1-1} \\
l_1(x) &= \frac{x+1}{0+1} \cdot \frac{x-1}{0-1} \\
l_2(x) &= \frac{x+1}{1+1} \cdot \frac{x-0}{1-0}
\end{aligned} \tag{24}
$$

Lagrange-Polynomial

$$l_i(x) := \prod_{\substack{k=0, \\ i \neq k}}^{n} \frac{x - x_k}{x_i - x_k} \tag{25}$$

with

$$x_0 < x_1 < \cdots < x_n \tag{26}$$

is basis of $\mathbf{R}^n$, d.h.,

$$P_n(x) = \sum_{i=0}^{n} b_i l_i(x) \tag{27}$$

Properties of the Lagrange-Polynomials

$$l_i(x_j) := \begin{cases} 1 & \text{für } x_j = x_i \\ 0 & \text{für } x_j \neq x_i \end{cases} \tag{28}$$

Polynomial interpolation

Geben:

- Points $x_0 < x_1 < \cdots < x_n$
- measurements $y_0, y_1, \ldots, y_n$

Goal:
Find a polynomial p of grade n

$$p(x) = b_n l_n(x) + \cdots + b_1 l_1(x) + b_0 l_0(x) \qquad (29)$$

with

$$p(x_i) = y_i \quad i \in \{0, 1, \ldots, n\} \qquad (30)$$

Allgemeiner

Solve the system of linear equations:
Find a polynomial $p(x) = b_n l_n(x) + \cdots + b_1 l_1(x) + b_0 l_0(x)$ with:

$$\begin{bmatrix} l_n(x_n) & \dots & l_0(x_n) \\ l_n(x_{n-1}) & \dots & l_0(x_{n-1}) \\ \vdots & \dots & \vdots \\ l_n(x_0) & \dots & l_0(x_0) \end{bmatrix} \begin{bmatrix} b_n \\ b_{n-1} \\ \vdots \\ b_0 \end{bmatrix} = \begin{bmatrix} y_n \\ y_{n-1} \\ \vdots \\ y_0 \end{bmatrix} \tag{31}$$

Lagrange-Interpolation

$$l_i(x_j) := \begin{cases} 1 & \text{für } x_j = x_i \\ 0 & \text{für } x_j \neq x_i \end{cases} \tag{32}$$

Lagrange-Interpolation

$$\begin{bmatrix} l_n(x_n) & \dots & l_0(x_n) \\ l_n(x_{n-1}) & \dots & l_0(x_{n-1}) \\ \vdots & \dots & \vdots \\ l_n(x_0) & \dots & l_0(x_0) \end{bmatrix} \begin{bmatrix} b_n \\ b_{n-1} \\ \vdots \\ b_0 \end{bmatrix} = \begin{bmatrix} y_n \\ y_{n-1} \\ \vdots \\ y_0 \end{bmatrix} \tag{33}$$

Lagrange-Interpolation

$$\begin{bmatrix} 1 & \dots & 0 \\ 0 & 1 & 0 \\ \vdots & \dots & \vdots \\ 0 & \dots & 1 \end{bmatrix} \begin{bmatrix} b_n \\ b_{n-1} \\ \vdots \\ b_0 \end{bmatrix} = \begin{bmatrix} y_n \\ y_{n-1} \\ \vdots \\ y_0 \end{bmatrix} \tag{34}$$

Existence and uniqueness

Proposition For fixed points $x_0 < x_1 < \cdots < x_n$ and arbitray points $y_0, y_1, \ldots, y_n$ there is a unique polynomial P_n of grade n with

$$p(x_i) = y_i \quad i \in \{0, 1, \ldots, n\} \tag{35}$$

Motivation

Setting: Error of the polynomial interpolation

$$|\epsilon_n(x)| = |f(x) - P_n(x)| \leq \max_{x \in [a,b]} \left| \frac{1}{(n+1)!} f^{(n+1)}(x) \right| \max_{x \in [a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

Goal: small error

Motivation

Setting: Error of the polynomial interpolation

$$|\epsilon_n(x)| = |f(x) - P_n(x)| \leq \max_{x \in [a,b]} \left| \frac{1}{(n+1)!} f^{(n+1)}(x) \right| \max_{x \in [a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

Motivation

Setting: Error of the polynomial interpolation

$$|\epsilon_n(x)| = |f(x) - P_n(x)| \leq \max_{x\in[a,b]} \left| \frac{1}{(n+1)!} f^{(n+1)}(x) \right| \max_{x\in[a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

More concrete goal: want

$$\max_{x\in[a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

to be small

How?

Motivation

Setting: Error of the polynomial interpolation

$$|\epsilon_n(x)| = |f(x) - P_n(x)| \le \max_{x\in[a,b]} \left| \frac{1}{(n+1)!} f^{(n+1)}(x) \right| \max_{x\in[a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

More concrete goal: want

$$\max_{x\in[a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

to be small

How?: smart choice of points x_i

Equidistant supporting points

Proposition:
For equidistant supporting points in the interval $[a, b]$ i.e.,

$$x_i = a + i\frac{(b-a)}{n} \quad i \in \{0, \dots, n\} \tag{36}$$

the interpolation error has the following upper bound:

$$|\epsilon_n(x)| \leq \left(\frac{b-a}{n}\right)^{n+1} \frac{1}{4(n+1)} \max_{x\in[a,b]} |f^{(n+1)}(x)| \tag{37}$$

Tschebyscheff-Polynomials

Definition

The Tschebyscheff-Polynomials of first order are defined as follows for $n \in \mathbb{N}$:

$$T_n : [-1, 1] \to \mathbb{R}, \quad T_n(x) = \cos\left(n \ \arccos x\right)$$

Tschebyscheff-Polynomials

Recursiv formular

$$T_{n+1}(t) = 2t \cdot T_n(t) - T_{n-1}(t) \text{ für } t \in [-1, 1] \tag{38}$$

with

$$T_0(t) = 1, \;\; T_1(t) = t \tag{39}$$

Roots

$T_n(t)$ has n roots $t_k^{(n)}$ on $[-1, 1]$: with

$$t_k^{(n)} := \cos\left(\frac{(2k-1)\pi}{2n}\right) \quad \text{für } k \in \{1, \ldots, n\} \tag{40}$$

for all $n \in \mathbb{N}$

Extrem points

$T_n(t)$ has $n+1$ extrem points $s_k^{(n+1)}$ on $[-1,1]$: with

$$s_k^{(n+1)} := \cos\left(\frac{k\pi}{n}\right) \quad \text{für } k \in \{0,\dots,n\} \tag{41}$$

and it holds that

$$T_n(s_k^{(n)}) = (-1)^k \quad \text{für } k \in \{0,\dots,n\} \tag{42}$$

for all $n \in \mathbb{N}$

Tschebyscheff- supporting points

Definition

The roots $\{t_0^{(n+1)}, \dots, t_n^{(n+1)}\}$ of the $n+1$-Tschebyscheff Polynomial $T_{n+1}(t)$ are the so called Tschebyscheff-Supporting-Points.

Optimality on $[-1, 1]$

Optimality on $[-1, 1]$:

$$\max_{x \in [a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

is minimal for the Tschebyscheff-Supporting-Points

Error

For Tschebyscheff-Supporting Points on the Intervall $[-1, 1]$ the interpolation error has the following upper bound:

$$|f(x) - P_n(x)| \leq \frac{1}{2^n} \max_{x \in [-1,1]} \left| \frac{1}{(n+1)!} f^{(n+1)}(x) \right|$$

Optimality on $[a, b]$

Optimality on $[a, b]$:

$$\max_{x \in [a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$$

is minimal for

$$\Phi : [-1, 1] \to [a, b] \tag{43}$$

shifted Tschebyscheff-Supporting Points $\Phi(t_k^{(n+1)})$.

Quadratur

Problem: determine Integral

$$I[f] = \int_a^b f(x) \, \mathrm{dx} \tag{44}$$

Quadraturformel

$$I[f] \approx I_n[f] = \sum_{i=0}^{n} g_i f(x_i) \, \mathrm{dx} \tag{45}$$

with

- knots $x_i \in [a, b]$ für i=0,...,n
- weights g_i für i=0,...,n

Newton-Cotes Formular

Idea: Determine Interpolation polynomial for $(x_i, f(x_i))$
$i = 0, 1, \ldots, n$

$$P_n(x) = \sum_{i=0}^{n} l_i(x) f(x_i) \qquad \text{mit } l_i(x) := \prod_{\substack{k=0,\\ i\neq k}}^{n} \frac{x - x_k}{x_i - x_k}$$

to approximate $f(x)$

Solution: Quadratur formulae

$$I[f] \approx I_n[f] = \int_a^b P_n(x)\,\mathrm{dx} = \sum_{i=0}^{n} \int_a^b l_i(x)\,\mathrm{dx}\; f(x_i) = \sum_{i=0}^{n} g_i f(x_i)$$

Newton-Cotes formulare

Simplification: Use equidistant supporting points

$$x_i = a + i\frac{(b-a)}{n} \quad i \in \{0, \dots, n\}$$

Ergebnis: Newton-Cotes formulare

$$I[f] \approx I_n[f] = \int_a^b P_n(x)\ \mathrm{dx} = (b-a)\sum_{i=0}^{n} \alpha_i^n f(x_i)$$

with

$$\alpha_i^n = \frac{1}{n}\int_0^n \prod_{\substack{j=0,\\ i\neq j}}^{n} \frac{x-j}{i-j}\ \mathrm{dx}$$

Newton-Cotes formulare

Trapez rule: $n = 1$

$$I[f] \approx I_1[f] = (b-a)\frac{f(a)-f(b)}{2} \tag{46}$$

Simpson rule: $n = 2$

$$I[f] \approx I_2[f] = \frac{(b-a)}{6}\left(f(a) + 4f\left(\frac{b+a}{2}\right) + f(b)\right) \tag{47}$$

Newton-Cotes formulare

Satz

The Newton-Cotes formulare $I_n[f]$ integrates polynomials of grade $\leq n$ exactly.

Idea Gauß-Quadratur: Use different points $x_0, \ldots, x_n$ to be able to exactly integrate polynomials of higher order

Error of the Newton-Cotes formulare

$\epsilon_n[f] = I_n[f] - I[f]$ is called **Error** of the Quadratur formulare

Reminder: Representation of the Interpolation error

$$f(x) - p_n(x) = \frac{1}{n+1!} f^{(n+1)}(\xi) \cdot \prod_{i=1}^{n} (x - x_i) \tag{48}$$

Example: For the Quadratur error of the Trapez rule $(n = 1)$ the following holds

$$\epsilon_1[f] = |I_n[f] - I[f]| \leq \frac{1}{12} ||f^{(2)}||_\infty \cdot h^3 \tag{49}$$

Gauß-Quadratur

Ziel:

Approximate for a fixed positive weight function:

$$\mu : (a, b) \to (0, \infty) \tag{50}$$

Integrals of the form

$$I[f] = \int_a^b f(x)\mu(x) \, \mathrm{dx} \tag{51}$$

via a Quadratur rule of the form:

$$I[f] \approx \sum_{i=0}^{n} f(x_i)\mu_i \tag{52}$$

with a special choice of the supporting pointsx_i and positive weights μ_i

Construction of Gauß-Quadratur formular

- Find orthogonal Polynomials $\{p_0, p_1, \dots, p_{n+1}\}$ with respect to
$$\langle p_k, p_j \rangle_\mu = \int_a^b p_k(x) p_j(x) \mu(x) \, \mathrm{d}x \tag{53}$$
mit $p_k \in \mathcal{P}_k$ und $\langle p_k, p_j \rangle = \delta_{kj}$
- use roots of p_{n+1} as knots
- determine weights
$$\mu_i = \int_a^b \mu(x) \prod_{\substack{k=0,\\ i\neq k}}^{n} \frac{x - x_k}{x_i - x_k} \, \mathrm{d}x \text{ für } 0 \leq i \leq n \tag{54}$$

Gauß-Quadraturformeln

Solution: Gauß-Quadratur Formulare

$$I_n[f] = \sum_{i=0}^{n} \mu_i f(x_i) \approx I[f] = \int_a^b f(x)\mu(x)\ \mathrm{dx} \tag{55}$$

with

$$I_n[p] = I[p] \quad \forall\ p \in \mathcal{P}_{2n+1} \tag{56}$$