Computational Mathematics 1

Lecture notes, University of Graz
based on the lecture by Olaf Steinbach

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Contents

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Introduction

Modelling of processes in nature and technology leads to systems of differential equations (usually partial differential equations), which in a minority of cases have an analytical solution. Computational mathematics considers the approximative solutions of these differential equations.

The university offers three courses:

1. Fundamentals
2. Numerics of Ordinary Differential Equations
3. Numerics of Partial Differential Equations

This course is the first. We will cover the following topics:

1. Numeric Integration
2. Linear Equation Systems (numeric linear algebra, GMRES, CG)
3. Non-linear Equation Systems
4. Eigenvalues

Approximation of functions

- as functional representation of measured data
- as solution of (e.g.) differential equations
- for numerical integration
- ...

Interpolation

Let $n+1$ supporting points be given. Let $x_i \in [0,1]$ be pairwise distinct, i.e. $x_i = x_j \implies i = j$. The associated measured data are the function values $f_i := f(x_i)$.

Find the global interpolation of n-th degree $f_n(x) = \sum_{k=0}^{n} a_k x^k$. Determine its coefficients a_k and the basis $\left\{x^k | k = 0, \dots, n\right\}$ of monoms.

Interpolation equations:

$$f_i = f_n(x_i) = \sum_{k=0}^{n} a_k x_i^k \qquad i = 0, \dots, n$$

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ \vdots & & & & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^n \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}$$

This gives a linear equation system of dimension $n+1$.

- Is it solvable? Is the solution unique?

$$A_n \in \mathbb{R}^{(n+1)\times(n+1)} \neq 0$$

- *How* can we compute the solutions?
- The error is given by $f(x) - f_n(x)$

Remark. *$A_n \in \mathbb{R}^{(n+1)\times(n+1)}$ has $(n+1)^2$ has non-zero elements.*

Supporting points $x_0, \ldots, x_n$, $n+1$ non-zero elements and information x_i^k data sparse matrix.

Example 1. *Let $n = 1$.*

$$A_1 = \begin{pmatrix} 1 & x_0 \\ 1 & x_0 \end{pmatrix}$$

$$\det(A_1) = x_1 - x_0 \neq 0$$

Lemma.

$$\det(A_n) = \prod_{j<i} (x_i - x_j)$$

Proof. Will be done in the practicals. □

Example 2 (Runge's phenomenon)**.** *Let $x \in [-5, 5]$, $f(x) = \frac{1}{1+x^2}$, $n = 2$.*

$$x_0 = -5 \qquad x_1 = 0 \qquad x_2 = 5$$

$$\begin{pmatrix} 1 & -5 & 25 \\ 1 & 0 & 0 \\ 1 & 5 & 25 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{26} \\ 1 \\ \frac{1}{26} \end{pmatrix}$$

$$a_0 = 1$$

$$\begin{aligned} -5a_1 + 25a_2 &= \frac{1}{26} - 1 \\ 5a_1 + 25a_2 &= \frac{1}{26} - 1 \\ \hline 10a_1 = 0 &\implies a_1 = 0 \\ 50a_2 &= -2 \cdot \frac{25}{26} \\ a_2 &= -\frac{1}{26} \\ f_2(x) &= 1 - \frac{1}{26}x^2 \end{aligned}$$

Compare with Figure 1.

Matrix A_n is badly conditioned. Hence, small changes on the right side trigger a huge change in the solution.

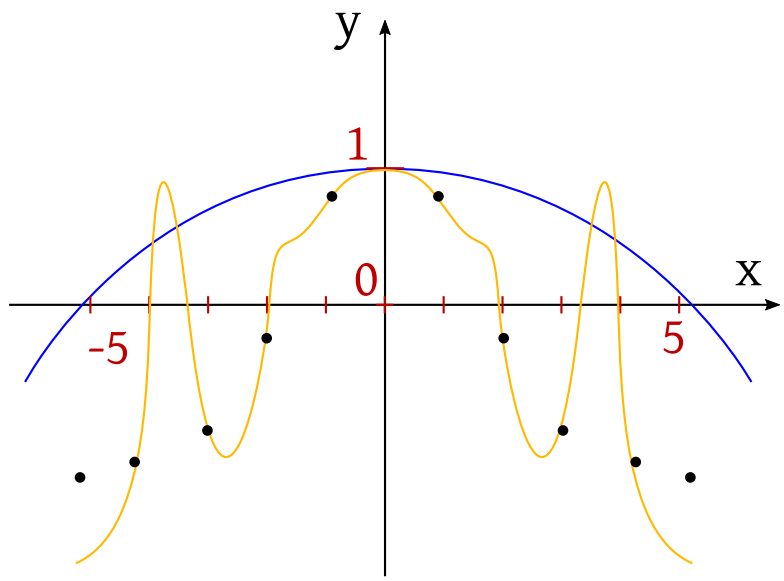


Figure 1: Runge's function (1901) illustrates the problem of oscillation at the edges of an interval that occurs when using polynomial interpolation with polynomials of high degree over a set of equispaced interpolation points

Question: Is interpolation *without* linear equation systems?

Approach:

$$f_n(x) = \sum_{k=0}^{n} a_k x^k = \sum_{k=0}^{n} d_k \varphi_k(x)$$

with $\varphi_k(x) = x^k$.

$$f_i = f_n(x_i) = \sum_{k=0}^{k} a_k \varphi_k(x_i)$$

$$\begin{pmatrix} \varphi_0(x_0) & \varphi_1(x_0) & \dots & \varphi_n(x_0) \\ \varphi_0(x_1) & \varphi_1(x_1) & \dots & \varphi_n(x_1) \\ \vdots & & & \vdots \\ \varphi_0(x_n) & \varphi_1(x_n) & \dots & \varphi_n(x_n) \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}$$

$$\varphi_k(x)\varphi_k(x_l) = \delta_{k,l} = \begin{cases} 1 & k = l \\ 0 & \text{else} \end{cases}$$

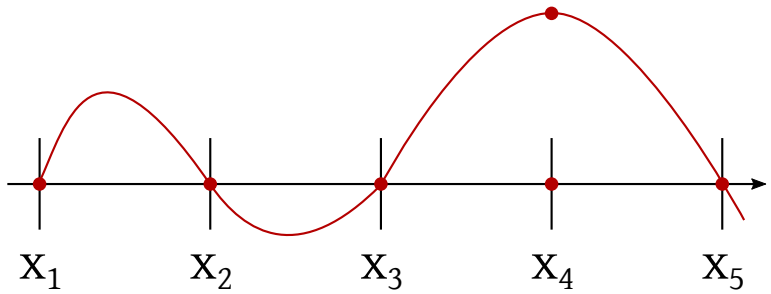


Figure 2: Lagrange polynomials $L_3^4(x)$

φ_k polynomial of degree n

$$\varphi_k(x) = \frac{(x-x_0)(x-x_1)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)(x_k-x_1)\dots(x_k-x_{k-1})(x-x_{k+1})\dots(x_k-x_n)}$$

$$L_k^n(x) = \prod_{\substack{l=0\\ l\neq k}}^{n} \frac{x-x_l}{x_k-x_l} \qquad \text{“Lagrange polynomials”}$$

Compare with Figure 2

Therefore, we get the interpolation polynomials

$$f_n(x) = \sum_{k=0}^{n} f(x_k)\cdot L_k^n(x)$$

Example 3.

$$
\begin{aligned}
f(x) &= \frac{1}{1+x^2} \qquad x_0 = -5, x_1 = 0, x_2 = 5, n = 3 \\
L_0^2(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{x(x-5)}{-5\cdot(-10)} = \frac{1}{50}x(x-5) \\
L_2^2(x) &= \frac{1}{50}x(x+5) \\
L_1^2(x) &= \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = -\frac{1}{25}(x^2-25) = \frac{1}{25}(25-x^2) \\
f_2(x) &= \frac{1}{26}\cdot\frac{1}{50}\cdot x\cdot(x-5) + \frac{1}{25}(25-x^2) + \frac{1}{26}\cdot\frac{1}{50}\cdot x\cdot(x+5) \\
&= 1 + x\cdot\left(-\frac{5}{26\cdot 50} + \frac{5}{26\cdot 50}\right) + x^2\cdot\left(\frac{1}{26}\cdot\frac{1}{25} - \frac{1}{25}\right) \\
&= 1 - \frac{1}{26}x^2
\end{aligned}
$$

Theorem 1. *For $n \in \mathbb{N}$ let $(x_i)_0^n \in [a,b]$ be pairwise distinct supporting points. Let $f(x)$ be $n+1$ times differentiable. Then it holds that,*

$$
f(x) - f_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi(x)) \prod_{i=0}^{n}(x-x_i)
$$

with some proper intermediate value $\xi(x)$.

Proof. Let $x = x_i$, the theorem is satisfied trivially.

Let $\bar{x} \in [a,b], \bar{x} \neq x_i$ and $i = 0, \ldots, n$ be arbitrary, but fixed.

Definition.

$$
g_\alpha(x) = f(x) - f_n(x) - \alpha \prod_{i=0}^{n}(x-x_i), \alpha \in \mathbb{R}
$$

$$
g_\alpha(x_j) = 0
$$

Choose $\alpha = \bar{\alpha}$: $g_{\bar{\alpha}}(\bar{x}) = 0$.

$$
\bar{a} = \frac{f(\bar{x}) - f_n(\bar{x})}{\prod_{i=0}^{n}(\bar{x}-x_i)}
$$

$g_{\bar{\alpha}}$ has roots $x_0, \ldots, \bar{x}_n, \bar{x}$ (which are $n+2$ values).

$f(x)$ is continuously differentiable, $f(a) = f(b) = 0$.

$$
\implies \exists \eta \in (a,b) : f'(\eta) = 0
$$

by Rolle's Theorem. Hence, $g'_{\bar{\alpha}}(x)$ has $n+1$ pairwise distinct zeros. $g''_{\bar{\alpha}}(x)$ has n pairwise different zeros. $g^{(n+2)}_{\bar{\alpha}}(x)$ has one zero $\xi = \xi(x_0, \ldots, x_n, \bar{x})$.

$$0 = g^{(n+1)}_{\bar{\alpha}}(\xi) = f^{(n+1)}(\xi) - \underbrace{f_n^{(n+1)}(\xi)}_{=0} - \alpha \left(\underbrace{\prod_{i=0}^{n} (x - x_i)}_{=(n+1)!} \right)^{(n+1)}_{x=\xi}$$

$$\implies \bar{\alpha} = \frac{1}{(n+1)!} f^{n+1}(\xi)$$

$$\implies f(\bar{x}) - f_n(\bar{x}) = \bar{\alpha} \prod_{i=0}^{n} (x - x_i) \forall \bar{x}$$

□

Interpolation:

$$f(x), f_n(x), f_n(x_i) = f_i, x_i \in [a, b] = [0, 1] \qquad i = 0, \ldots, n \quad i \neq j \implies x_i \neq x_j$$

$$f(x) - f_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi(x)) \prod_{i=0}^{n} (x - x_i)$$

Corollary.

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

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

$\max_{x \in [a,b]} \left| f^{(n+1)}(x) \right| < \infty$ regularity *or* differentiability *of the function to interpolate (given by the task assignment).*

$\max_{x \in [a,b]} \left| \prod_{i=0}^{n} (x - x_i) \right|$ *is the property resulting from choice of supporting points.*

Hence, the polynomial degree n and the choice of supporting points is influenceable.

Example 4.

$$[a, b] = [0, \frac{\pi}{2}] \qquad f(x) = \sin(x) \qquad \left| f^n(x) \right| \leq 1$$

$$\implies \max_{x \in [a,b]} \left| f(x) - f_n(x) \right| \leq \frac{1}{(n+1)!} \underbrace{\max_{x \in [0, \frac{\pi}{2}]} \left| f^{(n+1)}(x) \right|}_{\leq 1} = \left| \prod_{i=0}^{n} (x - x_i) \right| \leq \ldots$$

Let $n = 1, x_0 = 0, x_1 = \frac{\pi}{2}$.

$$f_n(x) = \frac{2}{\pi}x$$

$$\max_{x\in[0,\frac{\pi}{2}]} \left|f(x) - f_1(x)\right| \leq \frac{1}{2} \max_{x\in[0,\frac{\pi}{2}]} x \cdot (\frac{\pi}{2} - x) = \left(\frac{\pi}{4}\right)^2 \approx 0.3084$$

$$\max_{x\in[0,\frac{\pi}{2}]} \frac{\sin(x) - \frac{2}{\pi}x}{=} 0.2105$$

Example 5.

$$f(x) = \sqrt{x}, x \in [0,1]$$

Let $n = 1, x_0 = 0, x_1 = 1, f_1(x) = x$.

$$\max_{x\in[0,1]} \left|f(x) - f_1(x)\right| \leq \max_{x\in[0,1]} \underbrace{\left|f''(x)\right|}_{<\infty} \cdot \underbrace{\max_{x\in[0,1]} x(1-x)}_{=\frac{1}{2}}$$

$$f(x) = x^{\frac{1}{2}} \qquad f'(x) = \frac{1}{2}x^{-\frac{1}{2}} \qquad f''(x) = -\frac{1}{4}\frac{1}{x^{\frac{3}{2}}}$$

For $x \in [a,b], 0 < a < b$, we want to answer the question for choice of supporting points. In the error estimate, the following term occurs:

$$\max_{x\in[a,b]} \underbrace{\left|\prod_{i=0}^{n}(x - x_i)\right|}_{x^{n+1}+a_a x^n+\cdots+a_0 = a_0(\frac{1}{a_0}x^{n+1}+\cdots+1)} \rightarrow \min_{x_0,\ldots,x_n}$$

$$\max_{[a,b]} \left|p_{n+1}(x)\right| \rightarrow \min_{p_{n+1}, a_{n+1}=1}$$

This motivates the following exercise:

$$\min_{p_{n+1}\in\pi_1^{n+1}} \max_{x\in[a,b]} \left|p_{n+1}(x)\right| \text{ with } \prod_{1}^{n+1} = \left\{q_{n+1} \in \pi^{n+1} | q_{n+1}(0) = 1\right\}$$

This is a min-max problem. This gives the Chebyshev polynomials:

- solution of a differential equation
- orthogonal polynomials
- recursive definition

The Chebyshev polynomials

Recursive definition:

$$T_0(x) = 1, T_1(x) = x, T_{k+1}(x) = 2x \cdot T_k(x) - T_{k-1}(x) \qquad x \in \mathbb{R}$$

$$T_2(x) = 2x \cdot x - 1 = 2x^2 - 1, T_3(x) = 2x(2x^2 - 1) - x = 4x^3 - 3x$$

Lemma. *Let* $x \in [-1, +1], k \in \mathbb{N}$.

Then it holds that $T_k(x) = \cos(k \cdot \arccos(x))$

Proof. For $k = 0$ and $k = 1$, it is immediate. For $k \geq 2$, this will be part of the practicals. □

Properties

- $|T_k(x)| \leq 1$ if $x \in [-1, 1]$
- $T_k(1) = 1, T_k(-1) = (-1)^k$
- Zeros: $T_k(x) = \cos(k \cdot \arccos(x)) = 0$.

$$k \cdot \arccos(x) = \frac{\pi}{2} + l\pi$$

$$\implies x_l^k = \cos \frac{(1 + 2l)\pi}{2k} \qquad l = 0, \ldots, k - 1$$

Compare with Figure 3.

$$T_k(x) = +1 = k \cdot \arccos(x) = 2l\pi$$

$$\implies \hat{x}_{2l}^k = \cos\left(\frac{2l\pi}{k}\right)$$

$$T_k(x) = -1 \implies k \cdot \arccos(x) = (2l + 1)\pi$$

$$\implies \hat{x}_{2l+1} = \cos\left(\frac{(2l + 1)\pi}{k}\right)$$

Remark (An exercise for the practicals)**.** *Orthogonality of Chebyshev polynomials:*

$$\int_{-1}^{1} \frac{T_l(x)T_k(x)}{\sqrt{1 - x^2}} = \begin{cases} 0 & \text{if } k \neq l \\ \frac{\pi}{2} & \text{if } k = l \neq 0 \\ \pi & \text{if } k = l = 0 \end{cases}$$

Lemma.

$$T_k(x) = \frac{1}{2}\left[\left(x + \sqrt{x^2 - 1}\right)^k + \left(x - \sqrt{x^2 - 1}\right)^k\right] = \frac{1}{2}\left[(x + \sqrt{x^2 - 1})^k + (x + \sqrt{x^2 - 1})^{-k}\right]$$

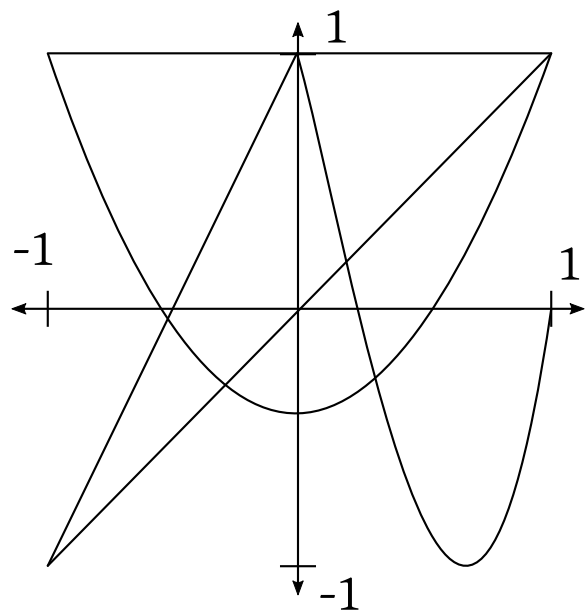


Figure 3: Chebyshev polynomials properties

Proof. Let $k = 0$. $T_0(x) = 1$. QED.
Let $k = 1$. $T_1(x) = x$.

$$
\begin{aligned}
T_{k+1}(x) &= 2xT_k(x) - T_{k-1}(x) \\
&= 2x\frac{1}{2}\left[\left(x + \sqrt{x^2-1}\right)^k + \left(x - \sqrt{x^2-1}\right)^k\right] - \left[(x + \sqrt{x^2-1})^{k-1} + (x - \sqrt{x^2-1})^{k-1}\right] \\
&= \frac{1}{2}\left(x + \sqrt{x^2-1}\right)^{k-1}\left[2x(x + \sqrt{x^2-1}) - 1\right] + \frac{1}{2}\left(x - \sqrt{x^2-1}\right)^{k-1}\left[2x(x - \sqrt{x^2-1} - 1\right] \\
&= \frac{1}{2}\left(x + \sqrt{x^2-1}\right)^{k+1} + \frac{1}{2}\left(x - \sqrt{x^2-1}\right)^{k+1}
\end{aligned}
$$

□

$$
\frac{(x - \sqrt{x^2-1})}{x + \sqrt{x^2-1}}\left(x + \sqrt{x^2-1}\right) = \frac{x^2 - (x^2-1)}{x + \sqrt{x^2-1}} = -\frac{1}{x + \sqrt{x^2-1}}
$$

Definition of Chebyshev polynomials: $x \in [-1, 1]$. Interpolation task: $[a, b], 0 < a < b$. This gives a min-max task for $p_n(x)$ with $p_n(0) = 1$.

$$
t \in [a, b] : x = \frac{b + a - 2t}{b - a} \qquad t = a : \quad x = 1 \qquad t = b : \quad x = -1
$$

Scaled Chebyshev polynomials:

$$\tilde{T}_k(t) = \frac{T_k\left(\frac{b+a-2t}{b-a}\right)}{T_k\left(\frac{b+a}{b-a}\right)}$$

Theorem 2. *Let* $0 < a < b$.

$$\min_{\substack{p_n(t) \\ p_n(0)=1}} \max_{t\in[a,b]} \left|p_n(t)\right|$$

$$= \max_{t\in[a,b]} \left|\tilde{T}_n(t)\right| = \frac{1}{T_n\left(\frac{b+a}{b-a}\right)}$$

$$= \frac{2q^n}{1+q^{2n}} \text{ with } q = \frac{\sqrt{b}+\sqrt{a}}{\sqrt{b}-\sqrt{a}} > 1$$

Indirect proof. Assume there exists $q_n(t), q_n(0) = 1$ and

$$\max_{t\in[a,b]} \left|q_n(t)\right| < \max_{t\in[a,b]} \left|\tilde{T}_n(t)\right|$$

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

$$x = \cos\frac{2l\pi}{n} = \hat{x}^n_{2l} \implies T_n(x) = 1$$

$$\tilde{T}_n(t^n_{2l}) = \frac{1}{T_n\left(\frac{b+a}{b-a}\right)}$$

$$x = \cos\frac{(2l+1)\pi}{n} = \hat{x}^n_{2l+1} \implies T_n(\hat{x}^n_{2l+1}) = -1$$

$$\tilde{T}_n(\hat{t}^n_{2l+1}) = -\frac{1}{T_n\left(\frac{b+a}{b-a}\right)}$$

$$q_n\left(\hat{t}^n_{2l}\right) < \frac{1}{T_n\left(\frac{b+a}{b-a}\right)}$$

$$q_n(\tilde{t}^n_{2l}) > -\frac{1}{T_n\left(\frac{b+a}{b-a}\right)}$$

Compare with Figure 4.

$$r_n(t) = \tilde{T}_n(t) - q_n(t)$$

$$\implies r(\hat{t}^n_{2l}) > 0$$

$$t(\hat{t}^n_{2l+1}) < 0$$

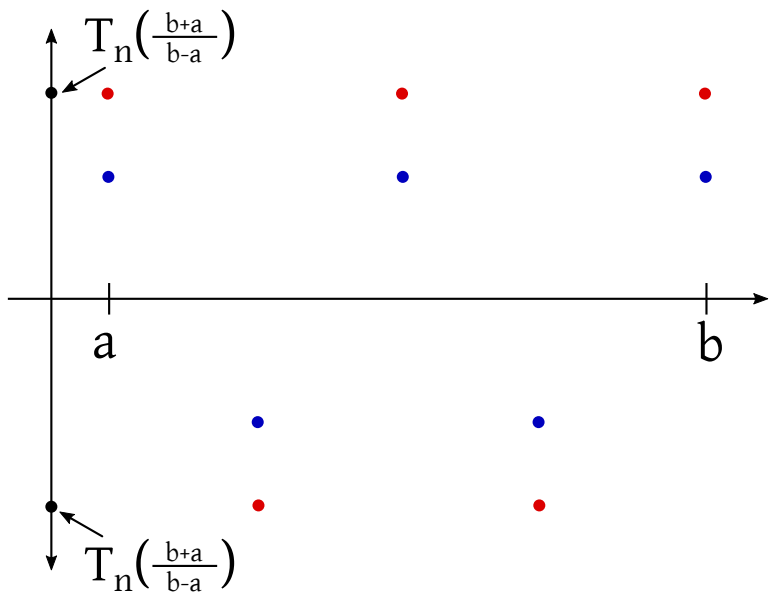


Figure 4: Construction for proving the scaled Chebyshev polynomial theorem

$r_n(t)$ has n zeros in $[a, b]$.

$$\begin{aligned} r_n(0) &= \tilde{T_n}(0) - q_n(0) = 0 \\ &\implies n+1 \text{ zeros} \implies r_n(t) = 0 \forall t \\ &\implies \tilde{T_n}(t) = q_n(t) \end{aligned}$$

This gives a contradiction.

It remains to determine $T_n\left(\frac{b+a}{b-a}\right)$.

$$\begin{aligned} T_n\left(\frac{b+a}{b-a}\right) &= \frac{1}{2}\left[q^n + q^{-n}\right] = \frac{q^{2n}+1}{2q^n} \text{ with } q = \frac{b+a}{b-a} + \sqrt{\frac{(b+a)^2}{(b-a)^2} - 1} \\ &= \frac{1}{b-a}\left[b + a + \sqrt{(b+a)^2 - (b-a)^2}\right] \\ &= \frac{1}{b-a}\left[b + a + 2\sqrt{a}\sqrt{b}\right] \\ &= \frac{(\sqrt{a} + \sqrt{b})^2}{(\sqrt{b} + \sqrt{a})(\sqrt{b} - \sqrt{a})} = \frac{\sqrt{a} + \sqrt{b}}{\sqrt{b} - \sqrt{a}} \end{aligned}$$

□

Remark. *This result also applies to the analysis of the so-called CG method (used to solve linear equation systems)*

Now consider the interpolation task in interval $[-1, 1]$.

$$f(x), f_n(x), f_n(x_i) = f(x_i) \qquad i = 0, \dots, n$$

Error estimate:

$$\max_{x\in[-1,1]} \left|f(x) - f_n(x)\right| \leq \frac{1}{(n+1)!} \max_{x\in[-1,1]} \left|f^{(n+1)}(x)\right| \qquad \max_{x\in[-2,1]} \left|\underbrace{\prod_{j=0}^{n}(x - x_j)}_{p_{n+1}(x)}\right|$$

As supporting points, we choose the zeros x_i of the $(n+1)$-th Chebyshev polynmial,

$$T_{n+1}(x_i^{n+1}) = 0 \qquad T_{n+1}(x_i^{n+1}) = 0$$

$$T_{n+1}(x) = \prod_{j=0}^{n}(x - x_j^{(n+1)}) \cdot a_{n+1} = a_{n+1}x^{n+1} + \dots$$

We compute the first intermediate values:

$$\begin{aligned}
T_0(x) &= 1 \\
T_1(x) &= x \\
T_{k+1}(x) &= 2xT_k(x) - T_{k-1}(x) \\
T_2(x) &= 2x^2 + \dots \\
T_3(x) &= 4x^3 + \dots \\
T_{k+1}(x) &= 2^k x^{k+1} + \dots
\end{aligned}$$

We continue to consider $T_{n+1}(x)$:

$$T_{n+1}(x) = 2^n x^{n+1} + \dots = \prod_{j=0}^{n}(x - x_j^{(n+1)}) = 2^{-n}T_{n+1}(x)$$

$$\max_{x\in[-1,1]} \left|\prod_{j=0}^{n}(x - x_j^{(n+1)})\right| \leq 2^{-n}$$

By interpolation in the zeros of the Chebyshev polynomial, we get,

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

Extension to a general interval $[a, b]$ by transformation.

Remark. *This holds independent of the representation of the interpolation polynomial. For example with monom x^k. For example with Lagrange polynomials, but also with Chebyshev polynomials.*

$$f_n(x) = \sum_{k=0}^{n} a_k T_k(x)$$

$$f_n(x_i^{(n+1)}) = \sum_{k=0}^{n} a_k T_k(x_i^{(n+1)}) = f(x_i^{(n+1)})$$

- Fully occupied matrix (an exercise in the practicals):

$$\int_{-1}^{1} \frac{T_k(x)T_l(x)}{\sqrt{1-x^2}}\, dx = 0 \qquad k \neq l$$

- Discrete orthogonality
  - direct computation of a_k
  - Fast Fourier Transformation

In the interpolation exercise, we have considered $n+1$ interpolation equations in pairwise different supporting points for determination of $n+1$ coefficients a_k of f_n. We now have to determine an interpolation polynomial of degree $2n+1$ with $2(n+1)$ coefficients. This gives $2(n+1)$ supporting points.

Our goal is $n+1$ supporting points.

Hence, we have 2 conditions per supporting point.

$$f_{2n+1}(x_i) = f(x_i) \qquad f'_{2n+1}(x_i) = f'(x_i) \qquad i = 0, \dots, n$$

Hermit interpolation

Error estimation of a Hermit interpolation:

$$\max_{x\in[a,b]} \left| f(x) - f_{2n+1}(x) \right| \leq \frac{1}{(2n+2)!} \cdot \max_{x\in[a,b]} \left| f^{(2n+2)}(x) \right| \cdot \max_{x\in[a,b]} \left| \prod_{j=0}^{n} (x-x_j)^2 \right|$$

$$f(x) - f_{2n+1}(x) = \underbrace{\frac{1}{(2n+2)!} f^{2n+2}(\xi)}_{\alpha} \prod_{j=0}^{n} (x-x_j)$$

$$f(x) = f_{2n+1}(x) + \alpha \prod_{j=0}^{n} (x-x_j)^2$$

$2n+2$ zeros.

$$x_0, \dots, x_n, \bar{x}, q(\bar{x}) = 0$$

Global interpolation tasks:

$$f(x), x \in [a,b], f_n(x), n \sim \text{ polynomial degree}$$

$$f_n(x_i) = f(x_i) \qquad i = 1, \dots, n$$

$$\max_{x\in[a,b]} \left| f_n(x) - f(x) \right| \leq \frac{1}{(n+1)!} \underbrace{\max_{x\in[a,b]} \left| f^{(n+1)}(x) \right|}_{\substack{\text{regularity of } f(x)=\sqrt{x} \\ x\in[0,1]}}$$

$$\max_{x\in[a,b]} \left| \prod_{i=1}^{n} (x - x_i) \right|$$

Question: Local interpretation with polynomials of low degree.

Piecewise linear interpolation

$$[a,b], n \in \mathbb{N}, h = \frac{b-a}{n} \text{ step size}$$

Uniform supporting points $x_k = a + kh$. Compare with Figure 5.

For *every* interval $[x_{k-1}, x_k]$, $k = 1, \dots, n$ we consider a local interpolation task. In the easiest case, this is a linear interpolation with

$$f_n(x_{k-1}) = f(x_{k-1}) \qquad f_n(x_k) = f(x_k)$$

This implies global continuity, but globally there is no continuous differentiability.

What is the error estimation?

$$\max_{x\in[x_{k-1},x_k]} \left| f(x) - f_n(x) \right| \leq \frac{1}{2} \max_{x\in[x_{k-1},x_k]} \max \left| f''(x) \right| \cdot \underbrace{\max_{x\in[x_{k-1},x_k]} \left| \underbrace{(x - x_{k-1})}_{\frac{h}{2}} \cdot \underbrace{(x - x_k)}_{\frac{h}{2}} \right|}_{\text{is given at } \frac{1}{2}(x_{k-1}+x_k)} = \frac{1}{8} h^2 \max_{x\in[x_k,x_{k-1}]} \left| f''(x) \right|$$

$$\Longrightarrow \max_{x\in[a,b]} \left| f(x) - f_n(x) \right| \leq \frac{1}{8} h^2 \max_{x\in[a,b]} \left| f''(x) \right|$$

if $\left| f''(x) \right|$ is bounded, $f(x) = \sqrt{x}$.

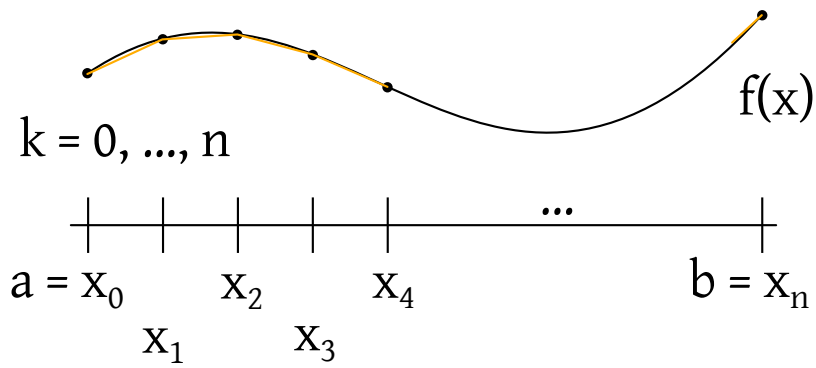


Figure 5: Piecewise linear interpolation

How about the error estimation in other norms? E.g.

$$\int_a^b [f(x) - f_n(x)]^2 \, dx = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} [f(x) - f_n(x)]^2 \, dx$$

$$x \in [x_{k-1}, x_k] \qquad f_n(x) : f(x_{k-1}) = f_n(x_{k-1}) \qquad f(x_k) = f_n(x_k)$$

$$f_n(x) = f(x_{k-1}) + \frac{f(x_k) - f(x_{k-1})}{h}(x - x_{k-1})$$

$x \in [x_{k-1}, x_k], x \in [x_{k-1}, \frac{x_{k-1}+x_k}{2}$

$$f(x) - f_n(x) = f(x) - f_n(x) - \underbrace{[f(x_{k-1}) - f_n(x_{k-1})]}_{=0} = \int_{x_{k-1}}^{x} [f'(s) - f_n'(s)] \, ds$$

$$
\begin{aligned}
[f(x) - f_n(x)]^2 &= \left[\int_{x_{k-1}}^{x} \mathbf{1} \cdot [f'(s) - f_n'(s)]\, ds\right]^2 \\
&\underbrace{\leq}_{\text{Cauchy-Schwarz}} \int_{x_{k-1}}^{x} 1^2\, ds \cdot \int_{x_{k-1}}^{x} [f'(s) - f_n'(s)]^2\, ds \\
&\leq (x - x_{k-1}) \cdot \int_{x_{k-1}}^{\frac{(x_{k-1}+x_k)}{2}} [f'(s) - f_n'(s)]^2\, ds
\end{aligned}
$$

$$
\implies \int_{x_{k-1}}^{\frac{x_{k-1}+x_k}{2}} [f(x) - f_n(x)]^2\, dx \leq \underbrace{\int_{x_{k-1}}^{\frac{x_{k-1}+x_k}{2}} (x - x_{k-1})\, dx}_{\frac{1}{2}(x-x_{k-1})^2\Big|_{x_{k-1}}^{\frac{x_k-x_{k-1}}{2}} = \frac{h^2}{8}} \cdot \frac{x_{k-1} + x_k}{2} [f'(x) - f_n'(x)]^2\, dx
$$

Analogously, it follows that

$$
\int_{\frac{x_k+x_{k-1}}{2}}^{x_k} [f(x) - f_n(x)]^2\, dx \leq \frac{h^2}{8} \int_{\frac{x_{k-1}+x_k}{2}}^{x_k} [f'(x) - f_n'(x)]^2\, dx
$$

$$
\implies \int_{x_{k-1}}^{x_k} [f(x) - f_n(x)]^2 \leq \frac{h^2}{8} \int_{x_{k-1}}^{x_k} [f'(s) - f_n'(s)]\, ds \leq \frac{h^4}{24} \int_{x_{k-1}}^{x_k} [f''(s)]^2\, ds
$$

We will see later, that this inequality holds.

$$
f_n'(s) = \frac{1}{h} [f(x_k) - f(x_{k-1})]
$$

Piecewise linear interpolation:

$$
[a, b], n \in \mathbb{N}, h = \frac{b-a}{n}, x_k = a + k \cdot h
$$

$x \in [x_{k-1}, x_k]$

$$
f_n(x) = f(x_{k-1}) + \frac{x - x_{k-1}}{h} \cdot [f(x_k) - f(x_{k-1})]
$$

$$
\int_{x_{k-1}}^{x_k} [f(x) - f_n(x)]^2\, dx \leq \frac{1}{8} h^2 \int_{x_{k-1}}^{x_k} [f'(x) - f_n'(x)]^2\, dx
$$

Sidenote:

$$
\frac{1}{h} \int_{x_{k-1}}^{x_k} [f'(s) - f_n'(s)]\, ds = \frac{1}{h} \underbrace{[f(s) - f_n(s)]}_{=0}\Bigg|_{x_{k-1}}^{x_k} = 0
$$

$$
\begin{aligned}
[f'(x) - f_n'(x)] &= \int_{x_{k-1}}^{x_k} \left[f'(x) - f_n'(x) - \frac{1}{h} \int_{x_{k-1}}^{x_k} f'(s) - f_n'(s)\, ds \right]^2 dx \\
&= \frac{1}{h} \int_{x_{k-1}}^{x_k} [f'(x) - f_n'(x)]\, ds \\
&= \frac{1}{h^2} \int_{x_{k-1}}^{x_k} \left[\int_{x_{k-1}}^{x_k} [[f'(x) - f_n'(x)] - [f'(s) - f_n'(s)]]\, ds \right]
\end{aligned}
$$

$$
\int_a^b g'(s)\, ds = g(b) - g(a)
$$

$$
\begin{aligned}
[f'(x) - f_n'(x)] &= \frac{1}{h^2} \int_{x_{k-1}}^{x_k} \left[\int_{x_{k-1}}^{x_k} \int_s^x f''(\eta) - \underbrace{f_n''(\eta)}_{=0 \text{ because } f_n \text{ is linear}} d\eta\, ds \right]^2 dx \\
&= \frac{1}{h^2} \cdot \int_{x_{k-1}}^{x_k} \left[\int_{x_{k-1}}^{x_k} \mathbf{1} \cdot \int_s^x f''(\eta)\, d\eta\, ds \right]^2 dx
\end{aligned}
$$

$$
\int_a^b f \cdot g\, dx \leq \left(\int_a^b f^2 \right)^{\frac{1}{2}} \cdot \left(\int_a^b g^2 \right)^{\frac{1}{2}}
$$

$$
\begin{aligned}
\left[\int_{x_{k-1}}^{x_k} 1 \int_s^x f''(\eta)\, d\eta\, ds \right]^2 &\leq \int_{x_{k-1}}^{x_k} 1^2\, ds \int_{x_{k-1}}^{x_k} [f''(\eta)\, d\eta]^2\, ds \\
&\leq \frac{1}{h} \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} \underbrace{\left[\int_0^x \mathbf{1} \cdot f''(\eta)\, d\eta \right]^2}_{\leq \left| \underbrace{\int_s^x 1^2\, d\eta}_{=(x-s)} \right| \cdot \left| \int_s^x f''(\eta)^2\, d\eta \right|} ds\, dx \\
&\leq (x - s) \underbrace{\int_{x_{k-1}}^{x_k} [f(\eta)]^2\, d\eta}_{\text{independent of } x,s} \\
&\leq \frac{1}{h} \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} |x - s|\, ds\, dx \cdot \int_{x_{k-1}}^{x_k} [f''(\eta)]^2\, d\eta
\end{aligned}
$$

$\hat{x} = x - x_{k-1}, \hat{s} = s - x_k - 1$

$$\begin{aligned}
\int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} |x - s| \; ds \, dx &= 2 \cdot \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x} (x - s) \, ds \, dx \\
&= 2 \cdot \int_0^h \underbrace{\int_0^x (x - s) \, ds}_{= -\frac{1}{2}(x-s)^2 \big|_0^x = \frac{1}{2}x^2} \; dx \\
&= \int_0^h x^2 \, dx = \frac{1}{3} h^3
\end{aligned}$$

Result:

$$\int_{x_{k-1}}^{x_k} \left[f'(x) - f_n'(x) \right]^2 \; dx \leq \frac{1}{3} h^2 \cdot \int_{x_{k-1}}^{x_k} \left[f''(x) \right]^2 \; dx$$

By insertion, we get

$$\int_{x_{k-1}}^{x_k} \left[f(x) - f_n(x) \right]^2 \; dx \leq \frac{1}{24} h^4 \cdot \int_{x_{k-1}}^{x_k} \left[f''(x) \right]^2 \; dx$$

Local for all k

$$\int_a^b \left[f(x) - f_n(x) \right]^2 \; dx \leq \frac{1}{24} h^4 \int_a^b \left[f''(x) \right]^2 \; dx$$

Norm for square-integrable functions:

$$\left\| f \right\|_{L^2([a,b])} := \left(\int_a^b \left[f(x) \right]^2 dx \right)^{\frac{1}{2}} < \infty$$

$$\left\| f - f_n \right\|_{L^2([a,b])} \leq \frac{1}{\sqrt{24}} h^2 \cdot \left\| f'' \right\|_{L^2([a,b])}$$

$\to 0$ for $k \to 0 \iff n \to \infty$.

Requirement: $\left\| f'' \right\|_{L^2([a,b])} < \infty$

Is not applicable for $f(x) = \sqrt{x}, x \in [0, 1]$.

$$\left\| f' - f_n' \right\| \leq \frac{1}{\sqrt{3}} h \left\| f'' \right\|_{L^2 \in ([a,b])}$$

$$x \in [x_{k-1}, x_k] : f_n(x) = f(x_{k-1}) + \frac{x - x_{k-1}}{h} \left[f(x_k) - f(x_{k+1}) \right]$$

$$f_n'(x) = \frac{1}{h}\left[f(x_k) - f(x_{k-1})\right] = \frac{1}{h}\int_{x_{k-1}}^{x_k} f'(s)\,ds$$

Recognize that $(a-b)^2 \leq 2(a^2+b^2)$, then

$$\int_{x_{k-1}}^{x_k}\left[\underbrace{f'(x)}_{a} - \underbrace{f_n'(x)}_{b}\right]^2 \leq 2\cdot\int_{x_{k-1}}^{x_k} f'(x)^2\,dx + 2\cdot\int_{x_{k-1}}^{x_k} \underbrace{f_n'(x)^3}_{\left[\frac{1}{h}\int_{x_{k-1}}^{x_k} f'(s)\,ds\right]^2}\,dx$$

with

$$\left[\frac{1}{h}\int_{x_{k-1}}^{x_k} f'(s)\,ds\right]^2 \leq \frac{1}{h}2\underbrace{\int_{x_{k-1}}^{x_k} 1^2\,ds}_{h}\int_{x_{k-1}}^{x_k}\left[f'(s)\right]^2\,ds$$

Hence,

$$\int_{x_{k-1}}^{x_k}\left[\underbrace{f'(x)}_{a} - \underbrace{f_n'(x)}_{b}\right]^2 \leq 4\cdot\int_{x_{k-1}}^{x_k}\left[f'(x)\right]^2\,dx$$

$$\left\|f' - f_n'\right\|_{L^2([a,b])} \leq 2\cdot\left\|f'\right\|_{L^2([a,b])}$$
$$\left\|f - f_n\right\|_{L^2([a,b])} \leq \frac{1}{\sqrt{2}}\cdot h\left\|f'\right\|_{L^2([a,b])}$$

In general, it holds that

$$\tau = 0,1 \qquad s = 1,2 \qquad s = p+1 \qquad p = \mathrm{grad}(f_n)$$
$$\left\|f^{(\tau)} - f_n^{(\tau)}\right\|_{L^2([a,b])} \leq c(s,\tau)h^{s-\tau}\left\|f^{(s)}\right\|_{L^2([a,b])}$$

$$
\begin{aligned}
\int_{x_{k-1}}^{x_k} [f'(x) - f_n'(x)]^2 \, dx &= \int_{x_{k-1}}^{x_k} \left[f'(x) - \frac{1}{h} \int_{x_{k-1}}^{x_k} f'(s) \, ds \right]^2 dx \\
&\leq h^{2\sigma} \cdot \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} \frac{f'(x) - f'(s)}{|x+s|^{1+2\sigma}} \, ds \, dx \\
&= \frac{1}{h^2} \int_{x_{k-1}}^{x_k} \left[\int_{x_{k-1}}^{x_k} [f'(x) - f'(s)] \, ds \right]^2 dx \\
&= \frac{1}{h^2} \left[\int_{x_{k-1}}^{x_k} \frac{f'(x) - f'(s)}{|x-s|^{\frac{1}{2}+\sigma}} |x-s|^{\frac{1}{2}+\sigma} \, ds \right]^2 \\
&\leq \int_{x_{k-1}}^{x_k} \frac{f'(x) - f'(s)^2}{|x-s|^{1+2\sigma}} \, ds \cdot \underbrace{\int_{x_{k-1}}^{x_k} |x-s|^{1+2\sigma} \, ds}_{\leq h \cdot h^{1+2\sigma}}
\end{aligned}
$$

$$
\begin{aligned}
\left\| f' - f_n' \right\|_{L^2([a,b])} &\leq h^{\sigma} \left\| f \right\|_S \\
\left\| f \right\|_s^2 &:= \int_a^b \int_a^h \frac{(f'(x) - f'(s))^2}{|x-s|^{1+2\sigma}} \, ds \, dx \qquad s \in (1,2), \sigma = s-1 \\
&= h^{s-1} \left\| f \right\|_s
\end{aligned}
$$

Theorem 3. *Let $f(x), x \in [a,b]$ be given with $\left| f \right|_s < \infty$, where,*

$$
\left| f \right|_1^2 = \int_a^b [f'(x)]^2 \, dx \qquad \left| f \right|_2^2 = \int_a^b [f''(x)]^2 \, dx \qquad 1 < s < 2
$$

$$
\left| f \right|_s = \int_a^b \int_a^b \frac{f'(x) - f'(s)}{|x-s|^{1+2\sigma}} \, ds \, dx
$$

Let $f_n(x)$ be the piecewise linear interpolation polynomial with

$$
f(x_k) = f_n(x_k) \qquad x_k = a + k \cdot h \qquad h = \frac{b-a}{n}
$$

Then it holds that

$$
\left\| f - f_n \right\|_\tau \leq c(s,\tau) \cdot h^{s-\tau} \cdot \left| f \right|_s
$$

with

$$
\left\| f \right\|_0^2 = \int_a^b [f(x)]^2 \, dx \qquad \left\| f \right\|_1^2 = \int_a^b [f'(x)]^2 \, dx
$$

Proof for $\tau \in \{0,1\}, s \in \{1,2\}$.

Remark.

- $\tau \in (0,1)$

$$
\left\| f \right\|_\tau^2 = \int_a^b \int_a^b \underbrace{[f(x) - f(s)]^2}_{|x-s|^{1+2\sigma}} \, ds \, dx
$$

- *The estimation stays correct for* $0 \leq \tau < \frac{3}{2}$.

$$\tau \leq s \leq \underbrace{p+1}_{\textit{polynomial degree}}$$

$$s > \frac{1}{2}$$

This assumes that $f(x)$ *is continuous.*

Error estimation:

$$\int_a^b [f(x) - f_n(x)]^2 \, dx \leq \frac{1}{24} \underbrace{\sum_{k=1}^{n} (x_k - x_{k-1})^4}_{[T_1]} \cdot \int_{x_{k-1}}^{x_k} \underbrace{[f''(x)]^2}_{[T_2]} \, dx$$

Here terms T_1 and T_2 balance out each other. If T_1 is large, T_2 will be "small". If T_1 is small, T_2 will be "large".

$$f(x) = \sqrt{x}, x \in [0,1], s < 1$$

This lecture took place on 18th of October 2017.

Piecewise linear interpolation

$$f(x), x \in [a,b], a = x_0 < x_1 < \ldots < x_n = b$$
$$f_n(x); x \in [x_{k-1}, x_k]$$

$$\begin{aligned} f_n(x) &= f(x_{k-1}) + \frac{x - x_{k-1}}{x_k - x_{k-1}} \left[f(x_k) - f(x_{k-1}) \right] \\ &= \left[1 - \frac{x - x_{k-1}}{x_k - x_{k-1}} \right] f(x_{k-1}) + \frac{x - x_{k-1}}{x_k - x_{k-1}} f(x_k) \\ &= \frac{x_k - x}{x_k - x_{k-1}} f(x_{k-1}) + \frac{x - x_{k-1}}{x_k - x_{k-1}} f(x_k) \end{aligned}$$

For $x \in [x_k, x_{k+1}]$

$$f_n(x) = \frac{x_{k+1} - x}{x_{k+1} - x_k} f(x_k) + \frac{x - x_k}{x_{k+1} - x_k} f(x_{k+1})$$

So we can find a representation, such that:

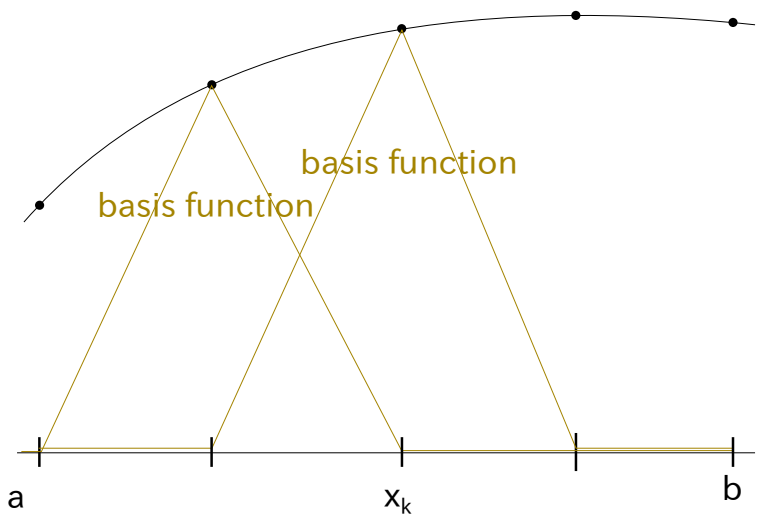


Figure 6: Visualization of the interpolation's basis functions

$$f_n(x) = \sum_{k=0}^{n} f(x_k)\varphi_k(x) \qquad x \in [a, b]$$

with the basis functios

$$\varphi_k(x) = \begin{cases} \frac{x - x_{k-1}}{x_k - x_{k-1}} & x \in [x_{k-1}, x_k] \\ \frac{x_{k+1} - x}{x_{k+1} - x_k} & x \in [x_k, x_{k+1}] \\ 0 & \text{else} \end{cases}$$

Our basis functions satisfy:

$$\varphi_k(x) = \begin{cases} 1 & x = x_k \\ 0 & x = x_l \neq x_k \end{cases}$$

"Lagrange bases" satisfy such a property. Hence our basis functions are also called *Lagrange bases*.

The functions

$$\frac{x - x_{k-1}}{x_k - x_{k-1}}, \frac{x_{k+1} - x}{x_{k+1} - x_k}$$

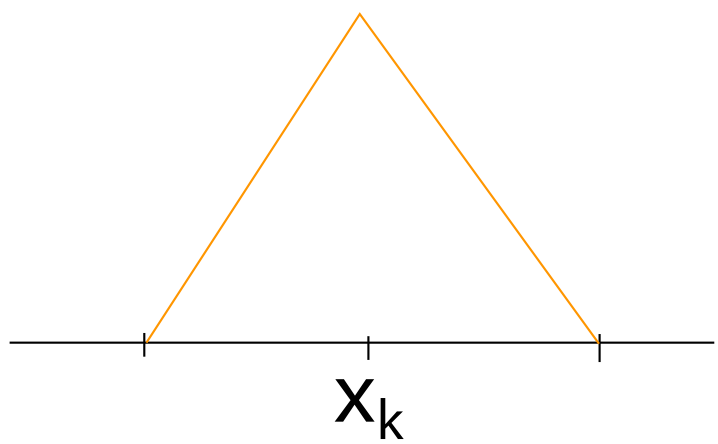


Figure 7: Visualization of Lagrange bases

are called "form functions".

We can generalize this to two dimensions. We get a so-called "hat function".

Interpolating function

$$f_n(x) = I_n$$

$$f(x) := \sum_{k=0}^{n} f(x_k)\varphi(x)$$

Error estimation

$$\|f - I_n f\|^2_{L^2([a,b])} \leq \frac{1}{24} h^4 \|f''\|^2_{L^2([a,b])}$$

Assuming this error estimation is optimal, is there another, piecewise linear function with smaller error?

In general, a representation of a piecewise linear function

$$f_n(x) = \sum_{k=0}^{n} a_k \varphi_k(x)$$

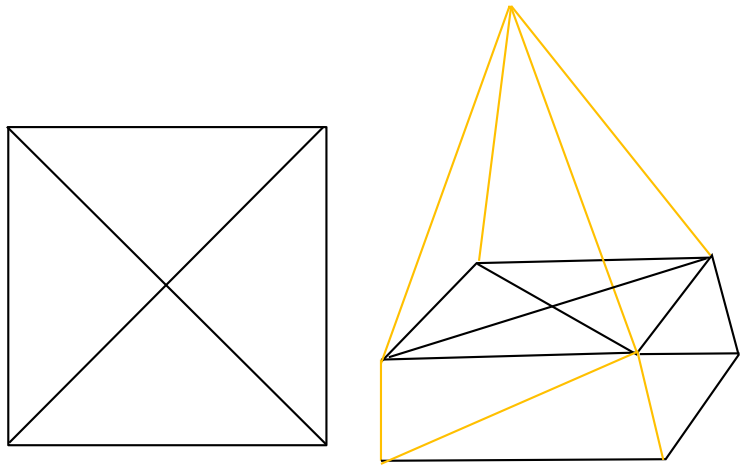


Figure 8: Visualization of a hat function

and we consider the minimization problem

$$\int_a^b \left[f(x) - \sum_{k=0}^{n} a_k \varphi(x) \right]^2 dx \implies \min_{a_0,\dots,a_n}$$

Projection methods

Minimization problem for the functional $F(\underline{a})$:

$$\begin{aligned}
F(\underline{a}) &:= \int_a^b \left[f(x) - \sum_{k=0}^{n} a_k \varphi(x) \right]^2 dx \\
&= \int_a^b \left[f(x) - \sum_{k=0}^{n} a_k \varphi(x) \right] \left[f(x) - \sum_{l=0}^{n} a_l \varphi_l(x) \right] dx \\
&= \int_a^b [f(x)]^2 \, dx - 2 \cdot \sum_{k=0}^{n} a_k \underbrace{\int_a^b f(x) \varphi_k(x) \, dx}_{f_k :=} + \sum_{k=0}^{n} \sum_{l=0}^{n} a_k a_l \underbrace{\int_a^b \varphi_k(x) \varphi_l(x) \, dx}_{m_{kl} = m_{lk} :=}
\end{aligned}$$

$$F(\underline{a}) = \int_a^b [f(x)]^2 \, dx - 2\sum_{k=0}^{n} f_k a_k + \sum_{k=0}^{n}\sum_{l=0}^{n} m_{kl} a_k a_l$$

is a quadratic function at coefficient q_k.

A necessary condition for the minimum is:

$$\frac{\partial}{\partial a_j} F(\underline{a}) = 0, j = 0, n$$

$$0 \stackrel{!}{=} \frac{\partial}{\partial a_j} F(\underline{a}) = \frac{\partial}{\partial a_j}\left[\int_a^b [f(x)]^2 \, dx - 2\sum_{k=0}^{n} f_k q_k + \sum_{k=0}^{n}\sum_{l=0}^{n} m_{kl} a_k a_l\right]$$

as $\frac{\partial}{\partial a_j}(\int_a^b [f(x)]^2) = 0$ and $\sum_{k=0}^{n} f_k q_k = f_0 a_0 + f_1 a_1 + \ldots + f_j a_j + \ldots$, we get

$$\begin{aligned}
&= -2f_j + \frac{\partial}{\partial a_j}\left[\sum_{l=0}^{n} m_{jl} a_j a_l + \sum_{k\neq j}\sum_{l=0}^{n} m_{kl} a_k a_l\right] \\
&= -2f_j + \frac{\partial}{\partial a_j}\left[m_{jj} a_j^2 + \sum_{l\neq j} m_{jl} a_j a_l + \sum_{k\neq j} m_{kj} a_k a_j + \sum_{k\neq j}\sum_{l\neq j} m_{kl} a_k a_l\right] \\
&= -2f_j + 2m_{jj} a_j + \sum_{l\neq j} m_{jl} a_l + \sum_{k\neq j} m_{kj} a_k \\
&= -2f_j + 2m_{jj} a_j + 2 \cdot \sum_{l\neq j} m_{jl} a_l \\
&= 2\left[\sum_{l=0}^{n} m_{jl} a_l - f_j\right] \stackrel{!}{=} 0 \qquad j = 0, n
\end{aligned}$$

Linear equation system:

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

$$M[j,l] = \int_a^b \varphi_l(x)\varphi_j(x)\, dx \qquad \text{“mass matrix”, also called “Gram’s matrix”}$$

$$f_j = \int_a^b f(x)\varphi(x)\, dx \qquad \text{“load vector”}$$

Ritz’ method.

$$\sum_{l=0} m_{jl} a_l = f_j$$

$$\sum_{l=0}^{n} a_l \int_a^b \varphi_l(x)\varphi_j(x)\, dx = \int_a^b f(x)\varphi(x)\, dx$$

$$f_n(x) = \sum_{l=0}^{n} a_l \varphi_l(x)$$

$$\int_a^b f_n(x)\varphi_j(x)\,dx = \int_a^b f(x)\varphi_j(x)\,dx \qquad \forall \varphi_j, j = 0, n$$

$$j_n(x) = \sum_{j=0}^{n} b_j \varphi_j$$

$$\int_a^b f_n(x)g_n(x)\,dx = \int_a^b f(x)g_n(x)\,dx$$

Ansatz space (or also trial space):

$$V_n := \operatorname{span}\{\varphi_k(x)\}_{k=0}^{n}$$

Find $f_n \in V_n : \int_a^b f_n(x)g_n(x)\,dx = \int_a^b f(x)g_n(x)\,dx \quad \forall g_n \in V_n$.

This is a so-called "variation form" (dt. Variationsformulierung). Especially, it is a "Galerkin-Bubnov variation form" because Ansatz and test space are the same.

The solution $f_n(x) = Q_n f(x)$, projection, L_2 projection

This lecture took place on 2017/10/23.

$$I_n f(x) = \sum_{k=0}^{n} f(x_k)\varphi_k(x)$$

$$\|f - f_n\|_{L^2([a,b])} \leq \frac{1}{\sqrt{24}} h^2 \|f''\|_{L^2([a,b])}$$
$$\|f' - f_n'\|_{L^2([a,b])} \leq \frac{1}{\sqrt{3}} h \|f''\|_{L^2([a,b])}$$

$$Q_n f : \|f - Q_n f\|^2_{L^2([a,b])} \to \min_{a_0,\ldots,a_n}$$

Linear equation system:

$$\sum_{k=0}^{n} a_k \int_a^b \varphi_k(x)\varphi_l(x)\,dx = \int_a^b f(x)\varphi_l(x)\,dx \qquad l = 0, n$$

Does it have a unique solution?

Ansatz space $V_n = \text{span}\{\varphi_k\}_{k=0}^n = S_k^1([a,b])$
Now we consider an arbitrary function $g_h \in V_h$.

$$g_h \in V_h \Leftrightarrow g_h(x) = \sum_{k=0}^n g_k \varphi_k(x) \Leftrightarrow \underline{g} = (g_k)_{k=0}^n \in \mathbb{R}^{n+1}$$

Isomorphism: $g_h \in V_h \leftrightarrow g \in \mathbb{R}^{n+1}$.

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

What do we know about the matrix (to determine uniqueness of the solution)?

$$M_h[l,k] = \int_a^b \varphi_k(x)\varphi_l(x)\,dx = M_h[k,l] \implies M_h = M_h^T \text{ symmetrical}$$

We test for positive definiteness:

$$\begin{aligned}
g \in \mathbb{R}^{n+1} : \left(M_h \underline{g}, \underline{g}\right) &= \sum_{k=0}^n \sum_{l=0}^n M_h[l,k] g_k g_l \\
&= \sum_{k=0}^n \sum_{l=0}^n g_k g_l \int_a^b \varphi_k(x)\varphi_l(x)\,dx \\
&= \int_a^b \underbrace{\sum_{k=0}^n g_k \varphi_k(x)}_{g_h(x)} \underbrace{\sum_{l=0}^n g_l \varphi_l(x)}_{g_h(x)}\,dx \\
&= \int_a^b [g_k(x)]^2\,dx \geq 0 \\
= 0 \Leftrightarrow 0 = g_h(x) &= \sum_{k=0}^n g_k \varphi_k(x) \Leftrightarrow g_0 = \ldots = g_n = 0, \underline{g} = \underline{0}
\end{aligned}$$

$$(M_h g, g) > 0 \quad \forall \underline{g}, \sum_{k=0}^n g_k^2 > 0$$

M_h is positive definite $\implies$ M_h is invertible.
What is the layout of M_h for piecewise linear basis functions.

$$\varphi_k(x) = \begin{cases} \frac{x - x_{k-1}}{x_k - x_{k-1}} & x \in (x_{k-1}, x_k) \\ \frac{x_{k+1} - x}{x_{k+1} - x_k} & x \in (x_k, x_{k+1}) \\ 0 & \text{otherwise} \end{cases}$$

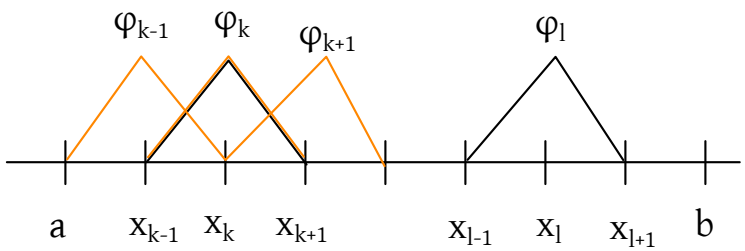


Figure 9: Layout of linear basis functions

$$M_k[l,k] = \int_a^b \varphi_k(x)\varphi_l(x)\,dx = 0 \text{ for } l+k, k\pm 1$$

$$l = k+0, n$$

$$\begin{aligned}
M_h[K,k] &= \int_a^b [\varphi_k(x)]^2\,dx = \int_{x_{k-1}}^{x_k} \left(\frac{x-x_{k-1}}{x_k-x_{k+1}}\right)^2 dx + \int_{x_k}^{x_{k+1}} \left(\frac{x_{k+1}-x}{x_{k+x}-x_k}\right)^2 dx \\
&= \frac{1}{3}(x_k - x_{k-1}) + \frac{1}{3}(x_{k+1}-x_k) = \frac{2}{3}h \\
M_h[0,0] &= \frac{1}{3}(x_1 - x_0) = \frac{1}{3}h \\
M_h[n,n] &= \frac{1}{3}(x_n - x_{n-1}) = \frac{1}{3}h
\end{aligned}$$

$$l = k \mp 1$$

$$\begin{aligned}
M_h[k+1,k] &= \int_a^b \varphi_k(x)\varphi_{k+1}(x)\,dx \\
&= \int_{x_k}^{x_{k+1}} \frac{x_{k+1}-x}{x_{k+1}-x_k}\frac{x-x_k}{x_{k+1}-x_k}\,dx \\
&\underbrace{\underbrace{\overset{s=x-x_k}{=}}_{}}_{h_k=x_{k+1}-x_k} \frac{1}{h^2}\int_0^{h_k}(h_k-s)s\,ds = \frac{1}{h_k^2}\left[\frac{1}{2}h_k s^2 - \frac{1}{3}s^2\right]_0^{h_k} = (\frac{1}{2}-\frac{1}{3})h_k = \frac{1}{6}h_k
\end{aligned}$$

$$h = \frac{b-a}{h}, x_k = a + kh, k = 0, n$$

$$M_h = \frac{1}{6}h \begin{pmatrix} 2 & 1 & \dots & & 0 \\ 1 & 4 & & & \\ \vdots & & \ddots & & \vdots \\ & & & 4 & 1 \\ 0 & & \dots & 1 & 2 \end{pmatrix} \in \mathbb{R}^{(n+1)\times(n+1)}$$

Properties of this matrix?

- tridiagonal ($n = 1$)
- diagonal dominant ($n = 1$)
- $M_h = M_h^T > 0$ (hence symmetrical, positive definite)
- matrix has few non-zero values (weakly assigned):

$$2 + 3(n-1) + 2 = 3n + 1 \text{ non-zero values}$$

- The inverse matrix is not weakly assigned (has many non-zero values)

$$g_h \in V_k : (M_h g, g) = \int_a^b [g_h(x)]^2\, dx = \sum_{k=1}^{n} \underbrace{\int_{x_{k-1}}^{x_k} [g_h(x)]^2\, dx}_{\int_{x_{k-1}}^{x_k}} \left[g_{k-1} \frac{x_k - x}{x_k - x_{k-1}} + g_k \frac{x - x_{k-1}}{x_k - x_{k-1}} \right]^2 dx$$

$$= g_{k-1}^2 \int_{x_{k-1}}^{x_k} \left(\frac{x_k - x}{x_k - x_{k-1}} \right)^2 dx + 2 g_{k-1} g_k \underbrace{\int_{x_{k-1}}^{x_k} \frac{x_k - x}{x_k - x_{k-1}} \frac{x - x_{k-1}}{x_k - x_{k-1}}\, dx}_{\frac{1}{6}h_k} + g_k^2 \underbrace{\int_{x_{k-1}}^{x_k} \left(\frac{x - x_{k-1}}{x_k - x_{k-1}} \right)^2 dx}_{\frac{1}{3}h_k}$$

$$= \frac{1}{6} h_k \left[2g_{k-1}^2 + 2g_{k-1}g_k + 2g_k^2 \right] = \frac{1}{6} h_k \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \vec{\begin{pmatrix} g_{k-1} \\ g_k \end{pmatrix}} \begin{pmatrix} g_{k-1} \\ g_k \end{pmatrix}$$

where $\frac{1}{6}h_k \left(\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \right)$ is $M_{h,k}$ is the *local* mass matrix. $\frac{x_k - x}{x_k - x_{k-1}}$ and $\frac{x - x_{k-1}}{x_k - x_{k-1}}$ are the form functions.

$$\implies M_h = \sum_{k=1}^{n} A_k^T M_{h,k} A_k$$

$n = 2$

$$M_{h,k} = \int_{\tau_k} \varphi_{k,l}(x) \varphi_{k,j}(x)\, dx \qquad i, j = 1, 3$$

$$M_{h,k} = \frac{\text{area}_k}{10} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}$$

$n = 3$

$$M_{h,k} = \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{pmatrix}$$

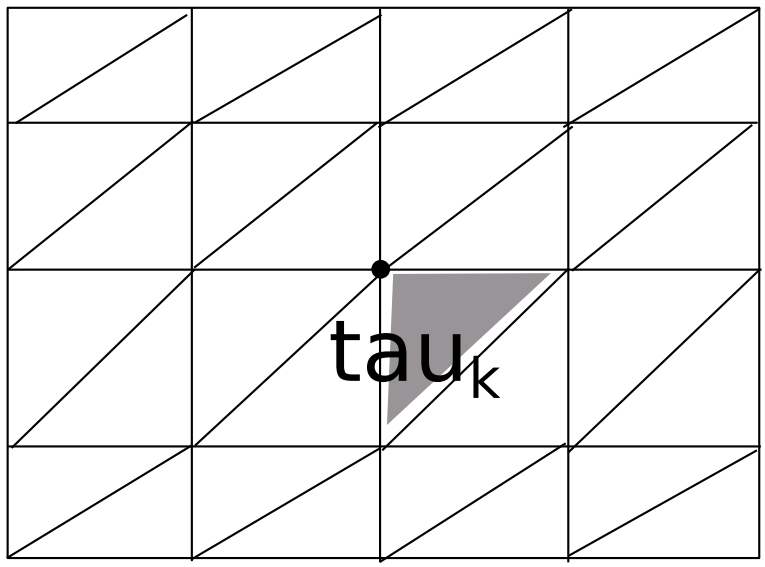


Figure 10: Area

Linear equation system:

$$M_h \underline{a} = \underline{f} \quad \Longrightarrow \quad \text{solution} \quad \underline{a} = M_h^{-1} \underline{f}$$

$$\Longrightarrow \; (Q_h f)(x) = \sum_{k=0}^{n} a_k \varphi_k(x)$$

$Q_n f$ is the solution of

$$\int_a^b (Q_n f)(x) g_h(x)\, dx = \int_a^b f(x) g_h(x)\, dx \qquad \forall g_h \in \operatorname{span}\{\varphi_l\}_{l=0}^{n}$$

$$\Longrightarrow \int_a^b \left[f(x) - (Q_h f)(x) \right] g_h(x)\, dx = 0 \forall g_h \in V_h \qquad \text{Galerkin orthogonality}$$

$$
\begin{aligned}
\|f - Q_h f\|^2_{L^2([a,b])} &= \int_a^b \left[f(x) - (Q_h f)(x)\right]\left[f(x) - (Qf)(x)\right]\, dx \\
&= \int_a^b \left[f(x) - (Q_h f)(x)\right] f(x)\, dx - \underbrace{\int_a^b \left[f(x) - (Q_h f)(x)\right](Q_h f)(x)\, dx}_{=0,\text{ Galerkin orthogonality}} \\
&= \int_a^b \left[f(x) - (Q_h f)(x)\right] f(x)\, dx - \underbrace{\int_a^b \left[f(x) - (Q_h f)(x)\right] g_h(x)\, dx}_{=0} \\
&= \int_a^b \left[f(x) - (Q_h f)(x)\right]\left[f(x) - g_h(x)\right]\, dx \\
&\leq \|f - Q_h f\|_{L^2([a,b])}\|f - g_h\|_{L^2([a,b])} \\
\implies \|f - Q_h f\|_{L^2([a,b])} &\leq \|f - g_h\|_{L^2([a,b])} \qquad \forall g_h \in V_h \\
\|f - Q_h f\|_{L^2([a,b])} &\leq \inf_{g_h \in V_k} \|f - g_h\|_{L^2([a,b])}
\end{aligned}
$$

The last line corresponds to a minimization problem. It's the so-called *Cea's Lemma*.

Lemma (Cea's lemma)**.**

$$
\|f - Q_h f\|_{L^2([a,b])} \leq \inf_{g_h \in V_k} \|f - g_h\|_{L^2([a,b])}
$$

$$
\implies \|f - Q_h f\|_{L^2([a,b])} \leq \inf_{g_h} \|f - g_h\|_{L^2([a,b])} \overset{\leq}{g_h = I_h f} \|f - I_h f\|_{L^2([a,b])} \leq \frac{1}{\sqrt{24}} h^2 \|f''\|_{L^2([a,b])}
$$

Given:

$$
\|f - Q_h f\|_{L^2([a,b])} \leq \|f - I_h f\|_{L^2([a,b])}
$$

Find whether it holds that:

$$
\|f - I_h f\|_{L^2([a,b])} \leq c\|f - Q_h f\|_{L^2([a,b])}
$$

This question is easy to answer for $n = 1$, but an open research question for $n \geq 2$.

We can show that c converges towards 1. So we can show how interpolation and projection errors behave towards each other.

$$
\begin{aligned}
\|f - Q_h f\|^2_{L^2([a,b])} &= \int_a^b [f(x) - (Q_h f)(x)] f(x)\, dx \\
&\overset{\text{c.s.u.}}{\leq} \|f - Q_h f\|_{L^2([a,b])}\|f\|_{L^2([a,b])}
\end{aligned}
$$

$$\|f - Q_h f\|_{L^2([a,b])} \leq \|f\|_{L^2([a,b])}$$

L_2 projection is also well-defined for $f \in L^2([a,b])$, hence also for non-continuous f.

Error estimation:

$$\|f - Q_h f\|_{L^2([a,b])} \leq \|f\|_{L^2([a,b])}$$

where $s = 0$.

$$\|f - Q_h f\|_{L^2([a,b])} \leq \frac{1}{\sqrt{24}} h^2 \|f''\|_{L^2([a,b])} = c(s) h^2 \|f\|_s \qquad , s = 2$$

In terms of interpolation error: $s \in [1, 2]$

Theorem 4. *$Q_h f$ is piecewise linear.*

$$\|f - Q_h f\|_{L^2([a,b])} \leq c(s) h^s \|f\|_s, \qquad s \in [0, 2]$$

Interpolation $s > \frac{1}{2}$.

Two major questions are left. We considered:

$$\|f - I_h f\|_{L^2}, \quad \|f' - (I_h f)'\|_{L^2}$$

$$\|f - Q_h f\|_{L^2} \leq \|f - I_h f\|_{L^2} \leq \dots$$

First question:

$$\|f' - (Q_h f)'\|_{L^2} \leq ?$$

Second question: If we consider the L^2 projection,

$$\int_a^b Q_h f g_h \, dx = \int_a^b f g_h \, dx$$

$$g_h = Q_h f$$

$$\implies \|Q_h f\|_{L^2([a,b])} \leq \|f\|_{L^2([a,b])}$$

This is called L^2 *stability of the L^2 projection*. This property does not hold for interpolation. Interpolation is not L^2 stable. Question raised:

$$\|(Q_h f)'\|_{L^2} \leq c \|f'\|_{L^2}$$

$$\|(I_h f)'\|_{L^2} \leq c \|f'\|_{L^2} \text{ interpolation}, n = 1, \text{ does not hold for } n \geq 2$$

This is comparatively simple for uniform nets. $h_k = h$. The question how about globally non-uniform nets? Ansatz function of higher order.

Interpolation versus projection:

+ interpolation is local
- projection is global, linear equation system

+ projection is very stable

- interpolation is unstable

Of course, locality and stability is desired and provided by "quasi interpolation" (implemented by the Scott-Zhang operator). Idea:

$$(R_h f)(x) = \sum_{k=0}^{n} F_k(f)\varpi_k(x)$$

$$(F_k f)(x) = f(x_k) \quad \text{"interpolation"}$$
$$(F_k f)(x) = (G_k f)(x_k)$$

This lecture took place on 2017/10/25.

Projection:

$$\int_a^b \left[f(x) - (Q_h f)(x)\right]^2 \, dx \to \min_{g_h \in V_h} \int_a^b \left[f(x) - g_h(x)\right]^2 \, dx$$

Ansatz space:

$$V_h = \operatorname{span}\{\varphi_k\}_{k=0}^n \qquad \text{piecewise linear } \varphi_k$$

VF:

$$Q_h f \in V_h : \int_a^b (Q_h f)(x) g_h(x) \, dx = \int_a^b f(x) g_h(x) \, dx \qquad \forall g_h \in V_h$$

We also consider different Ansatzräume, e.g.

$$V_h = \operatorname{span}\{\varphi_k(x)\}_{k=1}^n$$

with piecewise constant functions

$$\varphi_k(x) = \begin{cases} 1 & x \in (x_{k-1}, x_k) \\ 0 & \text{otherwise} \end{cases}$$

VF:

$$\sum_{k=1}^n a_k \underbrace{\int_a^b \varphi_k(x)\varphi_l(x)}_{=\begin{cases} 0 & l \neq k \\ x_l - x_{l-1} & l = k \end{cases}} dx = \int_a^b f(x)\varphi_l(x) \, dx = \int_{x_{l-1}}^{x_l} f(x) \, dx$$

$$\implies a_k = \frac{1}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} f(x) \, dx = f_h(x), x \in (x_{k_1}, x_k)$$

What about the error?

$$x \in (x_{k-1}, x_k), f(x) - (Q_h f)(x) = f(x) - \frac{1}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} f(y)\, dy = \frac{1}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} [f(x) - f(y)]\, dy$$

$$\int_{x_{k-1}}^{x_k} [f(x) - (Q_h f)(x)]^2\, dx = \frac{1}{(x_k - x_{k-1})^2} \int_{x_{k-1}}^{x_k} \left[\int_{x_{k-1}}^{x_k} [f(x) - f(y)]\, dy \right]^2 dx$$

$$= \frac{1}{(x_k - x_{k-1})^2} \int_{x_{k-1}}^{x_k} \underbrace{\left[\int_{x_{k-1}}^{x_k} 1 \cdot \int_y^x f'(s)\, ds\, dy \right]^2}_{\underbrace{\int_{x_{k-1}}^{x_k} 1^2\, dy}_{x_k - x_{k-1} \text{ cancels out}} \int_{x_{k-1}}^{x_k} \left[\int_y^x f'(s)\, ds \right]^2 dy} dx$$

$$\leq \frac{1}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} \underbrace{\left[\int_y^x 1 \cdot f'(s)\, ds \right]^2}_{\leq |x-y| \cdot \underbrace{\left| \int_y^x [f'(s)]^2\, ds \right|}_{\leq \int_{x_{k-1}}^{x_k} [f'(s)]^2\, ds}} dy\, dx$$

$$\leq \frac{1}{x_k - x_{k-1}} \underbrace{\int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} |x - y|\, dy\, dx}_{= \frac{1}{3}(x_k - x_{k-1})} \int_{x_{k-1}}^{x_k} [f'(s)]^2\, ds$$

Error estimation:

$$\int_a^b [f(x) - (Q_h f)(x)]^2\, dx \leq \frac{1}{3} \sum_{k=1}^{n} (x_k - x_{k-1})^2 \int_{x_{k-1}}^{x_k} [f'(x)]^2\, dx \; h \overset{=}{=} h_k \; \frac{1}{3} h^2 \int_a^b [f'(x)]^2\, dx$$

Assumptions:

$$f' \in L^2([a, b]), f(x) = \sqrt{x}, x \in (0, 1)$$

$$[f(x) - (Q_h f)(x)]^2 = \frac{1}{(x_k - x_{k-1})^2} \left[\int_{x_{k-1}}^{x_k} \frac{f(x) - f(y)}{|x - y|^{\frac{1}{2}+s}} |x - y|^{\frac{1}{2}+s}\, dy \right]^2$$

$$\leq \frac{1}{(x_k - x_{k-1})^2} \int_{x_{k-1}}^{x_k} \frac{[f(x) - f(y)]^2}{|x - y|^{1+2s}}\, dy \int_{x_{k-1}}^{x_k} \underbrace{|x - y|^{1+2s}}_{\leq h_k^{1+2s} \cdot h_k}\, dy$$

$$\int_{x_{k-1}}^{x_k} [f(x) - (Q_h f)(x)]^2\, dx \leq h_k^{2s} \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} \frac{[f(x) - f(y)]^2}{|x - y|^{1+2s}}\, dy\, dx$$

Error estimation:

$$\int_a^b [f(x) - (Q_h f)(x)]^2 \, dx \leq \sum_{k=1}^{n} (x_k - x_{k-1})^{2s} \int_{x_{k-1}}^{x_k} \int_{x_{k-1}}^{x_k} \frac{[f(x) - f(y)]^2}{|x-y|^{1+2s}} \, dy \, dx$$

$$\overset{\leq}{h_k} = h \, h^{2s} \int_a^b \int_a^b \frac{[f(x) - f(y)]^2}{|x-y|^{1+2s}} \, dy \, dx \qquad s \in (0,1)$$

$$\int_a^b [f(x) - (Q_h f)(x)]^2 \, dx \leq \int_a^b [f(x)]^2 \, dx$$

Let V_h^p be an Ansatz space of piecewise linear polynomials of degree p. Then for the projection of f to V_h^p it holds that:

$$\int_a^b [f(x) - (Q_h f)(x)]^2 \, dx \leq c h^{2s} |f|_s^2$$

with $|f|_s^2 = \int_a^b [f^{(n)}(x)]^2 \, dx \qquad s = n \in \mathbb{N}_0, s \leq p+1.$

$$|f|_s^2 = \int_a^b \int_a^b \frac{[f^{(n)}(x) - f^{(n)}(y)]}{|x-y|^{1+2\tilde{\sigma}}} \, dx \, dy \qquad s = n + \tilde{\sigma}, \tilde{\sigma} \in (0,1)$$

Convergence of h^s for $s \leq p+1$ assuming $|f|_s < \infty$.

Consider the function

$$f(x) = \sqrt{x} \quad , x \in (0,1), |f|_s < \infty, s < 1$$

This means we get the best possible convergence for $p = 0$. Every other choice of $p > 1$ gives asymptotically no better convergence order. So we always need to find a good tradeoff between the regularity of the function to interpolate and the choice of the polynomial ansatz order.

So we take about:

- adaptive mesh[1]
- a posteriori error estimation

Goal: precision versus effort.

Numerical Integration

$$I = \int_a^b f(x) \, dx \simeq I_n = \sum_{k=0}^{n} f(x_k) w_k$$

[1]Adaptivity comes in 4 dimensions here: the precision of the net, the polynomial degree p, a mixture of these or we adapt supporting points.

Integration point x_k, integration weight w_k.

Idea: Replace $f(x)$ by integration polynomial $f_n(x)$ with representation in Lagrange polynomials:

$$f_n(x) = \sum_{k=0}^{n} f(x_k) L_k^n(x), L_k^n(x) = \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{x - x_j}{x_k - x_j}$$

Assumption: Points $x_k \neq x_j$, $k \neq j$ pairwise different.

Approximation formula:

$$I_n = \int_a^b f_n(x)\,dx = \sum_{k=0}^{n} \int_a^b f(x_k) L_k^n(x)\,dx = \sum_{k=0}^{n} f(x_k) w_k, \quad w_k = \int_a^b L_k^n(x)\,dx$$

Integration formula:

$$I_n = \sum_{k=0}^{n} f(x_k) w_k, \quad w_k = \int_a^b L_k^n(x)\,dx$$

points x_k, pairwise different

Integration error:

$$I - I_n = \int_a^b \left[f(x) - f_n(x)\right]\,dx = \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n} (x - x_j)\,dx$$

If f is a polynomial of degree $\leq n$, then the integration formula is accurate. Or in general, an integrational formula is called "to be of degree m", if polynomials of degree $n \leq m$ can be interpolated accurately. Especially constant functions are integrated accurately. By arbitrary choice of points, we can go up to $m = n$. With a "proper" choice of points, we can reach $m = 2n + 1$.

$$f(x) = 1 \qquad I = \int_a^b 1\,dx = b - a = I_n = \sum_{k=0}^{n} \underbrace{f(x_k)}_{=1} w_k = \sum_{k=0}^{n} w_k$$

Or also, because $b - a = \sum_{k=0}^{n} w_k$,

$$\frac{1}{b-a} \sum_{k=0}^{n} w_k = 1$$

We might be able to additionally assume $x_k \in (a, b)$ or $w_k > 0$ (the latter avoids *point cancellation*).

Newton-Cotes Formulae

$$n \in \mathbb{N}, h = \frac{b-a}{n}, x_k = a + kh, k = 0, n$$

Integration weights:

$$w_k = \int_a^b L_k^n(x)\,dx = \int_a^b \prod_{\substack{j=0\\ j\neq k}}^{n} \frac{x - x_j}{x_k - x_j}\,dx = \int_a^b \prod_{\substack{j=0\\ j\neq k}}^{n} \frac{x-(a+jh)}{(a+kh)-(a+jh)}\,dx = \int_a^b \prod_{\substack{j=0\\ j\neq k}}^{n} \frac{x-(a+jh)}{(k-j)h}\,dx$$

We want to get rid of h in the enumerator. We apply substitution with $x = a + sh$.

$$\frac{dx}{ds} = h \qquad dx = h\,ds$$

$$x = a, s = 0, x = b, s = n, h = \frac{2-a}{n}$$

$$w_k = \frac{b-a}{n} \underbrace{\int_0^n \prod_{\substack{j=0\\ j\neq k}}^{n} \frac{s-j}{k-j}\,ds}_{\tilde{\omega}_k}$$

This way, we can determine $\tilde{w}_k$.

Hence, our interpolation formula is:

$$\implies I_n = \frac{b-a}{n} \sum_{k=0}^{n} f\left(a + k\frac{b-a}{n}\right)\tilde{\omega}_k$$

Example 6. *Let $n = 1$, $x_0 = a$, $x_1 = b$.*

$$\tilde{\omega}_0 = \int_0^1 \prod_{\substack{j=0\\ j\neq 0}}^{1} \frac{s-j}{0-j}\,ds = \int_0^1 \frac{s-1}{0-1}\,ds = \int_0^1 (1-s)\,ds = \frac{1}{2}$$

$$\tilde{\omega}_1 = \int_0^1 \prod_{\substack{j=0\\ j\neq 1}}^{1} \frac{s-j}{1-j}\,ds = \int_0^1 s\,ds = \frac{1}{2}$$

$$I_1 = (b-a)\left[f(a)\frac{1}{2} + f(b)\frac{1}{2}\right] = \frac{b-a}{2}\left[f(a) + f(b)\right]$$

This is the Trapezoidal Rule.

Error estimation:

$$I - I_n = \frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)\,dx$$

Substitution: $s = s(x), s'(x) = (x-a)(x-b)$. *Hence* $s(x) = \int^x (x-a)(x-b)\,dx = \frac{1}{3}x^3 - \frac{1}{2}(a+b)x^2 + abx$. $s'(x) = (x-a)(x-b) < 0$ *if* $x \in (a,b)$, *so* $s(x)$ *is strictly monotonically falling and continuous. The inverse function is* $x = x(s)$.

$$I - I_n = \frac{1}{2}\int_{s(a)}^{s(b)} f''(\xi(x(s)))\,ds \overset{\text{Mean value theorem for integration}}{=} = \frac{1}{2}f''(\underbrace{\xi(s(\bar{s}))}_{:=\eta})[s(b)-s(a)]$$

$$\begin{aligned} s(b) - s(a) &= \left(\frac{1}{3}b^3 - \frac{1}{2}(a+b)b^2 + ab^2\right) - \left(\frac{1}{3}a^3 - \frac{1}{2}(a+b)a^2 + a^2b\right) \\ &= \frac{1}{3}b^3 + \frac{1}{2}ab^2 - \frac{1}{2}b^3 - \frac{1}{3}a^3 + \frac{1}{2}a^3 - \frac{1}{2}a^2b \\ &= -\frac{1}{6}\left(b^3 - 3ab^2 + 3a^2b - a^3\right) = -\frac{1}{6}(b-a)^3 \end{aligned}$$

Trapezoidal Rule:

$$\int_a^b f(x)\,dx = \frac{b-a}{2}[f(a) - f(b)] - \frac{1}{12}f''(\eta)(b-a)^3$$

where $m = 1, n = 1$. *This means that this formula is accurate for linear functions.*

Example 7. *Let* $n = 0$, $X_0 = \frac{a+b}{2}$.

$$I_0 = (b-a)f\left(\frac{a+b}{2}\right)$$

This is the so-called midpoint rule (dt. Mittelpunktregel).

We consider a Taylor expansion along the mid point.

$$f(x) = f(x_0) + (x-x_0)f'(x_0) + \frac{1}{2}f''(\xi)(x-x_0)$$

$$\underbrace{\int_a^b f(x)\,dx}_{I} = \underbrace{\int_a^b f(x_0)\,dx}_{I_0=(b-a)f(\frac{a+b}{2})} + \underbrace{\int_a^b (x-x_0)f''(x_0)\,dx}_{=0} + \underbrace{\frac{1}{2}\int_a^b f''(\xi)(x-x_0)^2\,dx}_{=\frac{1}{24}f''(\eta)(b-a)^3}$$

As far as the midpoint rule is considered,

$$\Longrightarrow \int_a^b f(x)\,dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{1}{24}f''(\eta)(b-a^3)$$

for $m = 1$ *and* $n = 0$. *Here we have* $m > n$.

Example 8. *Let $n = 2$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$.*

$$\begin{aligned}
\tilde{\omega}_0 &= \int_0^2 \prod_{\substack{j=0\\ j\neq 0}}^{2} \frac{s-j}{0-j}\, ds = \int_0^2 \frac{s-1}{0-1}\frac{s-2}{0-2}\, ds \\
&= \frac{1}{2}\int_0^2 \left[s^2 - 3s + 2\right] ds = \frac{1}{2}\left[\frac{1}{3}8 - \frac{3}{2}4 + 4\right] = \frac{1}{2}\left(\frac{8}{3} - 2\right) = \frac{1}{3} \\
\tilde{\omega}_1 &= \int_0^2 \prod_{\substack{j=0\\ j\neq 1}}^{2} \frac{s-j}{1-j}\, ds = \int_0^2 \frac{s-0}{1-0}\frac{s-2}{1-2}\, ds \\
&= \int_0^2 s(2-s)\, ds = \int_0^2 (2s - s^2)\, ds = 4 - \frac{8}{3} = \frac{4}{3} \\
\tilde{\omega}_2 &= \frac{1}{3}
\end{aligned}$$

$$\begin{aligned}
I_2 &= \frac{b-a}{2}\left[f(a)\frac{1}{3} + f\left(\frac{a+b}{2}\right)\frac{4}{3} + f(b)\frac{1}{3}\right] \\
&= \frac{b-a}{2}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right]
\end{aligned}$$

This is the so-called "Simpson's rule".

Recall, the Trapezoidal Rule originates from,

$$f(x) = f(a) + \frac{x-a}{b-a}\left[f(b) - f(a)\right] + \frac{1}{2}f''(\xi)(x-a)(x-b)$$

"Rectangle rule" The Rectangle rule is given with:

$$f(x) = \underbrace{f(x_0) + (x - x_0)f'(x_0)}_{\substack{f_1(x), f_1(x_0)=f(x_0)\\ f_1'(x_0)=f'(x_0)}} + \underbrace{\frac{1}{2}f''(\xi)(x-x_0)^2}_{\text{Hermitian interpolation polynomial}}$$

For Simpson's Rule, we define,

$$f_3(x) : f_3(a) = f(a) \wedge f_3(b) = f(b) \wedge f_3(\frac{a+b}{2}) = f(\frac{a+b}{2}) \wedge f_3'(\frac{a+b}{2}) = f'(\frac{a+b}{2})$$

$$f(x) = f_3(x) + \frac{1}{4!}f^{(4)}(\eta)(x-a)(x-b)(x-x_0)^2$$

Hence, we get,

$$\int_a^b f(x)\, dx = \frac{b-a}{6}\left[f(a) + 4f(\frac{a+b}{2}) + f(b)\right] - \frac{1}{2880}(b-a)^5 f^{(4)}(\eta)$$

with $n = 2$ and $m = 3$.

Motivation: Let's consider,

$$I = \int_0^1 f(x)\,dx \qquad I_n = \sum_{k=0}^{n} f(x_k)\omega_k$$

$(n+1)$ parameters, (x_k, ω_k), hence $2n+2$ parameters. So we need $2n+2$ equations to determine $2n+2$ parameters.

Requirement of exact integration of polynomials of degree $2n+1$: hence, of the monomials x^k for $k = 0, 2n+1$.

For $k = 0$ to $2n+1$, we consider,

$$I = \int_0^1 x^k\,dx = \frac{1}{k+1} \stackrel{!}{=} I_n = \sum_{j=0}^{n} x_j^k \omega_j$$

Let $n = 2$, then we get Table 1.

K	I	I_2
0	1	$= \omega_0 + \omega_1 + \omega_2$
1	$\frac{1}{2}$	$= \omega_0 x_0 + \omega_1 x_1 + \omega_2 x_2$
2	$\frac{1}{3}$	$= \omega_0 x_0^2 + \omega_1 x_1^2 + \omega_2 x_2^2$
3	$\frac{1}{4}$	$= \omega_0 x_0^3 + \omega_1 x_1^3 + \omega_2 x_2^3$
4	$\frac{1}{5}$	$= \omega_0 x_0^4 + \omega_1 x_1^4 + \omega_2 x_2^4$
5	$\frac{1}{6}$	$= \ldots$ system of non-linear equations

Table 1: K, I and I_2 for $n = 2$

We try to solve the system of non-linear equations in Table 1.

Symmetry: Symmetry of integration points and weights.

$$x_0 = t \qquad x_1 = \frac{1}{2} \qquad x_2 = 1 - t$$
$$\omega_0 = \omega \qquad \omega_2 = \omega$$

$$k = 0 : 1 = \omega + \omega_1 + \omega \implies \omega_1 = 1 - 2\omega$$
$$k = 1 : \frac{1}{2} = \omega t + (1 - 2\omega)\frac{1}{2} + \omega(1 - t) = \frac{1}{2}$$
$$k = 2 : \frac{1}{12} = \omega[2t^2 - 2t + \frac{1}{2}]$$
$$k = 3 : \ldots$$

$$k = 4, 5 : \frac{11}{80} = \omega \left[2t^4 - 4t^3 + 6t^2 - 4t + \frac{7}{8} \right]$$

$t = \frac{1}{2} - \frac{\sqrt{15}}{10}$, $\omega = \frac{5}{18}$.

This will lead us to the discussion of Gauss-Legendre Quadrature.

This lecture took place on 2017/11/06.

We consider the numeric integration using a

$$I = \int_a^b f(x)\,dx \sim I_n = \sum_{k=0}^{n} f(x_k)\omega_k$$

$$f(x) \sim f_n(x) = \sum_{k=0}^{n} f(x_k) L_k^n(x), \omega_k = \int_a^b L_K^n(x)\,dx$$

$$x_k = a + k\frac{b-a}{n} \qquad k = 0, n \rightsquigarrow \text{Newton-Cotes formulae}$$

What is the optimal choice?

Independent of the choice of supporting points (pairwise different), (welche?) polynomials of degree $\leq n$ can be integrated accurately. Can the supporting points x_k be chosen in such a way that polynomials of degree $m > n$ can be integrated accurately.

So far:

- $2(n+1)$ unknown variables (x_k, ω_k)
- $2(n+1)$ equations for the integration of monoms (non-linear equation system)

Let $f(x) = f_m(x)$ is a polynomials of degree $m > n$. The associated interpolation polynomials of degree n is defined as,

$$f_n(x) = \sum_{k=0}^{n} f_m(x_k) L_k^n(x), \qquad f_n(x_j) = f_m(x_j), j = 0, n$$

The remainder is given with,

$$r_m(x) = f_m(x) - f_n(x)$$

as a polynomial of degree m. It satisfies,

$$r_m(x_j) = 0 \qquad j = 0, n$$

$$\implies r_m(x) = \underbrace{\prod_{j=0}^{n}(x - x_j)}_{\text{degree } n+1} \cdot g_{m-(n+1)}(x)$$

$$f_m(x) = f_n(x) + \prod_{j=0}^{n}(x - x_j) g_{m-(n+1)}(x)$$

$$I = \int_a^b f_m(x)\,dx = \int_a^b f_n(x)\,dx + \underbrace{\int_a^b \prod_{j=0}^{n}(x - x_j) g_{m-(n+1)}(x)\,dx}_{=0 \implies I = I_n \quad \forall g_{m-(n+1)}(x)}$$

$$= \sum_{k=0}^{n} f_m(x_k)\omega_k = I_n$$

Can $\int_a^b \prod_{j=0}^{n}(x - x_j) g_{m-(n+1)}(x)\,dx = 0$ be satisfied for all polynomials g? Let $p_{n+1}(x)$ denote $\prod_{j=0}^{n}(x - x_j)$.

Can $g_{m-(n+1)}(x) = p_{n+1}(x)$ be chosen, then

$$\int_a^b \left[p_{n+1}(x)\right]^2\,dx > 0$$

This case is impossible. hence, $\implies m - (n+1) < n + 1 \implies m < 2n + 2$ which equals $m \leq 2n + 1$. We consider a system of orthogonal polynomials $\{p_k(x)\}_{k=0}$.

$$\int_a^b p_k(x) p_l(x)\,dx = 0 \qquad \text{if } l \neq k$$

$$\implies g_{m-(n+1)}(x) = \sum_{l=0}^{m-(n+1)} \alpha_l p_l(x) \implies \int_a^b p_{n+1}(x) g_{m-(n+1)}(x)\,dx = 0$$

To construct orthogonal polynomials, we use the Gram-Schmidt method. We chose: $p_0(x) = 1$. Let $k = 0, 1, 2, \ldots$.

$$p_{k+1}(x) = x^{k+1} - \sum_{l=0}^{k} \beta_{kl} p_l(x)$$

$$0 = \int_a^b p_{k+1}(x) p_j(x)\,dx = \int_a^b x^{k+1} p_j(x)\,dx - \sum_{l=0}^{k} \beta_{kl} \underbrace{\int_a^b p_l(x) p_j(x)\,dx}_{=0, l \neq j}$$

In the sum, we can see the orthogonal polynomials, we already built.

$$\beta_{k,l} = \frac{\int_a^b x^{k+1} p_l(x)\,dx}{\int_a^b [p_l(x)]^2\,dx}$$

This leads to the following process:

1. Construction of orthogonal polynomials
2. Supporting points of the integration formula are the roots (dt. Nullstellen) of $p_{n+1}(x)$
3. $\rightsquigarrow L_k^n(x) \rightsquigarrow \omega_k(x)$

But this is incomplete. For the second step, we need to verify:

1. the roots must be real
2. must be $\in [a, b]$
3. and must be simple

Show that the roots of $p_{n+1}(x)$ are real, where $p_{n+1}(x)$ is real. Proof by contradiction:

$$x_0 \in \mathbb{C}, \qquad p_{n+1}(x_0) = 0, \qquad x_0 = \alpha + \beta_i, \qquad \beta \neq 0$$

$$\implies \overline{x_0} = \alpha - \beta_i, p_{n+1}(\overline{x_0}) = 0$$

$$\implies p_{n+1}(x) = (x - x_0)(x - \overline{x_0})q_{n-1}(x) = \left[(x-\alpha)^2 + \beta^2\right] q_{n-1}(x)$$

$$\implies 0 = \int_a^b p_{n+1}(x)q_{n-1}(x)\,dx = \int_a^b \frac{[p_{n+1}(x)]^2}{(x-\alpha)^2 + \beta^2}\,dx > 0$$

This is a contradiction, hence $x_0 \in \mathbb{R}$.

Consider $x_0 < a$.

$$p_{n+1}(x) = (x - x_0)q_n(x) \implies 0 = \int_a^b p_{n+1}(x)q_n(x)\,dx = \int_a^b \frac{[p_{n+1}(x)]^2}{\underbrace{x - x_0}_{>0}}\,dx > 0 \implies x_0 \geq a$$

$x_0 > b$ follows analogously (with < 0).

x_0 is not a simple root. $p_{n+1}(x) = (x - x_0)^2 q_{n-1}(x)$ leads to a contradiction.

Example: $[a, b] = [0, 1], n = 2$

$$
\begin{aligned}
p_0(x) &= 1 \\
p_1(x) &= x - \beta_{00} \\
\beta_{00} &= \frac{\int_0^1 x \cdot 1\, dx}{\int_0^1 1^2\, dx} = \frac{1}{2} \\
p_1 * x) &= x - \frac{1}{2} \\
p_2(x) &= x^2 - \beta_{11}\left(x - \frac{1}{2}\right) - \beta_{10} \cdot 1 \\
\beta_{11} &= \frac{\int_0^1 x^2(x - \frac{1}{2})\, dx}{\int_0^1 (x - \frac{1}{2})^2\, dx} = 1 \\
\beta_{10} &= \frac{1}{3} \\
\implies p_2(x) &= x^2 - x + \frac{1}{6} \\
\implies p_3(x) &= x^2 - \frac{3}{2}x^2 + \frac{3}{5}x - \frac{1}{20} \\
p_3(x) &= 0 \\
20x^3 - 30x^2 + 12x - 1 &= 0 \\
x_1 &= \frac{1}{2} \\
x_{0,2} &= \frac{1}{2} \pm \frac{\sqrt{15}}{10}
\end{aligned}
$$

So far: integration of polynomial $f_n(x)$, $m = 2n + 1$ (accurate). Error when applying for arbitrary given $f(x)$.

Let x_k be roots of orthogonal polynomials $p_{n+1}(x)$, ω_k with $0 \le k \le n$. Let $f_{2n+1}(x)$ be the Hermitian interpolation polynomial.

$$
f_{2n+1}(x_k) = f(x_k) \qquad f'_{2n+1}(x_k) = f'(x_k)
$$

$$
f(x) = f_{2n+1}(x) + \frac{1}{(2n+2)!} f^{(2n+2)}(\eta(x)) \prod_{j=0}^{n} (x - x_j)^2
$$

$$
I = \int_a^b f(x)\, dx = \underbrace{\int_a^b f_{2n+1}(x)\, dx}_{\substack{=\sum_{k=0}^n f_{2n+1}(x_k)\omega_k \\ =\sum_{k=0}^n f(x_k)\omega_k = I_n}} + \frac{1}{(2n+2)!} \int_a^b f^{(2n+2)}(\eta(x)) \prod_{j=0}^{n} (x - x_j)^2\, dx
$$

Let $[a, b] = [-1, +1]$. We apply Gram-Schmidt:

$$p_0(x) = 1$$
$$p_{k+1}(x) = x^{k+1} - \sum_{l=0}^{k} \beta_{kl} p_l(x)$$
$$\beta_{kl} = \frac{\int_a^b x^{k+1} p^l(x)\, dx}{\int_a^b [p_l(x)]^2\, dx}$$

$\{w_l(x)\}_{l=0}^{n+1}$ are linear independent. We want to get orthogonal $\{p_l(x)\}_{l=0}^{n+1}$.

$$p_0(x) = w_0(x)$$
$$p_{k+1}(x) = \omega_{k+1}(x) - \sum_{l=0}^{k} \beta_{kl} p_l(x)$$
$$\beta_{kl} = \frac{\int_a^b \omega_{k+1}(x) p_l(x)\, dx}{\int_a^b [p_l(x)]^2\, dx}$$

So far: $w_l(x) = x^l$.

Choose $\omega_{k+1}(x) = x p_k(x)$. The enumerator of β_{kl} is,

$$\int_a^b \omega_{k+1}(x) p_l(x)\, dx = \int_a^b x p_k(x) p_l(x)\, dx = \int_a^b p_k(x) \underbrace{x p_l(x)}_{\text{degree } l+1} dx$$

This is zero if $l + 1 < k$ (and $l = 0, k$).

$$\beta_{kl} = 0, \qquad l < k - 1$$
$$p_{k+1}(x) = x p_k(x) - \beta_{k,k-1} p_{k-1}(x) - \beta_{kk} p_k(x)$$

Consider $[-1, +1]$. Enumerator of β_{kk}:

$$\underbrace{\int_{-1}^{1} x\, [p_k(x)]^2\, dx}_{\text{symmetric function}} = 0 \implies p_{k+1}(x) = x p_k(x) - \beta_{k,k-1} p_{k-1}(x)$$

$$p_{k+1}(x) = x p_k(x) - \beta_k p_{k-1}(x)$$
$$\beta_k = \frac{\int_{-1}^{1} x p_k(x) p_{k-1}(x)\, dx}{\int_{-1}^{1} [p_{k-1}(x)]^2\, dx}$$

Lemma. $\int_{-1}^{1} [p_k(x)]^2 \, dx = \frac{2}{1+2k} [p_k(1)]^2$

Proof. By complete induction.

Consider $k = 0$. $p_0(x) = 1$. $\int_{-1}^{1} [p_0(x)]^2 \, dx = 2$ (correct)

Consider $k = 1$. $p_1(x) = x$. $\int_{-1}^{1} [p_1(x)]^2 \, dx = \frac{2}{3}$ (correct)

$\int_{-1}^{1} [p_k(x)]^2 \, dx = x[p_k(x)]^2\Big|_{-1}^{1} - 2\int_{-1}^{1} x p_k(x) p_k'(x) \, dx$

$$\begin{aligned} p_k(x) &= x^k + q_{k-1}(x) \\ p_k'(x) &= kx^{k-1} + q_{k-1}'(x) \\ xp_k'(x) &= kx^k + r_{k-1}(x) \end{aligned}$$

$$\implies \int_{-1}^{1} p_k(x) x p_k'(x) \, dx = k \int_{-1}^{1} [p_k(x)]^2 \, dx$$

$$\int_{-1}^{1} x p_k(x) p_{k-1}(x) \, dx = \int_{-1}^{1} [p_k(x)]^2 \, dx$$

$$\implies \beta_k = \frac{\int_{-1}^{1} [p_k(x)]^2 \, dx}{\int_{-1}^{1} [p_{k-1}(x)]^2 \, dx} = \frac{\frac{2}{1+2k}[p_k(1)]^2}{\frac{2}{1+2(k-1)}[p_{k-1}(1)]^2} = \frac{2k-1}{2k+1}$$

$$\implies (2k+1)p_{k+1}(x) = (2k+1)xp_k(x) - (2k-1)p_{k-1}(x)$$

These are the Legendre polynomials (leading to Gauss-Legendre integration).

In linear algebra, this method is known as *Arnoldi Iteration* (to transform symmetric matrices to a system of tridiagonal matrices). □

This lecture took place on 2017/11/08.

$$\int_{-1}^{1} f(x) \, dx \sim \sum_{k=0}^{n} f(x_k)\omega_k, \qquad p_{n+1}(x_k) = 0 \int_{-1}^{1} p_k(x) p_l(x) \, dx = 0, \qquad k \neq l$$

$$I = \int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} \, dx \simeq \sum_{k=0}^{n} f(x_k)\omega_k$$

$$f(x) \sim f_n(x) = \sum_{k=0}^{n} f(x_k) L_k^n(x)$$

$$I_n = \int_{-1}^{1} \frac{f_n(x)}{\sqrt{1-x^2}}\,dx = \sum_{k=0}^{n} f(x_k) \underbrace{\int_{-1}^{1} \frac{L_k^n(x)}{\sqrt{1-x^2}}\,dx}_{\omega_k}$$

$$I = I_n, f(x) = f_n(x)$$

For $m > n$

$$f_m(x) = \sum_{k=0}^{n} f_m(x_k) L_k^n(x) + \underbrace{\prod_{j=0}^{n}(x - x_j)}_{p_{n+1}(x)} g_{m-(n+1)}$$

$$\underbrace{\int_{-1}^{1} \frac{f_m(x)}{\sqrt{1-x^2}}\,dx}_{=I} = \underbrace{\sum_{k=0}^{n} f_m(x_k)\omega_k}_{=I_n} + \underbrace{\int_{-1}^{1} \frac{p_{n+1}(x) g_{m-(n+1)}(x)}{\sqrt{1-x^2}}\,dx}_{=0}$$

Because the LHS is I and the left term on RHS is I_n, the right term of RHS must be zero.

Orthogonality:

$$\int_{-1}^{1} \frac{p_k(x) p_l(x)}{\sqrt{1-x^2}}\,dx = 0, \qquad k \neq l$$

Chebyshev polynomials, $x \in [-1, +1]$

$$T_k(x) = \cos(k \arccos(x)) \qquad k = 0, \ldots, n+1$$

Lemma.

$$\int_{-1}^{1} \frac{T_k(x) T_l(x)}{\sqrt{1-x^2}}\,dx = \begin{cases} 0 & k \neq l \\ \frac{\pi}{2} & k = l \neq 0 \\ \pi & k = l = 0 \end{cases}$$

Proof. This proof will be posted as exercise in the practicals course. □

Supporting points x_k:

$$T_{n+1}(x_k) = 0$$

$$x_k^{(n+1)} = \cos \frac{(1+2k)\pi}{2(n+1)} \text{ for } k = 0, \ldots, n$$

Integration weights:

$$\omega_k = \int_{-1}^{1} \frac{L_k^n(x)}{\sqrt{1-x^2}}\,dx \stackrel{?}{=} \text{ yet unknown}$$

Consider that

$$L_k^n(x) = \prod_{\substack{j=0 \\ j\neq k}}^{n} \frac{x - x_j}{x_k - x_j} = \sum_{i=0}^{n} \alpha_i T_i(x)$$

$$\int_{-1}^{1} \frac{L_k^n(x) T_j(x)}{\sqrt{1-x^2}}\, dx = \sum_{i=0}^{n} \alpha_i \underbrace{\int_{-1}^{1} \frac{T_i(x) T_j(x)}{\sqrt{1-x^2}}\, dx}_{=0, i\neq j} = \alpha_j \int_{-1}^{1} \frac{[T_j(x)]^2}{\sqrt{1-x^2}}\, dx = \alpha_j \begin{cases} \pi & j = 0 \\ \frac{\pi}{2} & j \neq 0 \end{cases}$$

$$\implies \alpha_0 = \frac{1}{\pi} \underbrace{\int_{-1}^{1} \frac{L_k^n(x)}{\sqrt{1-x^2}}\, dx}_{=\omega_k}$$

$$\omega_k = \alpha_0 \cdot \pi$$

$$\alpha_i = \frac{2}{\pi} \int_{-1}^{1} \frac{L_k^n(x) T_i(x)}{\sqrt{1-x^2}}\, dx$$

Let $f_{n+i} := L_k^n(x) T_i(x)$ of degree $n+1$ with $n+1 \leq 2n+1 = m$. Because the integration formula is accurate, we get

$$= \frac{2}{\pi} \sum_{l=0}^{n} L_k^n(x_l) T_i(x_l) \omega_l$$

$$\alpha_i = \frac{2}{\pi} T_i(x_k) \omega_k$$

$$\begin{aligned} \int_{-1}^{1} \frac{[L_k^n(x)]^2}{\sqrt{1-x^2}}\, dx &= \sum_{i=0}^{n} \sum_{j=0}^{n} \alpha_i \alpha_j \int_{-1}^{1} \frac{T_i(x) T_j(x)}{\sqrt{1-x^2}}\, dx \\ &= \pi \alpha_0^2 + \frac{\pi}{2} \sum_{i=1}^{n} \alpha_i^2 \\ &= \pi \frac{\omega_k^2}{\pi^2} + \frac{\pi}{2} \sum_{i=1}^{n} \frac{4}{\pi^2} [T_i(x_k)]^2 \omega_k^2 \end{aligned}$$

$$\frac{\left[L_k^n(x)\right]^2}{\sqrt{1-x^2}} = \sum_{l=0}^{n} \left[L_k^n(x_l)\right]^2 \omega_l = \omega_k$$

$$
\begin{aligned}
\omega_k &= \omega_k^2 \left[\frac{1}{\pi} + \frac{2}{\pi} \sum_{i=1}^{n} [T_i(x_k)]^2 \right] \\
\frac{1}{\omega_k} &= \frac{1}{\pi} + \frac{2}{\pi} \sum_{i=1}^{n} [T_i(x_k)]^2 \\
&= \frac{1}{\pi} + \frac{2}{\pi} \sum_{i=1}^{n} \left[\cos i \frac{(1+2k)\pi}{2(n+1)} \right]^2
\end{aligned}
$$

We know that $\left(\cos \frac{\alpha}{2}\right)^2 = \frac{1}{2}(1 + \cos \alpha)$.

$$
\begin{aligned}
&= \frac{1}{\pi} \left[1 + \sum_{i=1}^{n} \left(1 + \cos \frac{i(1+2k)\pi}{n+1} \right) \right] \\
&= \frac{n+1}{\pi} + \frac{1}{\pi} \underbrace{\sum_{i=1}^{n} \cos \frac{i(1+2k)\pi}{n+1}}_{=0}
\end{aligned}
$$

Why is the sum of the cosine zero? Make a case distinction with $n = 2m$ and $n = 2m + 1$.

$$
\Longrightarrow \int_{-1}^{1} \frac{f_m(x)}{\sqrt{1-x^2}}\, dx = \frac{\pi}{n+1} \sum_{k=0}^{n} f_m(x_k^{(n+1)})
$$

$$
\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\, dx = \frac{\pi}{n+1} \sum_{k=0}^{n} f(x_k^{(n+1)}) + \frac{1}{(2n+2)!} \int_{-1}^{1} \frac{f^{(2n+2)}(\eta(x))}{\sqrt{1-x^2}} \prod_{j=0}^{n} (x - x_j)^2\, dx
$$

$$
f_m = T_k(x) T_l(x), k, l \leq n, k + l \leq 2n < 2n + 1
$$

$$
\frac{\pi}{n+1} \sum_{j=0}^{n} T_k(x_j) T_l(x_j) = \int_{-1}^{1} \frac{T_k(x) T_l(x)}{\sqrt{1-x^2}}\, dx = \begin{cases} 0 & k \neq l \\ \frac{\pi}{2} & k = l \neq 0 \\ \pi & k = l = 0 \end{cases}
$$

$$
\sum_{j=0}^{n} T_k(x_j^{(n+1)}) T_l(x_j^{(n+1)}) = \begin{cases} 0 & k \neq l \\ \frac{n+1}{2} & k = l \neq 0 \\ n+1 & k = l = 0 \end{cases}
$$

So additionally to the above-mentioned orthogonality, we have discrete orthogonality.

This lecture took place on 2017/11/13.

At the beginning, we considered an interpolation task: $f(x), x \in [-1, +1], f_n(x) : f_n(x_k) = f(x_k)$ where $k = 0, n$.

$$f_n(x) = \underbrace{\sum_{k=0}^{n} a_k x^k}_{\text{Linear equation system}} = \sum_{k=0}^{n} f(x_k) L_k^n(x) = \underbrace{\sum_{k=0}^{n} \tilde{a}_k T_k(x)}_{\text{Linear equation system}}$$

For Chebyshev polynomials, we were able to determine coefficients directly.

Supporting points: $x_k : T_{n+1}(x_k) = 0$.

$$\max \left| \prod_{j=0}^{n} (x - x_j) \right| \to \min$$

Interpolation with Chebyshev polynomials in roots of T_{n+1}:

$$f_n(x_i^{(n+1)}) = \sum_{k=0}^{n} a_k T_k(x_i^{(n+1)}) = f(x_i^{(n+1)})$$

Can we solve this equation system efficiently?

In the second chapter, we considered integration formulae. We want to solve integrals of structure:

$$I = \int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, dx \simeq I_n = \frac{\pi}{n+1} \sum_{k=0}^{n} f(x_k^{(n+1)})$$

We derived a discrete orthogonality.

$$\sum_{i=0}^{n} T_k(x_i^{(n+1)}) T_l(x_i^{(n+1)}) = \begin{cases} 0 & k \neq l \\ n+1 & k = l = 0 \\ \frac{n+1}{2} & k = l \neq 0 \end{cases}$$

Linear equation system:

$$\sum_{k=0}^{n} a_k T_K(x_i^{(n+1)}) = f_i \qquad i = 0, n$$

The direct solution, e.g. using Gaussian elimination requires n^3 multiplications. We want to consider methods to come close to a linear number of multiplications (n multiplications).

Consider the multiplication with $T_l(x_i^{(n+1)})$ over $l = 0, n$:

$$\begin{aligned}
\sum_{k=0}^{n} a_k T_k(x_i^{(n+1)}) T_l(x_i^{(n+1)}) &= f_i T_l(x_i^{(n+1)}) \\
\implies \sum_{i=0}^{n} \sum_{k=0}^{n} a_k T_k(x_i^{(n+1)}) T_l(x_i^{(n+1)}) &= \sum_{i=0}^{n} f_i T_l(x_i^{(n+1)}) \\
\implies \sum_{k=0}^{n} a_k \sum_{i=0}^{n} T_k(x_i^{(n+1)}) T_l(x_i^{(n+1)}) &= \sum_{i=0}^{n} f_i T_l(x_i^{(n+1)})
\end{aligned}$$

This corresponds to our formula for discrete orthogonality. The left-hand side is zero, if $k \neq l$.

$$a_l \underbrace{\sum_{i=0}^{n} T_l(x_i^{(n+1)}) T_l(x_i^{(n+1)})}_{\substack{=n+1, l=0 \\ =\frac{n+1}{2}, l\neq 0}} = \sum_{i=0}^{n} f_i T_L(x_i^{(n+1)})$$

$$\begin{aligned}
\implies a_0 &= \frac{1}{n+1} \sum_{i=0}^{n} f_i \\
a_l &= \frac{2}{n+1} \sum_{i=0}^{n} f_i T_l(x_i^{(n+1)}), \qquad l = 1, n
\end{aligned}$$

We derived a formula to evaluate a_l directly. This is a matrix-vector multiplication requiring $O(n^2)$ multiplications.

Let us consider it for $l = 1, n$.

$$\begin{aligned}
a_l &= \frac{2}{n+1} \sum_{i=0}^{n} f_i T_l(x_i^{(n+1)}) \\
&= \frac{2}{n+1} \sum_{i=0}^{n} f_i \cos l \arccos x_i^{(n+1)} \text{ with } x_i^{(n+1)} = \cos \frac{\frac{\pi}{2} + i\pi}{n+1} = \cos \frac{(1+2i)\pi}{2n+2} \\
a_l &= \frac{2}{n+1} \sum_{i=0}^{n} f_i \cos \frac{l(1+2i)\pi}{2n+2} \qquad \text{for } l = 0, n
\end{aligned}$$

How can we efficiently determine these coefficients?

From now on, we generally consider the evaluation of the following expression:

$$a_k = \sum_{j=0}^{n-1} f_j \cos \frac{2\pi kj}{n} \qquad \text{where } k = 0, n-1$$

$$b_k = \sum_{j=0}^{n-1} f_j \sin \frac{2\pi kj}{n}$$

$$c_k = \sum_{j=0}^{n-1} f_j e^{-i2\pi kj/n}$$

Let $n = 2m$.

$$a_k = \sum_{j=0}^{n-1} f_j e^{-i2\pi kj/n} = \sum_{j=0}^{2m-1} f_j e^{-i\pi kj/m} \qquad k = 0, n-1$$

Let $k = 2l$.

$$a_{2l} = \sum_{j=0}^{m-1} f_j e^{-i\pi 2lj/m} = \sum_{j=0}^{m} f_j e^{-i2\pi lj/m} + \underbrace{\sum_{j=m}^{2m-1} f_j e^{-i2\pi lj/m}\, e^{-i2\pi l(m+j)/m}}_{= \underbrace{\sum_{j=0}^{m-1} f_{m+j}}_{e^{-i2\pi lk/m}} \underbrace{e^{-2\pi l}}_{=1}}$$

$$a_{2l} = \sum_{j=0}^{m-1} \left[f_j + f_{m+j} \right] e^{-i2\pi lj/m}$$

Consider $k = 2l + 1$.

$$
\begin{aligned}
a_{2l+1} &= \sum_{j=0}^{2m-1} f_j e^{-i\pi(2l+1)j/m} \\
&= \sum_{j=0}^{m-1} f_j e^{-i\pi(2l+1)j/m} + \sum_{j=0}^{m-1} f_{m+j} e^{-i\pi(2l+1)(j+m)/m} \\
&= \sum_{j=0}^{m-1} f_j e^{-i\pi(2l+1)j/m} + \sum_{j=0}^{m-1} f_{m+j} e^{-i\pi(2l+1)j/m} e^{-i\pi(2l+1)} \\
a_{2l+1} &= \sum_{j=0}^{m-1} \left[f_j + f_{m+j} \cdot \underbrace{e^{-i\pi(2l+1)}}_{=-1} \right] e^{-i\pi(2l+1)j/m} \\
&= \sum_{j=0}^{m-1} \left[f_j + f_{m+j} \cdot e^{-i\pi(2l+1)} \right] e^{-i2\pi lj/m} \cdot e^{-i\pi j/m} \\
&= \sum_{j=0}^{m-1} \left[f_j + f_{m+j} \cdot e^{-i\pi(2l+1)} \right] e^{-i2\pi lj/m} \cdot e^{-i2\pi j/n}
\end{aligned}
$$

Hence,

$$
\begin{aligned}
a_{2l} &= \sum_{j=0}^{m-1} \underbrace{\left[f_j + f_{m+j} \right]}_{:=\hat{f_j}} e^{-i2\pi lj/m} \\
a_{2l+1} &= \sum_{j=0}^{m-1} \underbrace{\left[f - f_{m+j} \right] e^{-i2\pi j/n}}_{:=\hat{f_{m+j}}} e^{-i2\pi l_j/m}
\end{aligned}
$$

with $m = 2r$. The computation of one sum over n summands is reduced to computing 2 sums over $\frac{n}{2}$ summands.

Example 9. *Consider $n = 8$.*

$$
a_k = \sum_{j=0}^{7} f_j e^{-i2\pi kj/8} \qquad \textit{for } k = 0, 7
$$

$$
\begin{aligned}
a_0 &: f_0^1 = f_0 + f_4 \\
a_2 &: f_1^1 = f_1 + f_4 \\
a_4 &: f_2^1 = f_2 + f_4 \\
a_6 &: f_3^1 = f_3 + f_4 \\
\hline
a_1 &: f_4^1 = (f_0 - f_4)\omega_8^0 \\
a_3 &: f_5^1 = (f_1 - f_5)\omega_8^1 \\
a_5 &: f_6^1 = (f_2 - f_6)\omega_8^2 \\
a_7 &: f_7^1 = (f_3 - f_7)\omega_8^3
\end{aligned}
$$

$$
\begin{aligned}
a_0 &: f_0^2 = f_0^1 + f_2^1 \\
a_4 &: f_1^2 = f_1^1 + f_3^1 \\
\hline
a_2 &: f_2^2 = (f_0^1 - f_2^1)\omega_4^0 \\
a_6 &: f_3^2 = (f_1^1 - f_3^1)\omega_4^1 \\
\hline
a_1 &: f_4^2 = f_4^1 + f_6^1 \\
a_5 &: f_5^2 = f_5^1 + f_7^1 \\
\hline
a_3 &: f_6^2 = (f_4^1 - f_6^1)\omega_4^0 \\
a_7 &: f_7^2 = (f_5^1 - f_7^1)\omega_4^1
\end{aligned}
$$

$$
\begin{aligned}
a_0 &: f_0^3 = f_0^2 + f_1^2 \\
a_4 &: f_1^3 = f_0^2 + f_1^2 \\
\hline
a_2 &: f_2^3 = f_2^2 + f_3^2 \\
a_6 &: f_3^3 = f_2^2 - f_3^2 \\
\hline
a_3 &: f_6^3 = f_6^2 + f_7^2 \\
a_7 &: f_7^3 = f_6^2 + f_7^2
\end{aligned}
$$

One problem remains: The order of evaluation is mixed up. Is there any law behind the order? Consider that $n = 8$, hence every coefficient is one of $k = 0, 7$. So we can

represent k as $k = c_0 \cdot 2^0 + c_1 \cdot 2^1 + c_2 \cdot 2^2 = c_0 + 2c_1 + 4c_2$ *where* $c_i \in \{0, 1\}$.

$f_0^3 : 0000$	0000	a_0
$f_1^3 : 1100$	0014	a_4
$f_2^3 : 2010$	0102	a_2
$f_3^3 : 3110$	0116	a_6
$f_4^3 : 4001$	1001	a_1
$f_5^3 : 5101$	1015	a_5
$f_6^3 : 6011$	1103	a_3
$f_7^3 : 7111$	1117	a_7

Optimal recursion for $n = 2^p$: Required resources to compute $p\frac{n}{2} = \frac{n}{2} \ln n$ multiplications.

In general, we can do a prime number decomposition for n. In the worst case, n is a prime number. What we did is the "Fast Discrete Fourier Transformation"[2].

This lecture took place on 2017/11/15.

A small excursion: Vectors and matrices

Let $n \in \mathbb{N}, \underline{u} \in \mathbb{R}^n, \underline{u} = (u_i)_{i=1}^n, u_i \in \mathbb{R}$. The scalar product is defined as $\langle \cdot, \cdot \rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$. The Euclidean product is defined as $(\cdot, \cdot) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$.

$$(\underline{u}, \underline{v}) := \sum_{k=1}^{n} u_i v_i = \langle \underline{u}, \underline{v} \rangle_2$$

Norm: $\| \cdot \|_V : \mathbb{R}^n \to \mathbb{R}_+$

3 examples of norms:

1. Euclidean norm (for a vector a 2-norm): $\left\| \underline{u} \right\|_2 := \left(\sum_{i=1}^n u_i^2 \right)^{\frac{1}{2}} = \sqrt{(\underline{u}, \underline{u})}$
2. Maximum norm: $\left\| \underline{u} \right\|_\infty := \max_{i=1,n} |u_i|$
3. Sum norm: $\left\| \underline{u} \right\|_1 := \sum_{i=1}^n |u_i|$

[2] one historical implementation is *FFTPACK*

Cauchy-Schwarz inequality:

$$\begin{aligned}(\underline{u}, \underline{v}) &= \sum_{i=1}^{n} u_i v_i \\ &\leq \left(\sum_{i=1}^{n} u_i^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^{n} v_i^2\right)^{\frac{1}{2}}\end{aligned}$$

Definition. *Two norms* $\|\cdot\|_1$ *and* $\|\cdot\|_2$ *are called* equivalent*, if*

$$c_1 \left\|\underline{u}\right\|_1 \leq \left\|\underline{u}\right\|_2 \leq c_2 \left\|\underline{u}\right\|_1 \forall \underline{u} \in \mathbb{R}^n$$

with constants c_1 *and* c_2 *independent of* $\underline{u}$*, but they can depend on* n*. This inequality is called* precise*, if for certain* $\underline{u} \in \mathbb{R}^n$ *equality holds with* $\left\|\underline{u}\right\| > 0$*.*

Lemma. $\forall \underline{u} \in \mathbb{R}^n$*:*

$$\begin{aligned}\left\|\underline{u}\right\|_\infty \leq \left\|\underline{u}\right\|_1 &\leq n \left\|\underline{u}\right\|_\infty \\ \left\|\underline{u}\right\|_\infty \leq \left\|\underline{u}\right\|_2 &\leq \sqrt{n} \left\|\underline{u}\right\|_\infty \\ \left\|\underline{u}\right\|_2 \leq \left\|\underline{u}\right\|_1 &\leq \sqrt{n} \left\|\underline{u}\right\|_2\end{aligned}$$

All these inequalities are precise. The proof will be provided in the practicals.

Let $B \in \mathbb{R}^{m \times n}, B[K, l] = b_{Kl} \in \mathbb{R}, k \in \{1, \ldots, m\}, l \in \{1, \ldots, n\}$.

Matrix norm:	$\|\cdot\|_M : \mathbb{R}^{m \times n} \to \mathbb{R}_x$
Row sum norm:	$\|B\|_\infty = \max_{k=1,m} \sum_{l=1}^{n} \|b_{Kl}\|$
Column sum norm:	$\|B\|_1 = \max_{l=1,n} \sum_{k=1}^{n} \|b_{Kl}\|$
Frobenius norm (also Hilbert-Schmid norm):	$\|B\|_{\mathcal{F}} = \left(\sum_{k=1}^{m} \sum_{l=1}^{n} b_{Kl}^2\right)^{\frac{1}{2}}$

For a vector norm defined in $\mathbb{R}^n$ and $\mathbb{R}^m$, an *induced matrix norm* is

$$\|B\|_M := \sup_{\underline{0} \neq \underline{u} \in \mathbb{R}^n} \frac{\left\|B\underline{u}\right\|_V}{\left\|\underline{u}\right\|_V}$$

Especially,

$$\|B\|_2 := \sup_{\underline{0} \neq \underline{u} \in \mathbb{R}^n} \frac{\left\|B\underline{u}\right\|_2}{\left\|\underline{u}\right\|_2}$$

defines an *Euclidean matrix norm*.

Lemma. *The row sum norm is induced by the maximum norm. The column sum norm is induced by the sum norm.*

Proof. Will be provided in the practicals. □

Matrix norm $\|\cdot\|_M$ is called *compatible* with vector norm $\|\cdot\|_V$, if

$$\left\|B\underline{u}\right\|_V \leq \|B\|_M \left\|\underline{u}\right\|_V \qquad \forall \underline{u} \in \mathbb{R}^n$$

Every induced matrix norm is compatible with its inducing vector norm.

Remark. *Frobenius norm is compatible with the Euclidean vector space, but is not induced by* any *vector norm.*

Proof. Will be provided in the practicals. □

Let $V \in \mathbb{R}^{n\times n}$, i.e. $U \in \mathbb{R}^{m\times m}$. These are called *orthogonal*, if

$$V^T V = VV^T = I_n \in \mathbb{R}^{n\times n}$$
$$U^T U = UU^T = I_m \in \mathbb{R}^{m\times m}$$

Conclusions:

$$\underline{u} \in \mathbb{R}^n, \left\|V\underline{u}\right\|_2 = \left\|\underline{u}\right\|_2$$
$$\|B\|_2 = \|BV\|_2 = \|UB\|_2 = \|UBV\|_2$$

Hence, they are invariant in terms of orthogonal transformations.

It also holds that

$$\|B\|_{\mathcal{F}} = \|UB\|_{\mathcal{F}} = \|BV\|_{\mathcal{F}} = \|UBV\|_{\mathcal{F}}$$

Let $A \in \mathbb{R}^{n\times n}$ be invertible.

$$K_m(A) := \|A\|_M \left\|A^{-1}\right\|_M$$

where $K_m(A)$ is called *condition in terms of* $\|\cdot\|_M$

$$\kappa_2(A) := \|A\|_2 \left\|A^{-1}\right\|_2$$

is called *spectral condition number*

Family of $A \in \mathbb{R}^{n\times n}$ $(n \to \infty)$ is badly conditioned, if $K_2(A) \to \infty$ (as $n \to \infty$). Hint: Uniform grids are well conditioned whereas adaptive grids are badly conditioned.

This lecture took place on 2017/10/20.

3.2 Eigenvalue und singular values

Let $A \in \mathbb{R}^{n\times n}$. $\lambda(A)$ is the *eigenvalue* of A if the equation $Av = \lambda(A)\underline{v}$ has a non-trivial solution $\underline{v} \in \mathbb{R}^n$. Eigenvalues result from the roots of the characteristic polynomial.

$$p(\lambda) = \det(A - \lambda I) = \prod_{k=1}^{\mu} (\lambda_k(A) - \lambda)^{\alpha_k}$$

with μ pairwise different Eigenvalues λ_k of the algebraic multiplicities α_k, $\sum_{k=1}^{\mu} \alpha_k = n$.

$$\lambda_k \in \mathbb{C} \implies \overline{\lambda_k} \text{ is also a eigenvector}$$

The associated eigenvectors for eigenvalue $\lambda_k(A)$ construct a linear subspace:

$$\mathcal{L}(\lambda_k(A)) = \left\{\underline{x} \in \mathbb{R}^n | A\underline{x} = \lambda_k(A)\underline{x}\right\}$$

$$\beta_k := \dim(\mathcal{L}(\lambda_k(A)))$$

β_k is called *geometric multiplicity*. Spectral radius:

$$\gamma(A) := \max_{k=1,\mu \leq n} |\lambda_k(A)|$$

If $A = A^T$, then eigenvalue λ_k is real, eigenvectors $\left\{\underline{v}^k\right\}_{k=1}^n$ create an orthonormal system. $(\underline{v}^k, \underline{v}^l) = \delta_{kl}$.

Let $\underline{x} \in \mathbb{R}^n$.

$$\underline{x} = \sum_{k=1}^n \gamma_k \underline{v}^k \qquad \gamma_k = (\underline{x}, \underline{v}^k)$$

$$(\underline{x}, \underline{v}^l) = \sum_{k=1}^n \gamma_k (\underline{v}^k, \underline{v}^l) = \gamma_l$$

$$\left\|\underline{x}\right\|_2^2 = (\underline{x}, \underline{x}) = (\sum_{k=1}^n \gamma_k \underline{v}^k, \sum_{l=1}^n \gamma_l \underline{v}^l) = \sum_{k=1}^n \sum_{l=1}^n \gamma_k \gamma_k \underbrace{(\underline{v}^k, \underline{v}_l)}_{\delta_{kl}} = \sum_{k=1}^n \gamma_k^2$$

$$(A\underline{x}, \underline{x}) = \left(A \sum_{k=1}^n \gamma_k \underline{v}^k, \sum_{l=1}^n \gamma_l \underline{v}^l\right) = \sum_{k=1}^n \sum_{l=1}^n \gamma_k \gamma_l \underbrace{(A\underline{v}^k, \underline{v}^l)}_{=\lambda_k(\underline{v}^k, \underline{v}^l) = \lambda_k \delta_{kl}} = \sum_{k=1}^n \lambda_k(A) \gamma_k^2$$

$A = A^T$ is called positive definite, if $\lambda_k(A) > 0 \forall k = 1, \ldots, n$.

$$\implies (A\underline{x}, \underline{x}) = \sum_{k=1}^n \lambda_k(A) \underbrace{\gamma_k^2}_{\geq 0} \geq \min_{k=1,n} \lambda_k(A) \sum_{k=1}^n \gamma_k^2 = \lambda_{\min}(A)(\underline{x}, \underline{x})$$

$(\underline{x}, \underline{x}) > 0$,

$$\lambda_{\min}(A) \leq \frac{(A\underline{x}, \underline{x})}{(\underline{x}, \underline{x})} \qquad \forall \underline{x} \in \mathbb{R}^n, \|x\| > 0$$

$$\lambda_{\min}(A) = \min_{\underline{0} \neq \underline{x} \in \mathbb{R}^n} \frac{(A\underline{x}, \underline{x})}{(\underline{x}, \underline{x})}$$

$$\lambda_{\max}(A) = \max_{\underline{0} \neq \underline{x} \in \mathbb{R}^n} \frac{(A\underline{x}, \underline{x})}{(\underline{x}, \underline{x})} \text{ is called } \textit{Rayleigh quotient}$$

If the so-called *spectral equivalence inequalities* hold, it holds that

$$c_1^A(\underline{x},\underline{x}) \leq (A\underline{x},\underline{x}) \leq c_2^A(\underline{x},\underline{x})$$

$$\implies c_1^A \leq \frac{(A\underline{x},\underline{x})}{(\underline{x},\underline{x})} \leq c_2^A \qquad \forall \underline{x} \neq \underline{0}$$

$$\implies c_1^A \leq \lambda_{\min}(A) \leq \lambda_{\max}(A) \leq c_2^A$$

$A = A^T > 0$ is symmetrical and positive definite. Then

$$\langle \underline{u},\underline{v}\rangle = (A\underline{u},\underline{v}) = (\underline{u},A\underline{v})$$

defines the so-called *A-energetic scalar product* and the induced vector norm

$$\left\|\underline{x}\right\|_A = \sqrt{(A\underline{x},\underline{x})}$$

$$A\underline{v}^k = \lambda_k \underline{v}^k, A = A^T > 0, \left\{\underline{v}^k\right\}_{k=1}^n \text{ orthonormal system}$$

$$V = (\underline{v}^1, \underline{v}^2, \ldots, \underline{v}^n) \in \mathbb{R}^{n\times 1}$$

$$AV = (A\underline{v}^1, A\underline{v}^2, \ldots, A\underline{v}^n) = (\lambda_1\underline{v}^1, \lambda_2\underline{v}^2, \ldots, \lambda_n\underline{v}^n)$$

$$= (\underline{v}^1, \underline{v}^2, \ldots, \underline{v}^n)\begin{pmatrix}\lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n\end{pmatrix} = VD$$

$D = \operatorname{diag}(\lambda_k)$.

$$AV = VD \implies D = V^TAV \wedge A = VDV^T$$

$$VDV^T = \sum_{k=1}^n \lambda_k \underline{v}^k \underline{v}^{k,T}$$

I have a memory requirement of $O(n^2)$.

$$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_r \ggg \lambda_{r+1} \geq \ldots \geq 0$$

$$A_r = \sum_{k=1}^r \lambda_k \underline{v}^k \underline{v}^{k,T}$$

If $r \ll n$, we have a memory requirement of $O(\sqrt{n})$. This is called a *low rank approximation*.

Is invertability of A required, blockwise approximation, $\mathcal{H}$ matrices, hierarchical matrices.

$$A = VDV^T, D = \operatorname{diag}(\lambda_k), \lambda_k > 0$$

$$D^{\frac{1}{2}} := \operatorname{diag}(\sqrt{\lambda_k}), D^{\frac{1}{2}} \cdot D^{\frac{1}{2}} = D, (D^{\frac{1}{2}})^{-1} = \operatorname{diag}(\frac{1}{\sqrt{\lambda_k}}) = D^{-\frac{1}{2}}$$

$$A^{\frac{1}{2}} = VD^{\frac{1}{2}}V^T$$

$$A^{\frac{1}{2}} = A^{\frac{1}{2}} = V \underbrace{D^{\frac{1}{2}} \underbrace{V^T V}_{=I} D^{\frac{1}{2}}}_{D} V^T = VDV^T = A$$

This is purely theoretical approach and in the future, we will try to avoid using A.

$$\|A\|_2 = \left\|VDV^T\right\|_2 = \|D\|_2 = \max_{0 \neq \underline{x} \in \mathbb{R}^n} \frac{\left\|D\underline{x}\right\|_2}{\|x\|_2} = \lambda_{\max}(A) = \delta(A) \qquad A = A^T > 0$$

$A = A^T > 0$:

$$\kappa_2(A) = \|A\|_2 \left\|A^{-1}\right\|_2 = \delta(A)\delta(A^{-1}) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \leq \frac{c_2^A}{c_1^A} \ldots \text{spectral length equivalence inequality}$$

Let $B \in \mathbb{R}^{m \times n}$ with $\operatorname{rang}(B) \leq \min\{m, n\}$. We take $A = B^T B \in \mathbb{R}^{n \times n}$ and by construction, $A = A^T$.

$$\operatorname{rang}(A) \leq \min\{m, n\}$$

Then it follows that,

$$0 \leq \left\|B\underline{x}\right\|_2^2 = (B\underline{x}, B\underline{x}) = (B^T B\underline{x}, \underline{x}) = (A\underline{x}, \underline{x})$$

$$= \sum_{k=1}^{n} \lambda_k \gamma_k^2 \implies \lambda_k \geq 0$$

$$A = VDV^T$$

$$D = V^T AV = V^T B^T BV = \begin{pmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} in \mathbb{R}^{n \times n}, \lambda_k > 0, k = 1, r$$

$$\sigma_k = \sqrt{\lambda_k(A)} = \sqrt{\lambda_k(B^T B)} \geq 0$$

$$k = 1, \min\{m, n\}, \sigma_k(B) > 0, k = 1, r$$

σ_k is called *singular value*.

$$D = \begin{pmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_r & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{pmatrix} = \underbrace{\begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{r_0} \end{pmatrix}}_{\Sigma^T : n \times m} \cdot \underbrace{\begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{r_0} \end{pmatrix}}_{\Sigma : m \times n} ?????$$

$$D = \Sigma^T \Sigma$$

$$\Sigma = \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{pmatrix} \in \mathbb{R}^{m \times n}$$

Pseudo inverse:

$$\Sigma^+ = \begin{pmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_r} \end{pmatrix} \in \mathbb{R}^{n \times m}, \Sigma^+ \Sigma = \begin{pmatrix} I_r & \\ & \end{pmatrix} \in \mathbb{R}^{n \times n}$$

$$V^T B^T B V = D = \Sigma^T \Sigma$$

$$\implies \Sigma = \underline{\Sigma^{T,+} V^T B^T}_{U^T} B V = U^T B V$$

$$U = B V \Sigma^+ \in \mathbb{R}^{m \times m}, U^T U = \Sigma^{T,+} \underbrace{V^T \underbrace{B^T B}_{A} V}_{D} \Sigma^+ = I_m, V^T V = I_n$$

$$\implies B = U \Sigma V^T = \sum_{k=1}^{r} \sigma_k \underline{u}^k \underline{v}^{k,t}$$

This is the so-called *singular value decomposition*.

3.3 Orthogonalization of vector systems

Consider $\mathbb{R}^n$. $\left\{\underline{w}^k\right\}_{k=0}^{n-1}$ linear independent. We want to construct an orthogonal vector system $\left\{\underline{p}^k\right\}_{k=0}^{n-1}$. Gram-Schmidt

$$\underline{p}^0 = \underline{w}^0$$

For $k = 0, \ldots, n-2$, we determine $\underline{p}^{k+1} = \underline{w}^{k-1} - \sum_{l=0}^{k} \beta_{k,l} \underline{p}^l$ and $\beta_{k,l} = \frac{(\underline{w}^{k-1}, \underline{p}^l)}{(\underline{p}^l, \underline{p}^l)}$ We will see that it makes a huge difference which initial vector system is given.

Consider any $A \in \mathbb{R}^{n\times n}$ where A is invertible and $\operatorname{rank}(A) = n$.

$$A = (\underline{a}^1, \dots, \underline{a}^n)$$

$$\underline{\hat{v}}^k = \underline{a}^k - \sum_{l=1}^{k-1} (\underline{a}^k, \underline{v}^k)\underline{v}^l, \underline{v}^k = \frac{\underline{\hat{v}}^k}{\left\|\underline{\hat{v}}\right\|_2}$$

$$\implies \underline{a}^k = \left\|\underline{\hat{v}}^k\right\|_2 \underline{v}^k + \sum_{l=1}^{k-1} (\underline{a}^k, \underline{v}^l)\underline{v}^l \qquad k = 1, n$$

$$A = QR$$

$$Q^T Q = I, R = \text{(some upper triangular matrix)}$$

QR decomposition.

$A = A^T > 0$ $(A\underline{u}, \underline{v})$ is a scalar product.

$$\left\{\underline{p}^k\right\}_{k=0}^{n-1} : (A\underline{p}^k, \underline{p}^l) = 0, k \neq l$$

$$(A\underline{p}^k, \underline{p}^k) > 0$$

A-orthogonal, conjugated.

This lecture took place on 2017/11/22.

4. Linear equation system

We consider a family of linear equation systems, $A\underline{x} = \underline{f}$ with $A \in \mathbb{R}^{n\times n}, \underline{f} \in \mathbb{R}^n, \underline{x} \in \mathbb{R}^n$ for $n \to \infty$. Or: how do computational requirements behave when n is doubled? For all $n \in \mathbb{N}$, matrix $A \in \mathbb{R}^{n\times n}$ originates from a given problem setting, e.g. the L_2-projection.

Prerequisite: A is regular and invertible, hence has a unique solution.

Direct approaches Gaussian elimination, LR decomposition

Classical approaches Jacobi, Gauss-Seidel, successive over-relaxation (SOR method)

Gradient approaches (this will not be covered in this lecture)

Conjugate gradient method $A = A^T > 0$, or in general: generalized minimal residual method (GMRES)

Direct approaches

Gaussian elimination

We can easily solve matrices of upper triangular structure.

$$A\underline{x} = \underline{f}$$

$$\begin{pmatrix} a_{0,0} & a_{0,1} & \dots & a_{0,n} \\ 0 & a_{1,1} & \dots & a_{1,n} \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & a_{m,n} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{pmatrix}$$

We have to transform a general matrix into an upper triangular matrix.

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \dots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \dots & a_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \dots & a_{n,n} \end{pmatrix}$$

How can we achieve $\begin{pmatrix} a_{2,1} \\ a_{3,1} \\ \vdots \\ a_{n,1} \end{pmatrix} \overset{!}{=} \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$? We transform the first column values below the diagonal value to zero:

$$(\hat{2}) := (2) - \frac{a_{21}}{a_{11}}(1)$$

$$(\hat{f_2}) := (f_2) - \frac{a_{21}}{a_{11}}(f_1)$$

$$(\hat{3}) := (3) - \frac{a_{31}}{a_{11}}(1)$$

This goes on and on. Let's write it down in an algorithm:

Gaussian algorithm without pivotization

```
Preprocessing:

for i = 1, n-1 do    # iterate rows
  for j = i+1,n do   # iterate columns
    alpha := a_{ji} / a_{ii}
    for k = i,n do
```

```
      {\hat a}_{jk} := a_{jk} - alpha * a_{ik}
    {\hat f}_j := f_j - alpha * f_i

Backwards insertion:

x_n := f_n / a_{nn}
for i = n-1,1 do
  alpha = 0
  for j = i+1,n do
    alpha = alpha + a_{ij} * x_j
  x_i = 1/a_{ii} * (f_i - alpha)
```

What are the computational requirements? For the computer the *essential operations* are counted (multiplication and division for this algorithm). We have 6 multiplications and divisions in this algorithm. We will do an analysis.

For the preprocessing step:

$$\begin{aligned}
\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\left[1+\underbrace{\sum_{k=i}^{n}1}_{=n+1-i}+1\right] &= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(n+3-i)\\
&= \sum_{i=1}^{n-1}(n+3-i)(n-i)\\
&= \sum_{i=1}^{n-1}(n^2-(2n+3)i+i^2+3n)\\
&= n^2(n-1)+3n(n-1)-(2n+3)\underbrace{\sum_{i=1}^{n-1}i}_{\frac{1}{2}n(n-1)}+\underbrace{\sum_{i=1}^{n-1}i^2}_{\frac{1}{6}(n-1)n(2(n-1)+1)}\\
&= n^3(1-1+\frac{1}{3})+O(n^2)=\frac{1}{3}n^3+O(n^2)
\end{aligned}$$

Hence, we have cubic computational requirements.

For the backwards insertion:

$$1+\sum_{i=1}^{n-1}\left(\sum_{i=1}^{n}1+1\right)=1+\sum_{i=1}^{n-1}(n-i+1)=\frac{1}{2}n^2+O(n)$$

What do these estimates mean? We consider *time units*. One operation takes one unit of time (e.g. seconds). What does doubling of n mean?

$$n\to 2n,\ \frac{1}{3}n^3\to 8\left(\frac{1}{3}n^3\right)$$

$$n \to 1, 2n \to 8, 4n \to 64, 8n \to 3840$$

But what happens to the matrix? Can we improve our algorithm?

Fill-In happens. This means that entries, which have been zero before, become non-zero during the execution.

This lecture took place on 2017/11/27.

No lecture, because of the first practicals exam.

This lecture took place on 2017/11/29.

We continue with the topic of Gaussian elimination.

$$A := \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}$$

Can we describe the Gaussian elimination applied to A as a matrix multiplication?

$$L_1 := \begin{pmatrix} 1 & \dots & & \\ -\frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ \frac{a_{n1}}{a_{11}} & & & 1 \end{pmatrix}$$

$$L_2 := \begin{pmatrix} 1 & \dots & & \\ & 1 & & \\ & -\frac{a_{31}}{a_{22}} & & \\ \vdots & & \ddots & \\ & & & 1 \end{pmatrix}$$

Then

$$L_{n-1} \cdot \ldots \cdot L_2 \cdot L_1 A = R$$

$$L_1 = \begin{pmatrix} 1 & & & \\ -\frac{a_{21}}{a_{11}} & \ddots & & \\ \vdots & & \ddots & \\ -\frac{a_{n1}}{a_{11}} & & & 1 \end{pmatrix} = \begin{pmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{pmatrix} - \begin{pmatrix} 0 \\ \frac{a_{21}}{a_{11}} \\ \vdots \\ \frac{a_{n1}}{a_{11}} \end{pmatrix} = I - \underline{a}_1 \underline{b}_1^T$$

- Rank 1 disruption of the identity matrix (dt. Rang 1 Stöerung der Einheitsmatrix)
- Elementarmatrix

$$
\begin{aligned}
L_k &= I - \underline{a}_k \underline{b}_k^T \\
R &= \underbrace{(I - \underline{a}_{n-1}\underline{b}_{n-1}^T) \dots (I - \underline{a}_1 \underline{b}_1^T)}_{\text{inverse matrix}} A \\
L &= I - \underline{ab}^T
\end{aligned}
$$

How to get the inverse of L, L^{-1}? We have an idea:

$$
\begin{aligned}
L^{-1} &= I + \alpha \underline{ab}^T \\
I &= L^{-1}L = (I + \alpha \underline{ab}^T)(I - \underline{ab}^T) \\
&= I + \alpha \underline{ab}^T - \underline{ab}^T - \alpha \underline{ab}^T \underline{ab}^T \\
&= I + \underbrace{(\alpha - 1 - \alpha \underline{b}^T \underline{a})}_{\alpha(1-\underline{b}^T\underline{a})-1} \underline{ab}^T = I
\end{aligned}
$$

if $\alpha = \frac{1}{1-\underline{b}^T\underline{a}}$, $\underline{b}^T \underline{a} \neq 1$.

$$
\begin{aligned}
L_k = I - \underline{a}_k \underline{b}_k^T \implies \underline{b}_k^T \underline{a}_k = 0 \\
\implies L_k^{-1} = (I + \underline{a}_k \underline{b}_k^T) \\
\implies A = (I + \underline{a}_1 \underline{b}_1^T)(I + \underline{a}_2 \underline{b}_2^T) \dots (I + \underline{a}_{n-1}\underline{b}_{n-1}^T) R
\end{aligned}
$$

This is a LU decomposition.

Hence, we have a direct procedure to derive the LU decomposition of A.

$$
A = LR = \begin{pmatrix} 1 & & & 0 \\ b_1 & \ddots & & \\ \vdots & & \ddots & \\ \vdots & & & \ddots \\ b_{n_1} & \dots & \dots & 1 \end{pmatrix} \begin{pmatrix} r_{11} & \dots & \dots & r_{1n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ \vdots & 0 & & \ddots \\ & \dots & \dots & r_{nn} \end{pmatrix} = \begin{pmatrix} a_{11} & \dots & a_{1n} \\ a_{21} & \dots & a_{2n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{pmatrix}
$$

$$
r_{11} = a_{11} \qquad a_{21} = b_{21} r_{11} \implies l_{21} = \frac{a_{21}}{r_{11}} \qquad \dots
$$

$$
i < j = 1, n; r_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} r_{kj}
$$

$$i > j : l_{ij} = \frac{1}{r_{jj}} \left[a_{ij} - \sum_{k=1}^{j-1} l_{ik} r_{kj} \right]$$

This approach actually takes computational resources of $O(\frac{2}{3}n^3)$.

Solve the linear equation system $A\underline{x} = \underline{f}$, $A = LR$.

$$L \underbrace{R\underline{x}}_{\underline{z}} = \underline{f}$$

$$L\underline{z} = \underline{f}$$
$$R\underline{x} = \underline{z}$$

where L is an upper triangular matrix and R a lower triangular matrix.

This approach is useful for multiple computations of the linear equation system for various right-hand matrices (if not simultaneous).

Applications:

$$\begin{pmatrix} A_1 & & B_1 \\ & A_2 & B_2 \\ B_1^T & B_2^T & D \end{pmatrix} \begin{pmatrix} \underline{U}_1 \\ \underline{U}_2 \\ \underline{U}_3 \end{pmatrix} = \begin{pmatrix} \underline{f}_1 \\ \underline{f}_2 \\ \underline{f}_3 \end{pmatrix}$$

$$A_1 \underline{u}_1 + B_1 \underline{u}_3 = \underline{f}_1$$

$$\underline{u}_1 = A_1^{-1} \left[f_1 - B_1 \underline{u}_3 \right]$$

$$\underline{u}_2 = A_2^{-1} \left[f_2 - B_2 \underline{u}_3 \right]$$

$$\underline{f}_3 = D\underline{u}_3 + B_1^T \underline{u}_1 + B_2^T \underline{u}_2 = D\underline{u}_3 - B_1^T A_1^{-1} B_1 \underline{u}_3 - B_2^T A_2^{-1} B_2 \underline{u}_3 + B_1^T A_1^{-1} \underline{f}_1$$

$$\underbrace{\left(D - B_1^T A_1^{-1} B_1 - B_2^T A_2^{-1} B_2 \right)}_{S = S^T > 0} \underline{u}_3 = \underline{f}_3 - B_1^T A_1^{-1} \underline{f}_1 - B_2^T A_2^{-1} \underline{f}_2$$

which leads us to the CG method.

If a symmetrical, positive definite matrix A is given, then we can modify the procedure. We can decompose A with LL^T, a Cholesky decomposition.

This lecture took place on 2017/12/04.

Recall: $Ax = f$, $A \in \mathbb{R}^{n \times n}$ is regular, $f \in \mathbb{R}^n$.

In the following, we consider the transformation of a given matrix A to triangular form using *orthogonal matrices*. First, we consider the Householder transformation.

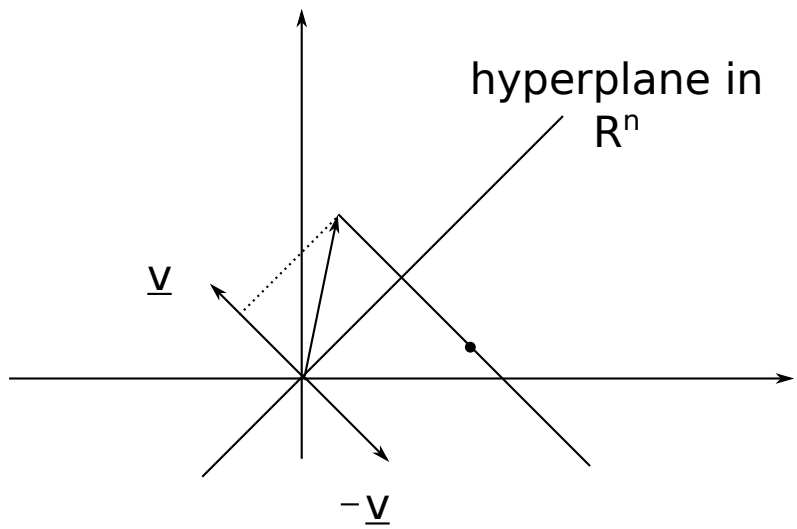


Figure 11: Transformation P

Householder transformation

First, for given $\underline{v} \in \mathbb{R}^n$ consider the symmetrical transformation

$$P(v) = I - \frac{2}{v^T v} v v^T \in \mathbb{R}^{n \times n}$$

Figure 11 illustrates the transformation.
with

$$\begin{aligned} P^T P &= \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \\ &= I - \frac{4}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T + \frac{4}{(\underline{v}^T \underline{v})^2} \underline{v}\underline{v}^T \underline{v}\underline{v}^T = I \end{aligned}$$

It holds that

$$P\underline{v} = \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \underline{v} = \underline{v} - 2\underline{v} = -\underline{v}$$

and for $\underline{w}$ with $\underline{v}^T \underline{w} = 0$:

$$P\underline{w} = \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \underline{w} = \underline{w}$$

For an arbitrary vector $\underline{x} \in \mathbb{R}^n$,

$$\underline{x} = \frac{\underline{x}^T \underline{v}}{\underline{v}^T \underline{v}} \underline{v} + \frac{\underline{x}^T \underline{w}}{\underline{w}^T \underline{w}} = \underline{w}$$

and therefore

$$P\underline{x} = \frac{\underline{x}^T \underline{v}}{\underline{v}^T \underline{v}} P\underline{v} + \frac{\underline{x}^T \underline{w}}{\underline{w}^T \underline{w}} P\underline{w} = -\frac{\underline{x}^T \underline{v}}{\underline{v}^T \underline{v}} \underline{v} + \frac{\underline{x}^T \underline{w}}{\underline{w}^T \underline{w}} \underline{w}$$

Hence, the Householder transformation p describes a reflection of $\underline{x}$. For the transformation of a given matrix A is upper triangular form, we consider the transformation of the first column $\underline{a}$ of A to a multiple of the first unit vector $\underline{e}$, i.e.

$$P\underline{a} = \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \underline{a} \overset{!}{=} \alpha \underline{e}$$

First step, we want to find a transformation P achieving the following transformation (as it turns out, this is the transformation P from above)

$$P\left(\begin{pmatrix} * & \dots & * \\ \vdots & & \vdots \\ * & \dots & * \end{pmatrix} \right) = \begin{pmatrix} * & * & \dots & * \\ 0 & * & & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & * & \dots & * \end{pmatrix}$$

The first columns are $\underline{a}$ and $\alpha \cdot \underline{e}$ respectively.

Question: For which $\underline{v}$ does $P\underline{a} = \alpha \underline{e}$ hold?

$$\underline{a} - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \underline{a} = \underline{a} - 2\frac{\underline{v}^T \underline{a}}{\underline{v}^T \underline{v}} \underline{v} \overset{!}{=} \alpha \underline{e}$$

i.e.

$$\underline{v} = \gamma(\underline{a} - \alpha \underline{e})$$

Because the definition of P contains the normalization of $\underline{v}$, it can be chosen that

$$\underline{v} = \underline{a} - \alpha \underline{e}$$

So, from

$$\begin{aligned} \alpha \underline{e} = P\underline{a} &= \left(I - \frac{2}{\underline{v}^T \underline{v}} \underline{v}\underline{v}^T \right) \underline{a} \\ &= \underline{a} - 2\frac{\underline{v}^T \underline{a}}{\underline{v}^T \underline{v}} \underline{v} \\ &= \underline{a} - 2\frac{\underline{v}^T \underline{a}}{\underline{v}^T \underline{v}} (\underline{a} - \alpha \underline{e}) \\ &= \left(1 - 2\frac{\underline{v}^T \underline{a}}{\underline{v}^T \underline{v}} \right) \underline{a} + 2\frac{\underline{v}^T \underline{a}}{\underline{v}^T \underline{v}} \alpha \underline{e} \end{aligned}$$

it follows that

$$2\underline{v}^T\underline{a} = \underline{v}^T\underline{v}$$

With

$$\begin{aligned}\underline{v}^T\underline{v} &= (\underline{a}^T - \alpha\underline{e}^T)(\underline{a} - \alpha\underline{e}) = \underline{a}^T\underline{a} - \alpha\underline{e}^T\underline{a} - \alpha\underline{a}^T\underline{e} + \alpha^2\underline{e}^T\underline{e} \\ &= \underline{a}^T\underline{a} - 2\alpha a_{11} + \alpha^2\end{aligned}$$

and

$$\underline{v}^T\underline{a} = (\underline{a}^T - \alpha\underline{e})\underline{a} = \underline{a}^T\underline{a} - \alpha\underline{e}^T\underline{a} = \underline{a}^T\underline{a} - \alpha a_{11}$$

and

$$2[\underline{a}^T\underline{a} - \alpha a_{11}] = 2\underline{v}^T\underline{a} = \underline{v}^T\underline{v} = \underline{a}^T\underline{a} - 2\alpha a_{11} + \alpha^2$$

results in

$$\alpha^2 = \underline{a}^T\underline{a}$$

To reduce the risk of decimal point cancellation

$$\alpha = \begin{cases} -\|a\|_2 & a_{11} \geq 0 \\ \|a\|_2 & a_{11} < 0 \end{cases}$$

Example:

$$A = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{pmatrix} \qquad \underline{a} = \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix} \qquad \|a\|_2 = \sqrt{5} \qquad \alpha = -\sqrt{5}$$

$$\underline{v} = \underline{a} - \alpha\underline{e} = \begin{pmatrix} 2 + \sqrt{5} \\ 1 \\ 0 \end{pmatrix}, \underline{v}^T\underline{v} = 10 + 4\sqrt{5}$$

We call it P_1, because after the first column, it has to be applied iteratively.

$$P_1 = I - \frac{2}{\underline{v}^T\underline{v}}\underline{v}\underline{v}^T = \frac{1}{5 + 2\sqrt{5}}\begin{pmatrix} -4 - 2\sqrt{5} & -2 - \sqrt{5} & 0 \\ -2 - \sqrt{5} & 4 + 2\sqrt{5} & 0 \\ 0 & 0 & 5 + 2\sqrt{5} \end{pmatrix}$$

$$P_1A = \ldots = \frac{1}{5 + 2\sqrt{5}}\begin{pmatrix} -10 - 5\sqrt{5} & -12 - 6\sqrt{5} & -2 - \sqrt{5} \\ 0 & 14 + 7\sqrt{5} & 4 + 2\sqrt{5} \\ 0 & 5 + 2\sqrt{5} & 10 + 4\sqrt{5} \end{pmatrix}$$

Application to the first column of the lower matrix.

$$\underline{a} = \begin{pmatrix} 0 \\ 14 + 7\sqrt{5} \\ 5 + 2\sqrt{5} \end{pmatrix}$$

Givens rotation

Especially for sparse matrices, the Givens rotation can help to eliminate specific entries.

$$G = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \text{ with } \alpha^2 + \beta^2 = 1$$

$$G^T G = \begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix} \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} = \begin{pmatrix} \alpha^2 + \beta^2 & 0 \\ 0 & \alpha^2 + \beta^2 \end{pmatrix} = I$$

Transformation:

$$\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \overset{!}{=} \begin{pmatrix} \overline{x} \\ 0 \end{pmatrix}$$

$$\beta x + \alpha y = 0 \implies \alpha = \frac{x}{\sqrt{x^2 + y^2}}, \beta = -\frac{y}{\sqrt{x^2 + y^2}}$$

Example:

$$A = \begin{pmatrix} 2 & 1 & 0 \\ 1 & 4 & 1 \\ 0 & 1 & 2 \end{pmatrix} \qquad \underline{a} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \qquad x = 2, y = 1, \alpha = \frac{2}{\sqrt{5}}, \beta = -\frac{1}{\sqrt{5}}$$

Rotation in the x_1-x_2-plane:

$$G_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 & 1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & -\sqrt{5} \end{pmatrix}$$

$$G_1 A = \frac{1}{\sqrt{5}} \begin{pmatrix} 5 & 6 & 1 \\ 0 & 7 & 2 \\ 0 & \sqrt{5} & 2\sqrt{5} \end{pmatrix}$$

$$\underline{a} = \frac{1}{\sqrt{5}} \begin{pmatrix} 7 \\ \sqrt{5} \end{pmatrix}, x = \frac{7}{\sqrt{5}}, y = 1, \alpha = \frac{7}{\sqrt{54}}, \beta = -\frac{\sqrt{5}}{\sqrt{54}}$$

$$G_2 = \frac{1}{\sqrt{54}} \begin{pmatrix} \sqrt{54} & 0 & 0 \\ 0 & 7 & \sqrt{5} \\ 0 & -\sqrt{5} & 7 \end{pmatrix}$$

$$R = G_2 G_1 A = \ldots = \frac{1}{\sqrt{220}} \begin{pmatrix} 5\sqrt{54} & 6\sqrt{54} & \sqrt{54} \\ 0 & 54 & 24 \\ 0 & 0 & 12\sqrt{15} \end{pmatrix}$$

$\rightarrow A = QR$ with $Q = (G_2 G_1)^T$.

Stationary iteration methods

Stationary refers to: $x^{k+1} = T(x^k)$ with $T \neq T^k$

$$A\underline{x} = \underline{f} \text{ with } \underline{x} = \underline{x} + \alpha B^{-1}(A\underline{x} - \underline{f}) \tag{1}$$

For a regular matrix $B \in \mathbb{R}^{n\times n}$ and a positive real parameter $\alpha \in \mathbb{R}$ is the solution of the linear equation system 1 equivalent to the solution of the fixed point equation 2.

$$\underline{x} = \underline{x} - \alpha B^{-1}(A\underline{x} - f) \tag{2}$$

This representation gives rise to the iteration process 10.4

$$\underline{x}^{k+1} := \underline{x}^k - \alpha B^{-1}(A\underline{x}^k - \underline{f}) = (I - \alpha B^{-1}A)\underline{x}^k + \alpha B^{-1}\underline{f}$$

(with an arbitrary chosen initial approximation $\underline{x} \in \mathbb{R}^n$) for $k = 0, 1, 2, \ldots$. The convergence of the process 10.4 follows from Banach's fixed point theorem.

Theorem 5. *The iteration matrix of the iteration process 10.4 is a contraction, hence it holds that*

$$\left\|I - \alpha B^{-1}A\right\|_M \leq q < 1 \tag{3}$$

in a vector norm $\|\cdot\|_V$ compatible to matrix norm $\|\cdot\|_M$. Then iteration process 10.4 converges against a uniquely defined solution $\underline{x} = A^{-1}\underline{f}$ of the linear equation system 1 and the following a priori error estimate is given:

$$\left\|\underline{x}^{k+1} - \underline{x}\right\|_V \leq \frac{q^{k+1}}{1-q}\left\|\underline{x}^1 - \underline{x}^0\right\|_V \tag{4}$$

as well as the posteriori error estimate

$$\left\|\underline{x}^{k+1} - \underline{x}\right\|_V \leq \frac{q}{1-q}\left\|\underline{x}^{k+1} - \underline{x}^k\right\|_V \tag{5}$$

Proof. The exact solution $\underline{x} = A^{-1}\underline{f}$ of the linear equation system 1 is the solution of the fixed point equation 2. Then it follows that,

$$\begin{aligned}\left\|\underline{x}^{k+1} - \underline{x}\right\|_V &= \left\|(I - \alpha B^{-1}A)(\underline{x}^k\underline{x})\right\|_V \\ &\leq \left\|I - \alpha B^{-1}A\right\|_M \left\|\underline{x}^k - \underline{x}\right\| \\ &\leq q\left\|\underline{x}^k - \underline{x}\right\|\end{aligned}$$

and by repetitive application, we get:

$$\left\|\underline{x}^{k+1} - \underline{x}\right\| \leq q^{k+1}\left\|\underline{x}^0 - \underline{x}\right\| \to 0 \text{ for } k \to \infty$$

because $q < 1$ for every arbitrary initial approximation $\underline{x}^0 \in \mathbb{R}^n$.

By the triangle inequality

$$\left\|\underline{x}^{k+1} - \underline{x}\right\|_V \leq q \left\|\underline{x}^k - \underline{x}\right\|_V \leq q \left(\left\|x^k - x^{k+1}\right\|_V + \left\|\underline{x}^{k+1} - \underline{x}\right\|_V\right)$$

$$\iff (1-q) \left\|x^{k+1} - x\right\|_V \leq q \left\|x^{k+1} - x^k\right\|_V$$

the a posteriori error estimate 5 follows.

From,

$$\left\|\underline{x}^{k+1} - \underline{x}\right\|_V \leq q^k \left\|\underline{x}^1 - \underline{x}\right\|_V$$

and by the a posteriori error estimate for $k = 0$,

$$\left\|x^1 - \underline{x}\right\|_V \leq \frac{q}{1-q} \left\|\underline{x}^1 - \underline{x}^0\right\|_V$$

the a priori error estimate can be derived. □

An arbitrary matrix $A \in \mathbb{R}^{n \times n}$ is representable as

$$A = L + D + R \tag{6}$$

where L refers to the lower triangular matrix slice, D to the diagonal values and R to the upper triangular matrix slice.

$$L = \begin{pmatrix} 0 & & & 0 \\ a_{21} & 0 & & \\ \vdots & & \ddots & \\ a_{n1} & \dots & a_{n,n-1} & 0 \end{pmatrix} \qquad R = \begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ & \ddots & & \vdots \\ & & \ddots & a_{n-1,n} \\ 0 & & & 0 \end{pmatrix} \qquad D = \begin{pmatrix} a_{11} & & 0 & \\ & a_{22} & & \\ & & \ddots & \\ & & & a_{nn} \end{pmatrix}$$

Because of invertibility of A we can (without loss of generality) assume the invertability of diagonal matrix D.

Then the linear equation system 1 is equivalent to fixed point equation:

$$D\underline{x} = f - (L + R)\underline{x}$$

resulting in the Jacobi method ("complete step procedure")

$$\underline{x}^{k+1} = D^{-1}(f - (L + R)\underline{x}^k) = \underline{x}^k - D^{-1}(A\underline{x}^k - f) \tag{7}$$

This lecture took place on 2017/12/06.

Can we apply Equation 1 to this process?

Jacobi method

Algorithm:

1. Let $\underline{x}^0 \in \mathbb{R}^n$ an arbitrary initial approximation.
2. For $k = 0, 1, 2, \ldots$
   (a) compute $\underline{r}^k = A\underline{x}^k - \underline{f}$, $g_k = (\underline{r}^k, \underline{r}^k) = \left\|\underline{r}^k\right\|_2^2$
3. If $g_k \leq \varepsilon^2 g_0$ with given error precision ε is achieved, terminate.
4. $x_i^{k+1} = \frac{1}{a_{ii}}\left[f_i - \sum_{j=1}^{i-1} a_{ij}x_j^k - \sum_{j=1+1}^{n} a_{ij}x_j^k\right]$ for $i = 1, \ldots, n$

Definition. *For matrix A, the* strong row sum criterion *is defined as*

$$\max_{i=1,\ldots,n} \sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{|a_{ij}|}{|a_{ii}|} \leq q < 1$$

Then the Jacobi method (equation 7) converges for any arbitrary initial approximation $\underline{x}^0$.

Proof.
- $\|\cdot\|_V = \|\cdot\|_\infty$ is compatible with $\|\cdot\|_M = \|\cdot\|_\infty$ where $\|\cdot\|_\infty$ is the row sum norm.
- Iteration matrix

$$\left\|\underbrace{I - D^{-1}A}_{\substack{0 \text{ at diagonal} \\ \frac{a_{ij}}{a_{ii}} \text{ otherwise}}}\right\|_\infty = \max_{i=1,\ldots,n} \sum_{\substack{i=1 \\ j\neq 1}}^{n} \frac{|a_{ij}|}{|a_{ii}|} \leq q < 1$$

  Hence, by Equation 1, convergence of the Jacobi method is given.

□

Starting from Equation 6, the linear equation system 1 is equivalent to the fixed point equation

$$(D + L)\underline{x} = \underline{f} - R\underline{x}$$

resulting in the derivation of the forwarding[3] Gauss-Seidel method ("single step method")

$$\underline{x}^{k+1} = (D + L)^{-1}\left[\underline{f} - R\underline{x}^k\right] = \underline{x}^k - (D + L)^{-1}[A\underline{x}^k - f] \tag{8}$$

$$= (D + L)^{-1}R\underline{x}^k + (D + L)^{-1}\underline{f} \tag{9}$$

[3]Using forward insertion.

$$(D+L)\underline{x}^{k+1} = \underline{b}$$

$$\begin{pmatrix} a_{11} & & & \\ a_{21} & a_{22} & & \\ \vdots & & \ddots & \\ a_{n1} & \dots & & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} x_1^{k+1} \\ x_2^{k+1} \\ \vdots \\ x_n^{k+1} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \rightsquigarrow \begin{matrix} x_1^{k+1} = \frac{b_1}{a_{11}} \\ x_2^{k+1} = \frac{1}{a_{22}}(b_2 - a_{21}x_1^{k+1}) \\ \vdots \end{matrix}$$

Forwarding Gauss-Seidel method

1. Let $\underline{x}^0 \in \mathbb{R}^n$ be an arbitrary initial approximation.
2. For $k = 0, 1, 2, \dots$, determine
   (a) $\underline{r}^k = A\underline{x}^k - f, g_k = (\underline{r}^k, \underline{r}^k) = \left\|\underline{r}^k\right\|_2^2$
3. If $g_k \leq \varepsilon^2 g_0$ for given ε, terminate
4. $x_i^{k+1} = \frac{1}{a_{ii}}\left[f_i - \sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k\right]$ for $i = 1, \dots, n$

Theorem 6. *For matrix A, let the strong row sum criterion be satisfied (compare with Theorem 10.5). Then the Gauss-Seidel method 9 converges for an arbitrary initial approximation $\underline{x}^0$.*

Proof. Show $\left\|(D+L)^{-1}R\right\|_\infty \leq q < 1$ (then the statement from Equation 1 follows).

For arbitrary $\underline{y} \in \mathbb{R}^n$, consider the linear equation system

$$(D+L)\underline{z} = R\underline{y}$$

Then it holds that

$$z_1 = \frac{1}{a_{11}} \sum_{j=2}^{n} a_{1j}y_j$$

and therefore

$$|z_1| \leq \sum_{j=2}^{n} \frac{|a_{1j}|}{|a_{11}|} |y_j| \leq \max_{l=1,\dots,n} |y_l| \sum_{j=2}^{n} \frac{|a_{1j}|}{|a_{1i}|} \leq q \left\|y\right\|_\infty$$

Hence, it holds that

$$|z_l| \leq q \left\|y\right\|_\infty < \left\|y\right\|_\infty \text{ for } l = 1, \dots, k-1$$

Then it follows that

$$
\begin{aligned}
\|z_k\| &= \frac{1}{|a_{kk}|}\left|-\sum_{l=1}^{k-1} a_{kl} z_l + \sum_{l=k+1}^{n} a_{kl} y_l\right| \\
&\leq \frac{1}{|a_{kk}|}\left[\max_{l=1,\ldots,k-1}]\,|z_l| \sum_{l=1}^{k-1} |a_{kl}| + \max_{l=k+1,\ldots,n} \left|y_l\right| \sum_{l=k-1}^{n} |a_{kl}|\right] \\
&\leq \left\|y\right\|_\infty \sum_{l=1}^{n} \frac{|a_{kl}|}{|a_{kk}|} \leq q \left\|y\right\|_\infty
\end{aligned}
$$

for $k = 2, \ldots, n$ and therefore it holds that

$$
\left\|(D+L)^{-1} R \underline{y}\right\|_\infty = \|z\|_\infty \leq q \left\|y\right\|_\infty
$$

Because the row sum norm is induced by the maximum norm, it follows that

$$
\left\|(D+L)^{-1} R\right\|_\infty = \sup_{\substack{y \in \mathbb{R}^n \\ y \neq 0}} \frac{\left\|(D+L)^{-1} R y\right\|_\infty}{\left\|y\right\|_\infty} \leq q < 1
$$

The convergence of the Gauss-Seidel method (acc. to Equation 1) follows. □

This lecture took place on 2017/12/11.

Revision of Jacobi and Gauss-Seidel methods

$$
A\underline{x} = \underline{f}
$$

For $i = 1, \ldots, n$,

$$
\hat{x}_i^{k+1} = \frac{1}{a_{ii}}\left[f_i - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j^k\right]
$$

$$
x_i^{k+1} = (1-\omega) x_i^k + \hat{x}_i^{k+1}
$$

where ω is called relaxation parameter with $\omega \in (0, 1]$.

$$\begin{aligned}
x_i^{k+1} &= (1-\omega)x_i^k + \omega \hat{x}_i^{k+1} \\
&= (1-\omega)x_i^k + \omega \frac{1}{a_{ii}} \left[f_i - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j^k \right] \\
&= x_i^k + \omega \frac{1}{a_{ii}} \left[f_i - \sum_{j=1}^{n} a_{ij} x_j^k \right] \\
&= x_i^k - \omega \frac{1}{a_{ii}} \left[\sum_{j=1}^{n} a_{ij} x_j^k - f_i \right] \qquad i = 1, \ldots, n \\
\underline{x}^{k+1} &= \underline{x}^k - \omega D^{-1}(A\underline{x}^k - \underline{f})
\end{aligned}$$

This method is called *Richardson Iteration* or *ω-Jacobi method*.

Another interpretation is given with:

$$\begin{aligned}
& A\underline{x} = \underline{f} \\
\iff & \underline{0} = A\underline{x} - \underline{f} \\
& \underline{0} = -gB^{-1}(A\underline{x} - \underline{f}) \\
& \underline{x} = \underline{x} - gB^{-1}(A\underline{x} - \underline{f})
\end{aligned}$$

Where $g \neq 0$ and B is regular. Fixed point equation.

Richardson Iteration:

$$\underline{x}^{k+1} = x^k - gB^{-1}(A\underline{x}^k - \underline{f})$$

For example $b = \operatorname{diag}(A), \gamma = w$.

Gauss-Seidel method: for $i = 1, \ldots, n$,

$$\begin{aligned}
\hat{x}_i^{k+1} &= \frac{1}{a_{ii}} \left[f_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij} x_j^k \right] \\
x_i^{k+1} &= (1-\omega)x_i^k + \omega \hat{x}_i^{k+1} \\
&= (1-\omega)x_i^k + \frac{\omega}{a_{ii}} \left[f_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij} x_j^k \right] \\
x_i^{k+1} &= x_i^k + \frac{\omega}{a_{ii}} \left[f_i - \sum_{j=i}^{n} a_{ij} x_j^k \right] - \frac{\omega}{a_{ii}} \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} \\
a_{ii} x_i^{k+1} + \omega \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} &= a_{ii} x_i^k + \omega \left[f_i - \sum_{j=i}^{n} a_{ij} x_j^k \right]
\end{aligned}$$

Consider matrix $A = L + D + R$ where L is a lower triangular matrix, D only contains diagonal elements and R is the right upper triangular matrix. Then,

$$\begin{aligned} D\underline{x}^{k+1} + \omega L\underline{x}^{k+1} &= D\underline{x}^k + \omega\left[\underline{f} - \omega(D+R)\underline{x}^k\right] && = D\underline{x}^k + \omega\left[\underline{f} - A\underline{x}^k + L\underline{x}^k\right] \\ (D+\omega L)\underline{x}^{k+1} &= (D+\omega L)\underline{x}^k - \omega(A\underline{x}^k - \underline{f}) \end{aligned}$$

Successive Over-Relaxation (SOR) method:

$$\implies \underline{x}^{k+1} = \underline{x}^k - \omega(D+\omega L)^{-1}(A\underline{x}^k - \underline{f})$$

Theorem 7. *Ostrowski, 1947*

Let A be a symmetric matrix and be positive definite. Then the SOR method converges if and only if $\omega \in (0, 2)$.

Proof. To be done in the practicals. □

Ostrowski's theorem applied to $\omega = 1$ shows the convergence of the Gauss-Seidel method for symmetric, positive definite matrices A.

But one problem occurs. Even for a symmetric matrix the recursion matrix won't become symmetric: $g = \omega$, $B = D + \omega L$, $A = A^T \implies B \neq B^T$.

Thus, we want to derive a symmetric method.

SOR (in forwards direction[4]:

$$\underline{x}^{k+1} = \underline{x}^{k+1} - \omega(D+\omega L)^{-1}\left[A\underline{x}^k - \underline{f}\right]$$

Let us consider again,

$$x_i^{k+1} = (1-\omega)x_i^k + \frac{\omega}{a_{ii}}\left[f_i - \sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k\right]$$

but we replace some k and $k+1$:

$$x_i^{k+1} = (1-\omega)x_i^k + \frac{\omega}{a_{ii}}\left[f_i - \sum_{j=1}^{i-1} a_{ij}x_j^k - \sum_{j=i+1}^{n} a_{ij}x_j^{k+1}\right]$$

We get some SOR in backwards direction:

$$\underline{x}^{k+1} = \underline{x}^{k+1} - \omega(D+\omega R)^{-1}\left[A\underline{x}^k - \underline{f}\right]$$

[4]Corresponds to "top to bottom" in the matrix

Now we combine these two SOR variants.

$$\begin{aligned}
\underline{x}^{k+\frac{1}{2}} &= \underline{x}^k - \omega(D+\omega L)^{-1}\left[A\underline{x}^k - \underline{f}\right] \\
\underline{x}^{k+1} &= \underline{x}^{k+\frac{1}{2}} - \omega(D+\omega R)^{-1}\left[A\underline{x}^{k+\frac{1}{2}} - \underline{f}\right] \\
&\dots \\
\underline{x}^{k+1} &= \underline{x}^k - \underbrace{\omega(2-\omega)}_{g}\underbrace{(D+\omega R)^{-1}D(D+\omega L)^{-1}}_{B=B^T>0 \text{ for } A=A^T>0}\left[A\underline{x}^k - \underline{f}\right]
\end{aligned}$$

Symmetric Successive OverRelaxation (ISSOR method):

$$A = A^T > 0 \implies \text{convergence} \iff \omega \in (0,2)$$

B acts as a precondition.

All these methods can be considered as Richardson iteration.

Richardson iteration, Methods of single iteration

$$\underline{x}^{k+1} = \underline{x}^k - \alpha(A\underline{x}^k - \underline{f})$$

α is constant and therefore this is called a stationary method.

$$A = A^T > 0 \qquad \left\|\underline{x}^{k+1} - \underline{x}\right\|_V \le \underline{q}\left\|\underline{x}^k - \underline{x}\right\|_V \qquad q < 1$$

$$\begin{aligned}
\underline{x}^{k+1} &= \underline{x}^k - \alpha(A\underline{x}^k - \underline{f}) \\
\underline{x} &= \underline{x} - \alpha(A\underline{x} - \underline{f}) \\
\underline{x}^{k+1} - \underline{x} &= \underbrace{(I-\alpha A)}_{M}(\underline{x}^k - \underline{x})
\end{aligned}$$

$$\|\cdot\|_V = \|\cdot\|_2$$

$$\begin{aligned}
\left\|\underline{e}^{k+1}\right\|_2^2 &= \left\|(I-\alpha A)\underline{e}^k\right\|_2^2 = \left((I-\alpha A)\underline{e}^k, (I-\alpha A)\underline{e}^k\right) \\
&= \left\|g^k\right\|_2^2 - 2\alpha\underbrace{(A\underline{e}^k, \underline{e}^k)}_{\ge c_1^A\|\underline{e}^k\|_2^2} + \alpha^2\underbrace{(A\underline{e}^k, A\underline{e}^k)}_{\le (c_2^A)^2\|\underline{e}^k\|_2^2} \\
&\le \underbrace{(1 - 2\alpha c_1^A + (c_2^A)^2)}_{<1}\left\|\underline{e}^k\right\|_2^2
\end{aligned}$$

when is it minimal for α^*? It depends on c_1^A and c_2^A.

So how do we choose α^* and $\|\cdot\|_V$. For the latter we can use $A = A^T > 0$ or $A \neq A^T$ indefinit. Those lead us to the gradient methods and orthogonalization/CG method.

This lecture took place on 2017/12/13.

Gradient methods

Let $A \in \mathbb{R}^{n\times n}$ be regular, $\underline{x} = A^{-1}\underline{f}$ be the solution of Equation 1 ($A\underline{x} = \underline{f}$). Additionally, we assume A is symmetric and positive definite.

Now we reformulate the problem as an optimization problem. Consider,

$$F : \mathbb{R}^n \to \mathbb{R}$$
$$F(\underline{z}) = \left\|\underline{z} - \underline{x}\right\|_A^2 = (A(\underline{z} - \underline{x}), \underline{z} - \underline{x}) = (A\underline{z}, \underline{z}) - 2(\underbrace{A\underline{x}}_{=\underline{f}}, \underline{z}) + \left\|\underline{x}\right\|_A^2$$

with the vector norm $\|\cdot\|_A$ induced by A.

For the solution $\underline{x} = A^{-1}f$ of Equation 1 it holds that,

$$0 = F(\underline{x}) = \min_{\underline{z}\in\mathbb{R}^n} F(\underline{z})$$

Let $\underline{x}^k$ be the given approximate solution and $\underline{r}^k = A\underline{x}^k - \underline{f}$ is the corresponding residue. We consider a new approach with approximate solution,

$$\underline{x}^{k+1} = \underline{x}^k + \alpha_k f^k$$

where $\underline{p}^k$ (the direction of search) is chosen in direction of the negative gradient.

$$-\left(\nabla F(\underline{z})\Big|_{\underline{z}=\underline{x}^k}\right) = -\left(2(A\underline{z} - \underline{f})\Big|_{\underline{z}=\underline{x}^k}\right) = 2(A\underline{x}^k - \underline{f}) = -2\underline{r}^k$$

By neglecting the factor 2 we get,

$$\underline{x}^{k+1} = \underline{x}^k - \alpha_k \underline{r}^k$$

The real parameter α_k is chosen such that F is minimal:

$$F(\underline{x}^{k+1}) = F\left(\underline{x}^k - \alpha_k \underline{r}^k\right) \overset{!}{=} \min_{\alpha\in\mathbb{R}} F\left(\underline{x}^k - \alpha \underline{r}^k\right)$$

Because

$$\begin{aligned}
F(\underline{x}^k - \alpha\underline{r}^k) &= \left\|\underline{x}^k - \alpha\underline{r}^k - \underline{x}\right\|_A^2 \\
&= (A(\underline{x}^k - \alpha\underline{r}^k - \underline{x}), \underline{x}^k - \alpha\underline{r}^k - \underline{x}) \\
&= (A(\underline{x}^k - \underline{x}), \underline{x}^k - \underline{x}) - 2\alpha(A(\underline{x}^k - \underline{x}), \underline{r}^k) + \alpha^2(A\underline{r}^k, \underline{r}^k) \\
&= F(\underline{x}^k) - 2\alpha(\underline{r}^k, \underline{r}^k) + \alpha^2(A\underline{r}^k, \underline{r}^k)
\end{aligned}$$

the minimum is assumed for

$$\alpha_k = \frac{(\underline{r}^k, \underline{r}^k)}{(A\underline{r}^k, \underline{r}^k)}$$

The resulting method is called *gradient method of steepest decent*.
Algorithm:

1. Given initial approximation $\underline{x}^0$ (arbitrary), $\underline{r}^0 = A\underline{x}^0 - \underline{f}$
2. For $k = 0, 1, 2, \ldots$
   (a) $g_k = (\underline{r}^k, \underline{r}^k) = \left\|\underline{r}^k\right\|_2^2$
3. Terminate if $g_k \leq \varepsilon^2 g_0$ with given error precision ε.
4. $\underline{v}^k = A\underline{r}^k, \alpha_k = \frac{(\underline{r}^k, \underline{r}^k)}{(\underline{v}^k, \underline{r}^k)}, \underline{x}^{k+1} = \underline{x}^k - \alpha_k \underline{r}^k, \underline{r}^{k+1} = \underline{r}^k - \alpha_k \underline{v}^k$

Theorem 8. *Let A be symmetric and positive definite. Furthermore it holds that*

$$(A\underline{x}, \underline{x}) \geq c_1^A \left\|\underline{x}\right\|_2^2 \qquad \left\|A\underline{x}\right\|_2 \leq c_2^A \left\|\underline{x}\right\|_2$$

for all $\underline{x} \in \mathbb{R}^n$. Then the gradient method of steepest decent converges towards

$$\left\|\underline{x}^{k+1} - \underline{x}\right\|_A^2 \leq \left(1 - \left(\frac{c_1^A}{c_2^A}\right)^2\right)^{k+1} \left\|\underline{x}_0 - \underline{x}\right\|_A^2$$

In case if A is not symmetrically positive definite,

- $$\tilde{F}(z) = \left\|z - \underline{x}\right\|_{A^TA}^2$$
  where A^TA is symmetrically positive definite.
  $$\implies \underline{p}^k = -\nabla\tilde{F}(z)\Big|_{z=\underline{x}^k} = -2A^T\underline{r}^k$$
  α_k such that
  $$\tilde{F}(\underline{x}^{k+1}) = \tilde{F}(\underline{x}^k - \alpha_k A^T\underline{r}^k) \overset{!}{=} \min_{\alpha\in\mathbb{R}} \tilde{F}(x^k - \alpha A^T\underline{r}^k)$$
  $$\implies \alpha_k = \frac{(A^T\underline{r}^k, A^T\underline{r}^k)}{(AA^T\underline{r}^k, AA^T\underline{r}^k)}$$
- Gradient method of minimal defect
  The direction of search is the negative residue
  $$\underline{x}^{k+1} = \underline{x}^k - \alpha_k\underline{r}^k$$

k	x_1^k	x_2^k	$F(x^k)$
0	0	0	14
1	1.680	1.344	$2.213 \cdot 10^{-1}$
2	1.968	0.984	$3.499 \cdot 10^{-3}$
3	1.995	1.005	$5.530 \cdot 10^{-5}$

where α_k such that

$$\tilde{F}(\underline{x}^{k+1}) = \tilde{F}(\underline{x}^k - \alpha_k \underline{r}^k) \overset{!}{=} \min_{\alpha \in \mathbb{R}} \tilde{F}(\underline{x}^k - \alpha \underline{r}^k)$$

$$\implies \alpha_k = \frac{(A\underline{r}^k, \underline{r}^k)}{(A\underline{r}^k, A\underline{r}^k)}$$

Convergence behavior is analogously to $\|\cdot\|_{A^TA}$ instead of $\|\cdot\|_A$.

Example 10. *Gradient method of steepest decent for*

$$\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5 \\ 4 \end{pmatrix} \text{ with initial value } \underline{x}^0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\underline{r}^0 = A\underline{x}^0 - f = \begin{pmatrix} -5 \\ -4 \end{pmatrix}, \alpha_0 = \frac{(\underline{r}^0, \underline{r}^0)}{(A\underline{r}^0, \underline{r}^0)} = \frac{41}{122}$$

$$\underline{x}^1 = \underline{x}^0 - \alpha_0 \underline{r}^0 \approx \begin{pmatrix} 1.680 \\ 1.344 \end{pmatrix}$$

Exact solution: $\underline{x} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$.

$$F(\underline{z}) = \left(\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} z_1 - 2 \\ z_2 - 1 \end{pmatrix}, \begin{pmatrix} z_1 - 2 \\ z_2 - 1 \end{pmatrix} \right)$$

$$\implies \underline{r}^2 \approx \begin{pmatrix} -0.08 \\ -0.064 \end{pmatrix} \left\| \begin{pmatrix} -5 \\ -4 \end{pmatrix} = \underline{r}^0 \right.$$

Advantage of the gradient method:

> Parallel oder almost parallel search directions can be traversed multiple times in one iteration. Compare with Figure 12.

This motivates the *orthogonalization of search directions*.

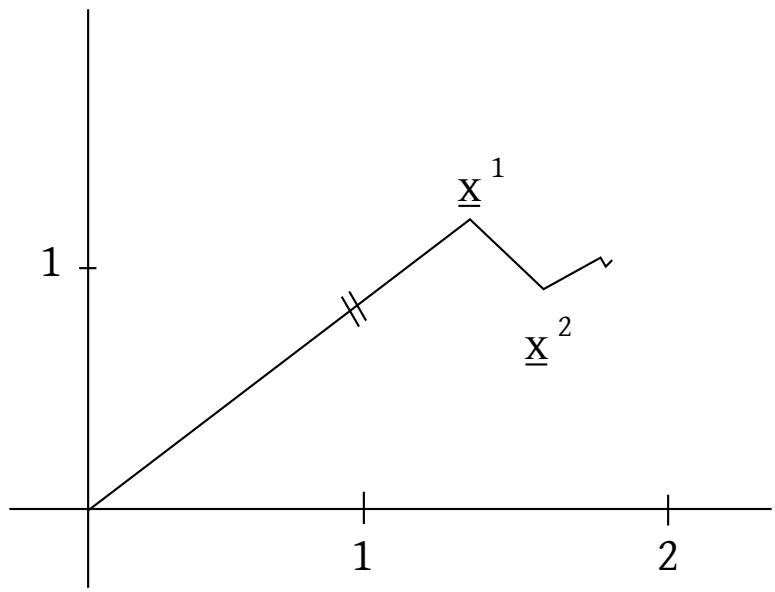


Figure 12: Gradient method search direction

This lecture took place on 2018/01/08.

Conjugate Gradient method, CG method

Assumption: $A = A^T$, symmetrical and positive definite

A system of linear independent vectors $\left\{\underline{p}^k\right\}_{k=0}^{n-1}$ is called *A-orthogonal* or *conjugated*, if

$$(A\underline{p}^k, \underline{p}^l) = 0 \text{ for } k, l = 0, \ldots, n-1 \text{ with } k \neq l \text{ and}$$

$$(A\underline{p}^k, \underline{p}^k) > 0 \text{ for } k = 0, \ldots, n-1$$

For linear independent $\left\{\underline{w}^k\right\}_{k=0}^{n-1}$, using the Gram-Schmidt orthogonalization method, we can construct a system of A-orthogonal vectors $\left\{\underline{p}^k\right\}_{k=0}^{n-1}$.

- Let $\underline{p}^0 := \underline{w}^0$

- For $k = 0, \ldots, n-2$ compute

$$\underline{p}^{k+1} := \underline{w}^{k+1} - \sum_{l=0}^{k} \beta_{kl} \underline{p}^l$$

with

$$\beta_{kl} = \frac{(A\underline{w}^{k+1}, \underline{p}^l)}{(A\underline{p}^l, \underline{p}^l)}$$

In the 2D-case (hence, if $n = 2$), then the ideal situation would be to make one step ahead and the next orthogonal step leads us directly to the solution.

We insert our solution approach:

$$\underline{x} = \underline{x}^0 - \sum_{l=0}^{n-1} \alpha_l \underline{p}^l$$

into the linear equation system $A\underline{x} = \underline{f}$ results in

$$A\underline{x} = A\underline{x}^0 - \sum_{l=0}^{n-1} \alpha_l A\underline{p}^l = \underline{f}$$

$$\implies (A\underline{x}, \underline{p}^k) = (A\underline{x}^0, p^k) - \sum_{l=0}^{n-1} \alpha_l (A\underline{p}^l, \underline{p}^k) = (\underline{f}, \underline{p}^k)$$

for $k = 0, \ldots, n-1$. Here $(A\underline{p}^l, \underline{p}^k) = 0$ if $l \neq k$ because $\left\{\underline{p}^k\right\}_{k=0}^{n-1}$ is A-orthogonal. Hence,

$$\implies \alpha_k = \frac{(A\underline{x}^0 - f, \underline{p}^k)}{(A\underline{p}^k, \underline{p}^k)}$$

for $k = 0, \ldots, n-1$.

For approximative solution

$$\underline{x}^{k+1} = \underline{x}^0 - \sum_{l=0}^{k} \alpha_l \underline{p}^l = \underline{x}^0 - \sum_{l=0}^{k-1} \alpha_l \underline{p}^l - \alpha_k \underline{p}^k = \underline{x}^k - \alpha_k \underline{p}^k$$

is the associated residue given by

$$\underline{r}^{k+1} = A\underline{x}^{k+1} - f = A\underline{x}^0 - \sum_{l=0}^{k} \alpha_l A\underline{p}^l - f = A\underline{x}^k - f - \alpha_k A\underline{p}^k = \underline{r}^k - \alpha_k A\underline{p}^k$$

Because $(A\underline{p}^l, \underline{p}^k) = 0$ for $k \neq l$, it follows that

$$\left(A\underline{x}^0 - f, \underline{p}^k\right) = \left(A\underline{x}^0 - \sum_{l=0}^{k-1} \alpha_l A\underline{p}^l - f, \underline{p}^k\right) = (\underline{r}^k, \underline{p}^k)$$

and therefore

$$\alpha_k = \frac{(\underline{r}^k, \underline{p}^k)}{(A\underline{p}^k, \underline{p}^k)}$$

Hence for $k = 0, \ldots, n-2$ we get the iteration step

$$\underline{x}^{k+1} = \underline{x}^k - \alpha_n \underline{p}^k \qquad \underline{r}^{k+1} = \underline{r}^k - \alpha_k A\underline{p}^k \qquad \alpha_k = \frac{(\underline{r}^k, \underline{p}^k)}{(A\underline{p}^k, \underline{p}^k)}$$

After this construction it holds that

$$(\underline{r}^{k+1}, \underline{r}^k) = (\underline{r}^k - \alpha_k A\underline{p}^k, \underline{r}^k) = 0 \tag{10}$$

for $k = 0, \ldots, n-2$.

Lemma. *It holds that* $(\underline{r}^{k+1}, \underline{p}^l) = 0$ *for* $l = 0, \ldots, k$ *and* $k = 0, \ldots, n-2$

Proof. By induction over k.

Base step $k = 0$, $(\underline{r}^1, \underline{p}^0) = 0$ holds because of Equation 10 with $k = 0$.

Induction hypothesis $(\underline{r}^k, \underline{p}^l) = 0$ for $l = 0, \ldots, k$

Induction step

- $l = k$: $(\underline{r}^{k+1}, \underline{p}^k) = 0$ because of Equation 10.
- $l < k$:

$$(\underline{r}^{k+1}, \underline{p}^k) = \underbrace{(\underline{r}^k, \underline{p}^l)}_{=0\text{, by induction hypothesis}} - \underbrace{\alpha_k (A\underline{p}^k, \underline{p}^l)}_{=0\text{, by } A\text{-orthogonality}}$$

□

By construction of the search direction, we get

$$\underline{p}^l = \underline{w}^l - \sum_{j=0}^{l-1} \beta_{l-1,j} \underline{p}^k \text{ or equivalently } \underline{w}^l = \underline{p}^l + \sum_{j=0}^{l-1} \beta_{l-1,j} \underline{p}^j$$

it follows

$$(\underline{r}^{k+1}, \underline{w}^l) = (\underline{r}^{k+1}, \underline{p}^l) + \sum_{j=0}^{l-1} \beta_{l-1,j} (\underline{r}^{k+1}, \underline{p}^j) = 0$$

for $l = 0, \ldots, k$.

Therefore the residue $\underline{r}^{k+1}$ is orthogonal to all base vectors $\underline{w}^l$ for $l = 0, \ldots, k$. The vector system

$$\left\{\underline{w}^0, \underline{w}^1, \ldots, \underline{w}^k, \underline{r}^{k+1}\right\}$$

is linear independent such that the search direction can be chosen as

$$\underline{w}^{k+1} = \underline{r}^{k+1} \text{ or equivalently } \underline{w}^{l} = \underline{r}^{l} \text{ for } l = 0, \dots, n-1$$

Hence, it follows that

$$(\underline{r}^{k+1}, \underline{p}^{l}) = (\underline{r}^{k+1}, \underline{r}^{l} - \sum_{j=0}^{l-1} \beta_{l-1,j} \underline{p}^{j}) \underbrace{=}_{\text{by Lemma}} (\underline{r}^{k+1}, \underline{r}^{l}) = 0 \text{ for } l = 0, \dots, k \text{ and } k = 0, \dots, n-2$$

By the orthogonalization method by Gram-Schmidt, we get

$$\underline{p}^{0} = \underline{w}^{0} = \underline{r}^{0} \qquad \underline{p}^{k+1} = \underline{r}^{k+1} - \sum_{l=0}^{k} \beta_{k,l} \underline{p}^{l} \text{ for } k = 0, \dots, n-2$$

with

$$\beta_{k,l} = \frac{(A\underline{r}^{k+1}, \underline{p}^{l})}{(A\underline{p}^{l}, \underline{p}^{l})} = \frac{(\underline{r}^{k+1}, A\underline{p}^{l})}{(A\underline{p}^{l}, \underline{p}^{l})}$$

Without loss of generality, let $\alpha_l \neq 0$. Otherwise, by recursion $r^{l+1} = r^{l} - \alpha_l A\underline{p}^{l}$ and orthogonality $(\underline{r}^{l+1}, \underline{r}^{l}) = 0$, equality

$$0 = (\underline{r}^{l+1}, \underline{r}^{l}) = (\underline{r}^{l}, \underline{r}^{l})$$

follows and therefore $\underline{r}^{l} = 0$ holds. Hence $\underline{x}^{l} = \underline{x}$ is the exact solution of $A\underline{x} = \underline{f}$. The recursion for residues was given by

$$\underline{r}^{l+1} = \underline{r}^{l} - \alpha_l A\underline{p}^{l} \tag{11}$$

By Equation 11, it follows that

$$A\underline{p}^{l} = \frac{1}{\alpha_l}\left(\underline{r}^{l} - \underline{r}^{l+1}\right)$$

and therefore the counter of β_{kl}

$$(\underline{r}^{k+1}, A\underline{p}^{l}) = \frac{1}{\alpha_l}(\underline{r}^{k+1}, \underline{r}^{l} - \underline{r}^{l+1}) = 0 \text{ for } l = 0, \dots, k-1$$

and therefore $\beta_{k,l} = 0$ for $l = 0, \dots, k-1$. It still holds that

$$(\underline{r}^{k+1}, A\underline{p}^{k}) = \frac{1}{\alpha_k}(\underline{r}^{k+1}, r^{k} - r^{k+1}) = -\frac{1}{\alpha_k}(r^{k+1}, r^{k+1}) \text{ for } l = k$$

This results in

$$\underline{p}^{k+1} = \underline{r}^{k+1} - \beta_k \underline{p}^{k}$$

with

$$\beta_k := \beta_{kk} = \frac{(\underline{r}^{k+1}, A\underline{p}^k)}{(A\underline{p}^k, \underline{p}^k)} = -\frac{1}{\alpha_k}\frac{(\underline{r}^{k+1}, \underline{r}^{k+1})}{(A\underline{p}^k, \underline{p}^k)}$$

By Equation 11 (now replace l with k), it follows that

$$\alpha_k A\underline{p}^k = \underline{r}^k - \underline{r}^{k+1}$$

and therefore

$$\alpha_k(A\underline{p}^k, \underline{p}^k) = (r^k - r^{k+1}, \underline{p}^k) \underbrace{=}_{\text{by Lemma}} (\underline{r}^k, \underline{p}^k) = (\underline{r}^k, \underline{r}^k - \beta_{k-1}\underline{p}^{k-1}) \underbrace{=}_{\text{by Lemma}} (\underline{r}^k, \underline{r}^k) =: \rho_k$$

Followingly, it holds that

$$\beta_k = -\frac{\rho_{k+1}}{\rho_k}$$

or equivalently,

$$\alpha_k = \frac{(\underline{r}^k, \underline{p}^k)}{(A\underline{p}^k, \underline{p}^k)} = \frac{\rho_k}{(A\underline{p}^k, \underline{p}^k)}$$

The resulting method is the method of conjugate gradients (CG), developed by Hestenes and Stiefel.

Algorithm: Iteration steps of conjugate gradient method

1. Choose an arbitrary initial vector $\underline{x}^0 \in \mathbb{R}^n$, $\underline{r}^0 = A\underline{x}^0 - f$.
2. Let $\underline{p}^0 := \underline{r}^0$ and $\rho_0 = (\underline{r}^0, \underline{r}^0)$. Terminate if $\rho_0 < \varepsilon^2$ with a given error precision ε is achieved.
3. Compute for $k = 0, 1, \ldots, n-2$
   (a) $\underline{s}^k = A\underline{p}^k$, $\sigma_k = (\underline{s}^k, \underline{p}^k)$, $\alpha_k = \frac{\rho_k}{\sigma_k}$
   (b) $\underline{x}^{k+1} := \underline{x}^k - \alpha_k \underline{p}^k$
   (c) $\underline{r}^{k+1} := \underline{r}^k - \alpha_k \underline{s}^k$
   (d) $\rho_{k+1} := (\underline{r}^{k+1}, \underline{r}^{k+1})$
   (e) Terminate if $\rho_{k+1} < \varepsilon^2 \rho_0$ with a given error precision ε is achieved. Otherwise compute the new search direction

$$\underline{p}^{k+1} := \underline{r}^{k+1} + \beta_k \underline{p}^k, \qquad \beta_k := \frac{\rho_{k+1}}{\rho_k}$$

By the induction hypotheses

$$\underline{r} \in \operatorname{span}\left\{\underline{r}^0\right\}, \underline{p}^0 = \underline{r}^0 \in \operatorname{span}\{\underline{r}^0\}$$

and because

$$\underline{r}^{l+1} = \underline{r}^l - \alpha_l A\underline{p}^l, \underline{p}^{l+1} = \underline{r}^{l+1} + \beta_l \underline{p}^l$$

by complete induction over $l = 0, \dots, k-1$

$$\underline{p}^k \in \operatorname{span}\left\{\underline{r}^0, A\underline{r}^0, A^2\underline{r}^0, \dots, A^k\underline{r}^0\right\} =: S_k(A, \underline{r}^0)$$

In this case, $S_k(A, \underline{r}^0)$ specifies the k-th Krylov space of matrix A for initial residue $\underline{r}^0$. After construction,

$$S_k(A, \underline{r}^0) = \operatorname{span}\{\underline{p}^1, \underline{p}^2, \dots, \underline{p}^k\}$$

is a A-orthogonal basis of $S_k(A, \underline{r}^0)$.

This lecture took place on 2018/01/10.

Revision: We defined the Krylov space as $\underline{p}^k \in S_k(A, \underline{r}^0) = \operatorname{span}\left\{\underline{p}^0, \underline{p}^1, \dots, \underline{p}^k\right\}$.

Theorem 9. *Given a symmetrical and positive definite matrix $A = A^T > 0$. The CG method converges with convergence estimate*

$$\left\|\underline{x}^k - \underline{x}\right\|_A \leq \frac{2q^k}{1+q^{2k}} \left\|\underline{e}^0\right\|_A$$

with

$$q = \frac{\sqrt{K_2(A)}+1}{\sqrt{K_2(A)}-1} \qquad K_2(A) = \|A\|_2 \left\|A^{-1}\right\|_2 = \frac{\lambda_{max}(A)}{\lambda_{min}(A)}$$

Proof. For an exact solution $\underline{x}$ and (by the CG method constructed) approximate solution $\underline{x}^k$,

$$\underline{x} = \underline{x}^0 - \sum_{l=0}^{n-1} \alpha_l \underline{p}^l \qquad \underline{x}^k = \underline{x}^0 - \sum_{l=0}^{k-1} \alpha_l \underline{p}^l$$

it follows that

$$\left\|\underline{x}^k - \underline{x}\right\|_A^2 = \left\|\sum_{l=k}^{n-1} \alpha_l \underline{p}^l\right\|_A^2 = \sum_{l=k}^{n-1}\sum_{j=k}^{n-1} \alpha_l \alpha_j (A\underline{p}^l, \underline{p}^j) = \sum_{l=k}^{n-1} \alpha_l^2 \left\|\underline{p}^l\right\|_A^2$$

by A-orthogonality of search directions $\underline{p}^l$.

For an arbitrary linear combination

$$\underline{w} = \sum_{l=0}^{k-1} w_l \underline{p}^l$$

with arbitrary coefficients $w_0, \ldots, w_{k-1}$ it follows analogously,

$$\left\|\underline{x}^0 - \underline{w} - \underline{x}\right\|_A^2 = \left\|-\sum_{l=0}^{k-1} w_l \underline{p}^l + \sum_{l=0}^{n-1} \alpha_l \underline{p}^l\right\|_A^2 = \sum_{l=0}^{k-1} (w_l - \alpha_l)^2 \left\|\underline{p}^l\right\|_A^2 + \sum_{l=k}^{n-1} \alpha_l^2 \left\|\underline{p}^l\right\|_A^2$$

And therefore,

$$\left\|\underline{x}^k - \underline{x}\right\|_A \leq \left\|\underline{x}^0 - \underline{w} - \underline{x}\right\|_A \text{ for all } \underline{w} \in S_{k-1}(A, \underline{r}^0)$$

The approximate solution $\underline{x}^k$ is also the solution of minimization problem,

$$\left\|\underline{x}^k - \underline{x}\right\|_A = \min_{\underline{w} \in S_{k-1}(A, \underline{r}^0)} \left\|\underline{x}^0 - \underline{w} - \underline{x}\right\|_A$$

With

$$\underline{r}^0 = A\underline{x}^0 - \underline{f} = A(\underline{x}^0 - \underline{x}) = A\underline{e}^0 \qquad \underline{e}^0 = \underline{x}^0 - \underline{x}$$

it follows that

$$\underline{x}^0 = \underline{w} - \underline{x} = \underline{e}^0 - \sum_{l=0}^{k-1} w_l A^l \underline{r}^0 = A^0 \underline{e}^0 - \sum_{l=0}^{k-1} w_l A^{l+1} \underline{e}^0 = \sum_{l=0}^{k} \tilde{w}_l A^l \underline{e}^0$$

with $\tilde{w}_0 = 1$ and $\tilde{w}_l = -w_{l-1}$ for $l = 1, \ldots, k$. Then it holds that

$$\underline{x}^0 - \underline{w} - \underline{x} = p_k(A)\underline{e}^0$$

with a matrix polynomial $p_k \in \pi_k^1 \in \{f \in \pi_k | f(0) = 1\}$, hence $\underline{x}^k$ is the solution of the minimization problem

$$\left\|\underline{x}^k - \underline{x}\right\|_A = \min_{p_k \in \pi_k^1} \left\|p_k(A)\underline{e}^0\right\|_A$$

Matrix A is symmetric and positive definite $\Longrightarrow$ the eigenvectors $\left\{\underline{v}^j\right\}_{j=1}^n$ define an orthonormal system with associated eigenvalues $\lambda_j(A)$.

$$\rightarrow \underline{e}^0 = \sum_{j=1}^{n} (\underline{e}^0, \underline{v}^j)\underline{v}^j$$

and furthermore,

$$\begin{aligned} p_k(A)\underline{e}^0 = p_k(A) \sum_{j=1}^{n} (\underline{e}^0, \underline{v}^j)\underline{v}^j &= \sum_{j=1}^{n} (\underline{e}^0, \underline{v}^j) p_k(A)\underline{v}^j \\ &= \sum_{j=1}^{n} (\underline{e}^0, \underline{v}^j) p_k(\lambda_j(A))\underline{v}^j \end{aligned}$$

Remark.

$$A\underline{x} = \lambda \underline{x}$$
$$A^2\underline{x} = AA\underline{x} = A\lambda\underline{x} = \lambda Ax = \lambda^2\underline{x}$$
$$p(A)\underline{x} = p(\lambda)x$$

By the orthonormality of eigenvectors $\underline{v}^j$ it follows that,

$$\begin{aligned}
\left\|p_k(A)\underline{e}^0\right\|_A^2 &= (Ap_k(A)\underline{e}^0, p_k(A)\underline{e}^0) \\
&= \left(\sum_{j=1}^{n}(\underline{e}^0, \underline{v}^j)p_k(\lambda_j(A)) \underbrace{A\underline{v}^j}_{=\lambda_j(A)\underline{v}^j} \sum_{i=1}^{n}(\underline{e}^0, \underline{v}^i)p_k(\lambda_i(A)\underline{v}^i)\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n}(\underline{e}^0, \underline{v}^i)(\underline{e}^0, \underline{v}^j)p_k(\lambda_i(A))p_k(\lambda_j(A))\lambda_j(A)(\underline{v}^j, \underline{v}^i) \\
&= \sum_{j=1}^{n}(\underline{e}^0\underline{v}^j)^2 p_k(\lambda_j(A))^2\lambda_j(A) \\
&\leq \max_{j=1,\dots,n}\left[p_k(\lambda_j(A))\right]^2 \sum_{j=1}^{n}(\underline{e}^0, \underline{v}^j)^2\lambda_j(A) \\
&= \max_{j=1,\dots,n}\left[p_k(\lambda_j(A))\right]^2 \left\|\underline{e}^0\right\|_A^2
\end{aligned}$$

and therefore,

$$\left\|\underline{x}^k - \underline{x}\right\|_A \leq \min_{p_k\in\pi_k^1}\max_{j=1,\dots,n}\left\|p_k(\lambda_j(A))\right\| \left\|\underline{e}^0\right\|_A \leq \min_{p_k\in\pi_k^1}\max_{\lambda\in[\lambda_{\min}(A),\lambda_{\max}(A)]}\left|p_k(\lambda)\right| \left\|\underline{e}^0\right\|_A$$

With the theorem about Chebyshev polynomials it follows that

$$\min_{p_k\in\pi_k^1}\max_{\lambda\in[\lambda_{\min}(A),\lambda_{\max}(A)]}\left|p_k(\lambda)\right| = \frac{2q^k}{1+q^{2k}}$$

$$q = \frac{\sqrt{\lambda_{\max}(A)} + \sqrt{\lambda_{\min}(A)}}{\sqrt{\lambda_{\max}(A)} + \sqrt{\lambda_{\min}(A)}} = \frac{\sqrt{K_2(A)}+1}{\sqrt{K_2(A)}-1}$$

□

This lecture took place on 2018/01/15.

CG method:

$$A\underline{x} = \underline{f}, A \in \mathbb{R}^{n\times n}, n \to \infty, A = A^T > 0$$

Theorem 10.

$$\left\|\underline{x}^k - \underline{x}\right\|_A \leq \frac{2q^k}{1+q^{2k}} \left\|\underline{x}^0 - \underline{x}\right\|_A, q = \frac{\sqrt{K_2(A)}+1}{\sqrt{K_2(A)}-1}$$

Applications (PGD):

$$K_2(A) \sim \left(\frac{1}{h}\right)^2, d = 1 : h = \frac{1}{n}$$

Question: Is there any method for convergence independent of n? The answer is "preconditioning".

$$A\underline{x} = \underline{f}, A = A^T > 0$$

Let $B \in \mathbb{R}^{n\times n}$ be chosen appropriately. $B = B^T > 0$.

$$B = B^{\frac{1}{2}}B^{\frac{1}{2}}, B = V^T D V \qquad B^{\frac{1}{2}} := V^T D^{\frac{1}{2}} V$$

$$D = \operatorname{diag}(\lambda_K(B)) \qquad D^{\frac{1}{2}} := \operatorname{diag}(\sqrt{\lambda_K(B)})$$

$$\begin{aligned}
A\underline{x} &= \underline{f} \\
B^{-\frac{1}{2}}AB^{-\frac{1}{2}}B^{\frac{1}{2}}\underline{x} &= B^{-\frac{1}{2}}\underline{f} \\
\tilde{A}\underline{\tilde{x}} &= \underline{\tilde{f}} \\
\tilde{A} &= B^{-\frac{1}{2}}AB^{-\frac{1}{2}} \\
\underline{\tilde{x}} &= B^{\frac{1}{2}}\underline{x} \\
\underline{\tilde{f}} &= B^{-\frac{1}{2}}\underline{f}
\end{aligned}$$

$\tilde{A} = \tilde{A}^T > 0 \implies$ CD-method.

$$\underline{\tilde{x}}^0, \underline{\tilde{r}}^0 = \tilde{A}\underline{\tilde{x}} - \underline{\tilde{f}} = \underline{\tilde{r}}^0$$

$$\tilde{g}_0 = (\underline{\tilde{r}}^0, \underline{\tilde{r}}^0)$$

For $k = 0, 1, 2, \ldots, n-2$:

$$\underline{\tilde{s}}^k = \tilde{A}\underline{\tilde{p}}^k, \tilde{\sigma}_k = (\underline{\tilde{s}}^k, \underline{\tilde{p}}^k), \tilde{\alpha}_k = \frac{\tilde{g}_k}{\tilde{\sigma}_k}$$

$$\underline{\tilde{x}}^{k+1} = \underline{\tilde{x}}^k - \tilde{\alpha}_k\underline{\tilde{p}}^k, \underline{\tilde{r}}^{k+1} - \tilde{\alpha}_k\underline{\tilde{s}}^k$$

$$\tilde{g}_{k+1} = (\underline{\tilde{r}}^{k+1}, \underline{\tilde{r}}^{k+1})$$

$$\tilde{g}_{k+1} < \varepsilon^2\tilde{g}_0 \implies \text{terminate}$$

$$\tilde{\beta}_k = \frac{\tilde{g}_{k+1}}{\tilde{g}_k}, \underline{\tilde{p}}^{k+1} = \underline{\tilde{r}}^{k+1} + \beta_k \underline{\tilde{p}}^k$$

Convergence:

$$\left\|\underline{\tilde{x}}^k - \underline{\tilde{x}}\right\|_{\tilde{A}} \leq \frac{2q^k}{1+q^{2k}} \left\|\underline{\tilde{x}}^0 - \underline{\tilde{x}}\right\|_{\tilde{A}}, q = \frac{\sqrt{K_2(\tilde{A})}+1}{\sqrt{K_2(\tilde{A})}-1}$$

$$K_2(\tilde{A}) \leq \frac{c_2^A}{c_1^A} : c_1^A(\underline{\tilde{x}}, \underline{\tilde{x}}) \leq (\tilde{A}, \underline{\tilde{x}}) \leq c_2^A(\underline{\tilde{x}}, \underline{\tilde{x}}) \quad \forall \underline{\tilde{x}} \in \mathbb{R}^n$$

where $(\tilde{A}\underline{\tilde{x}}, \underline{\tilde{x}}) = (B^{-\frac{1}{2}}AB^{-\frac{1}{2}}B^{-\frac{1}{2}}\underline{x}, B^{\frac{1}{2}}\underline{x})$ and $(\underline{\tilde{x}}, \underline{\tilde{x}}) = (B^{\frac{1}{2}}\underline{x}, B^{\frac{1}{2}}\underline{x})$.

$$c_1(B\underline{x}, \underline{x}) \leq (A\underline{x}, \underline{x}) \leq c_2^A(B\underline{x}, \underline{x}) \quad \forall \underline{x} \in \mathbb{R}^n$$

We call it preconditioning if the following conditions are met:

1. spectral equivalence $A \tilde{-} B$ with $\frac{c_2^A}{c_1^A} \leq$ const.
2. efficient computation of $\underline{r} = B^{-1}\underline{r}$.

CG method with preconditioning

1. $\underline{x}^0, \underline{r}^0 = A\underline{x}^0 - \underline{f}, \underline{v}^0 = B^{-1}\underline{r}^0, \underline{p}^0 = \underline{v}^0, g_0 = (\underline{v}^0, \underline{r}^0)$
2. for $k = 0, \ldots, n-2$
   (a) $\underline{s}^k = A\underline{p}^k, \sigma_k = (\underline{s}^k, \underline{p}^k), \alpha_k = \frac{g_k}{\sigma_k}, \underline{x}^{k+1} = \underline{x}^k - \alpha_k \underline{p}^k, \underline{r}^{k+1} - B^{-1}\underline{r}^{k+1}$
   (b) $g_{k+1} = (\underline{v}^{k+1}, \underline{r}^{k+1}), g_{k+1} \leq \varepsilon^2 g_0 \implies$ terminate
   (c) $\beta_k = \frac{g_{k+1}}{g_k}, \underline{p}^{k+1} = \underline{v}^{k+1} + \beta_k \underline{p}^k$

Hence, the major difference is the introduction of $\underline{r}^{k+1}$.

Given A, find B with $B^{-1}\underline{r}$ is efficiently realizable. $K_2(B^{-1}A) \leq$ is constant independent of "bad parameters".

1. dimension n
2. discretion parameter h
3. degree of Ansatz function
4. uniformity of mesh
5. region, distortion, material parameter, ...

Example 11. *L_2-projection, piecewise linear, general grid.*

$$0 = x_0 < x_1 < \ldots < x_n = 1, h_k = x_k - x_{k-1}$$

$$M_h \underline{u} = \underline{f}, \underline{u} \in \mathbb{R}^n \leftrightarrow \underline{u}_h \in S_k^1(0,1)$$

$B = \underline{T}$

$$\begin{aligned}(M_h \underline{u}, \underline{u}) &\leq \int_0^1 [u_h(x)]^2 \, dx \\ &= \sum_{k=1}^n \int_{x_{k-1}}^{x_k} [u_h(x)]^2 \, dx \\ &\leq \sum_{k=1}^n (M_k \underline{u}^k, \underline{u}^k)\end{aligned}$$

$$M_k = \tfrac{h_k}{6} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \qquad \lambda_{\min}(M_k) = \tfrac{1}{6} h_k \qquad \lambda_{\max}(M_k) = \tfrac{1}{2} h_k$$

$$\begin{aligned}&\leq \frac{1}{2} \sum_{k=1}^n h_k (u_{k-1}^2 + u_k^2) \leq \underbrace{h_{max}}_{C_2^A} \sum_{k=0}^n u_k^2 \\ &\geq \frac{1}{6} \sum_{k=1}^n h_k (u_{k-1}^2 + u_k^2 \geq \underbrace{\frac{1}{6} h_{min}}_{C_1^A} \sum_{k=0}^n u_k^2\end{aligned}$$

$$h_{max} = h_{min} \implies K_2(M_h) = 6$$

$$\frac{h_{max}}{h_{min}} \to \infty \implies K_2(M_h) \to \infty$$

What about B?

$$\begin{aligned}(M_h \underline{u}, \underline{u}) &\leq \frac{1}{2} \underbrace{\sum_{k=1}^n h_k (u_{k-1}^2 + u_k^2)}_{h_1 u_0^2 + h_1 u_1^2 + h_2 u_1^2 + h_2 u_2^2 + \ldots = \frac{1}{2}(D\underline{u}, \underline{u})} \\ &= \frac{1}{2} \left[h_1 u_0^2 + \sum_{k=1}^{n-1} (h_k + h_{k+1}) u_k^2 + h_n u_h^2 \right]\end{aligned}$$

where D is a diagonal matrix with values h_1 to h_n where $h_k + h_{k+1}$ can be found in the middle.

$$\implies \frac{1}{6}(D\underline{u}, \underline{u}) \leq (M_h \underline{u}, \underline{u}) \leq \frac{1}{2}(D\underline{u}, \underline{u}) \forall \underline{u} \in \mathbb{R}^{n+1}$$

$$K_2(D^{-1}M_h) \leq 3$$

This actually works for arbitrary dimensions.

For the CG method, we considered: $A\underline{x} = \underline{f}, A = A^T > 0$. But now, we consider: $A\underline{x} = \underline{f}$, A invertible.

$$\rightarrow A^T A\underline{x} = A^T \underline{f}$$

$$M = M^T > 0$$

CG? convergence? preconditioning?

There is a variety of methods to tackle this problem. In this lecture, we will look at the "Generalized Minimal RESidual" method (GMRES) (by Saad, Schultz, 1987)

Krylov-Space:

$$S_k(A, \underline{r}^0) = \operatorname{span}\left\{\underline{r}^0, A\underline{r}^0, A^2\underline{r}^0, \ldots, A^k\underline{r}^0\right\}$$

Orthonormal vector system:

$$\left\{\underline{v}^k\right\}_{k=0}^{n-1} : (\underline{v}^k, \underline{v}^l) = \delta_{kl}$$

$$\underline{r}^0, \underline{v}^0 = \frac{\underline{r}^0}{\left\|\underline{r}^0\right\|_2}$$

For $k = 0, \ldots, n-2$:

$$\underline{\hat{v}}^{k+1} = A\underline{v}^k - \sum_{l=0}^{k} \beta_{kl}\underline{v}^l \qquad \beta_{kl} = (A\underline{v}^k, \underline{v}^l)$$

$$\left\|\underline{\hat{v}}^{k+1}\right\|_2 = 0 \implies \text{terminate}$$

$$\underline{v}^{k+1} = \frac{\hat{v}^{k+1}}{\left\|\underline{\hat{v}}^{k+1}\right\|_2}$$

$\rightarrow$ Arnoldi iteration

Approach:

$$\underline{x}^{k+1} = \underline{x}^0 - \sum_{l=0}^{k} \alpha_l \underline{r}^l$$

$$\underline{r}^{k+1} = A\underline{x}^{k+1} - \underline{f} = \underline{r}^0 - \sum_{l=0}^{k} \alpha_l A\underline{v}^l$$

$$\left\|\underline{r}^{k+1}\right\|_2 = \left\|\underline{r}^0 - \sum_{l=0}^{k} \alpha_l A\underline{v}^l\right\|_2 \rightarrow \min_{\alpha_1, \ldots, \alpha_k}$$

Arnoldi:

$$A\underline{v}^l = \underbrace{\left\|\hat{\underline{v}}^{l+1}\right\|_2}_{\beta_{l,l+1}} \underline{v}^{l+1} + \sum_{j=0}^{l} \beta_{l,j}\underline{v}^j = \sum_{j=0}^{l+1} \beta_{l,j}\underline{v}^j$$

$$\underline{r}^{k+1} = \underline{r}^0 - \sum_{l=0}^{k} \alpha_k A\underline{v}^l = \underline{r}^0 - \sum_{l=0}^{k} \alpha_l \sum_{j=0}^{l+1} \beta_{l,j}\underline{v}^j$$

where

$$\begin{aligned}
\sum_{l=0}^{k} \alpha_l \sum_{j=0}^{l+1} \beta_{l,j}\underline{v}^j] &\overset{l=0}{=} \alpha_0 \left[\beta_{00}\underline{v}^0 + \beta_{0,1}\underline{v}^1\right] \\
&\overset{l=1}{+} \alpha_1 \left[\beta_{10}\underline{v}^0 + \beta_{11}\underline{v}^1 + \beta_{12}\underline{v}^2\right] \\
&+ \alpha_2 \left[\beta_{20}\underline{v}^0 + \beta_{21}\underline{v}^1 + \beta_2 1\underline{v}^2 + \beta_{23}\underline{v}^3\right] + \dots \\
&= \left[\beta_{00}\alpha_0 + \beta_{10}\alpha_1 + \beta_{20}\alpha_2 + \dots\right] \underline{v}^0 \\
&+ \left[\beta_{01}\alpha_0 + \beta_{11}\alpha_1 + \beta_{21}\alpha_2 + \dots\right] \underline{v}^1 \\
&+ \left[\beta_{12}\alpha_1 + \beta_{22}\alpha_2 + \dots\right] \underline{v}^2
\end{aligned}$$

$$\underbrace{\begin{pmatrix} \underline{v}^0 & \underline{v}^1 & & \\ & & & \end{pmatrix}}_{V_{k+1}\in\mathbb{R}^{n\times(k+2)}} \underbrace{\begin{pmatrix} \beta_{00} & \beta_{10} & \beta_{20} & \cdots & \beta_{k0} \\ \beta_{01} & \beta_{11} & \beta_{21} & \cdots & \beta_{k1} \\ & \beta_{12} & \ddots & & \\ & & \ddots & \ddots & \\ & & & \ddots & \beta_{kk} \\ & & & & \beta_{k,k+1} \end{pmatrix}}_{H_k\in\mathbb{R}^{(k+2)\times(k+1)}} \underbrace{\begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_k \end{pmatrix}}_{\underline{\alpha}\in\mathbb{R}^{k+1}}$$

$$\underline{r}^{k+1} = \underline{r}^0 - V_{k+1}H_k\underline{\alpha}$$

$$\underline{v}^0 = \frac{\underline{r}^0}{\left\|\underline{r}^0\right\|_2}, \qquad \underline{r}^0 = \left\|\underline{r}^0\right\|_2 \underline{v}^0 = V_{k+1}\left\|\underline{r}^0\right\|_2 \underline{e}^0 \text{ where } \underline{e}^0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\begin{aligned}
\left\|\underline{r}^{k+1}\right\|_2 &= \left\|V_{k+1}\left(\left\|\underline{r}^0\right\| \underline{e}^0 - H_k\underline{\alpha}\right)\right\|_2 \\
&= \left\| \left\|\underline{r}^0\right\|_2 \underline{e}^0 - H_k\underline{\alpha}\right\|_2 \\
&= \left\|G_K\left(\left\|\underline{r}^0\right\|_2 \underline{e}^0 - H_k\underline{\alpha}\right)\right\|_2
\end{aligned} \qquad V_{k+1}^T V_{k+1} = I_{k+2}$$

$$G_K^T G_K = I_{K+2}$$

$$G_H G_K = \begin{pmatrix} \boxed{} \\ \\ \\ \\ \end{pmatrix} \begin{pmatrix} \\ \underline{\alpha} \\ \\ \end{pmatrix} = \begin{pmatrix} \\ \\ \\ \overline{0} \end{pmatrix}$$

This lecture took place on 2018/01/17.

GMRES: Arnoldi iteration

$$\underline{x}^0 (= \underline{0}), \underline{r}^0 = A\underline{x}^0 - \underline{f}, \underline{v}^0 = \frac{\underline{r}^0}{\left\|\underline{r}^0\right\|_2}$$

For $k = 0, 1, \ldots, n-2$

$$\hat{v}^{k+1} = A\underline{v}^k - \sum_{l=0}^{k} \beta_{kl} \underline{v}^l, \beta_{kl} = (A\underline{v}^k, \underline{v}^k)$$

$$\underline{v}^{k+1} = \frac{\underline{\hat{v}}^{k+1}}{\left\|\underline{\hat{v}}^{k+1}\right\|_2}, \left\|\underline{\hat{v}^{k+1}}\right\|_2 = \beta_{k,k+1} \neq 0, \beta_{k,k+1} = 0 \implies \text{terminate}$$

$$A\underline{x} = \underline{f}$$

$$\begin{aligned}
\underline{x}^{k+1} &= \underline{x}^0 - \sum_{l=0}^{k} \alpha_l \underline{v}^l \\
\underline{r}^{k+1} &= \underline{r}^0 - \sum_{l=0}^{k} \alpha_l A \underline{v}_l \\
\left\|\underline{r}^{k+1}\right\|_2 &= \left\|\underline{r}^0 - V_{k+1} H_k \underline{\alpha}\right\|_2 \\
&= \left\|\left\|\underline{r}^0\right\|_2 \underline{e}^0 - H_k \underline{\alpha}\right\|_2 \\
&= \left\| \underbrace{Q_k \left(\left\|\underline{r}^0\right\|_2 \underline{e}^0 - H_k \underline{\alpha} \right)}_{\underline{z} \in \mathbb{R}^{k+2}} \right\|_2 \qquad Q_k \in \mathbb{R}^{(k+2)\times(k+2)}, Q_k^T Q_k = I
\end{aligned}$$

$$V_{k+1} = (\underline{v}^0 \ldots, \underline{v}^k)$$

$$H_k = \begin{pmatrix} \beta_{00} & \beta_{10} & \cdots & \\ \beta_{01} & \beta_{11} & & \vdots \\ & \beta_{12} & \ddots & \\ & & \ddots & \beta_{kk} \\ & & & \beta_{kk+1} \end{pmatrix}$$

$$Q_k \overbrace{\begin{pmatrix} \cdots & & & & \\ & \cdots & & & \\ & & \cdots & & \\ & & & \cdots & \\ & & & & \cdots \end{pmatrix}}^{k+1} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_k \end{pmatrix} = Q_k \begin{pmatrix} r \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\downarrow$$

$$\begin{pmatrix} 0 & & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 0 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_k \end{pmatrix} = \begin{pmatrix} f_0 \\ \vdots \\ f_k \\ f_{k+1} \end{pmatrix}$$

$$\begin{aligned} \left\|\underline{z}\right\|_2^2 &= \sum_{l=0}^{k+1} z_l^2 - \sum_{l=0}^{k} z_l^2 + z_{k+1}^2 \\ &= f_{k+1}^2 + \left\| \underbrace{\left(Q_k H_k \underline{\alpha} - Q_k \left\|\underline{r}^0\right\|_2 \underline{e}^0\right)_{l=0,k}}_{\neq 0} \right\|_2 \\ &= f_{k+1}^2 \\ \min_{\alpha_0,\ldots,\alpha_k} \left\|\underline{r}^{k+1}\right\|_2 &= \left|f_{k+1}\right| \text{ if } \left(Q_k H_k \underline{\alpha} - Q_k \left\|\underline{r}^0\right\|_2\right)_{l=0,k} = \underline{0} \end{aligned}$$

$Q_k \rightsquigarrow$ Givens-Rotation

1st column of H_k:

$$\underbrace{\begin{pmatrix} a_0 & b_0 & & & \\ -b_0 & a_0 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix}}_{G_0} \begin{pmatrix} \beta_{00} \\ \beta_{01} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$a_0 = \frac{\beta_{00}}{\sqrt{\beta_{00}^2 + \beta_{01}^2}}$$

$$b_0 = \frac{\beta_{01}}{\sqrt{\beta_{00}^2 + \beta_{01}^2}}$$

$$\implies -b_0\beta_{00} + a_0\beta_{01} = \frac{-\beta_{01}\beta_{00}\beta_{00}\beta_{01}}{\sqrt{\beta_{00}^2 + \beta_{01}^2}} = 0$$

$$\underbrace{\begin{pmatrix} 1 & & & & & \\ & a_1 & b_1 & & & \\ & -b_1 & a_1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & \ddots \\ & & & & & & 1 \end{pmatrix}}_{G_1} G_0 H_k = G_1 \begin{pmatrix} \tilde{\beta}_{00} & \tilde{\beta}_{10} & \tilde{\beta}_{20} & \cdots \\ 0 & \tilde{\beta}_{11} & \tilde{\beta}_{21} & \cdots \\ 0 & \tilde{\beta}_{12} & \tilde{\beta}_{22} & \cdots \\ \vdots & \vdots & \vdots & \\ 0 & & & \end{pmatrix}$$

$$= \begin{pmatrix} \tilde{\beta}_{00} & \tilde{\beta}_{10} & \cdots & & \beta_{k0} \\ 0 & \tilde{\beta}_{11} & \tilde{\beta}_{21} & \cdots & \\ 0 & 0 & \tilde{\beta}_{22} & \cdots & \\ \vdots & \vdots & \vdots & & \\ 0 & 0 & & & \end{pmatrix} \underbrace{G_k \dots G_2 G_1 G_0}_{Q_k} H_k = \begin{pmatrix} * & & & & \\ 0 & * & & & \\ & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \ddots & * \\ & & & & & 0 \end{pmatrix}$$

G_j:

$$a_j = \frac{\beta_{jj}}{\sqrt{\beta_{jj}^2 + \beta_{jj+1}^2}}, b_j = \frac{\beta_{jj+1}}{\sqrt{\beta_{jj} + \beta_{jj+1}^2}}$$

$$Q_k \begin{pmatrix} \left\|\underline{r}^0\right\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$G_1 G_0 \left\|\underline{r}^0\right\|_2 \underline{e}^0 = G_1 \begin{pmatrix} a_0 & b_0 & & & \\ -b_0 & a_0 & & & \\ & & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{pmatrix} \begin{pmatrix} \left\|\underline{r}^0\right\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = G_1 \begin{pmatrix} a_0 \left\|\underline{r}^0\right\|_2 \\ -b_0 \left\|\underline{r}^0\right\|_2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} a_0 \left\|\underline{r}^0\right\|_2 \\ -a_1 b_0 \left\|\underline{r}^0\right\|_2 \\ (-b_1)(-b_0) \left\|\underline{r}^0\right\|_2 \\ \vdots \end{pmatrix}$$

$$Q_k \left\| \underline{r}_2 \right\| \underline{e}^0 = \underline{f}$$

$$f_{k+1} = \prod_{l=0}^{k} (-b_l) \left\| \underline{r}^0 \right\|_2$$

$$\left\| \underline{r}^{k+1} \right\|_2 = \prod_{l=0}^{k} \frac{\left| \beta_{ll+1} \right|}{\sqrt{\beta_{ll}^2 + \beta_{l,l+1}^2}} \left\| \underline{r}^0 \right\|_2 = 0, \beta_{k,k+1} = 0$$

Remark on GMRES algorithm:

1. Combination of Arnoldi and Minimieg (application of Givens rotation)
2. Are other search directions considered, then we have to apply *all* previous Givens rotations
3. The Arnoldi termination criterion is very robust: $p_{kk+1} = 0 \implies \underline{x} = \underline{x}^{k+1}$
4. Preconditioning is analogously applicable, $A\underline{x} = \underline{f} \rightsquigarrow B^{-1}A\underline{x} = B^{-1}\underline{f}$ where $B^{-1}A = \tilde{A}$
5. Computation of $\underline{x}^{k+1}$ after minimization requires knowledge about *all* search directions $\underline{v}^l$, $v_k \sim k_n$, memory requirement f
   - GMRES(K): restart with k iterations, $\underline{x}^0 \to \underline{x}^k, \underline{x}^k \dots \underline{x}^{2k+1}$, H_k convergence?
   - BiCGStab (short recurrences, interruption)

In practice: if you preconditioning is very good, the method is neglectible. If your preconditioning is bad, you are screwed.

This lecture took place on 2018/01/22.

Non-linear equations

Find $\overline{x} \in [a, b] : f(\overline{x}) = 0$.

$$f \in C([a, b]) \text{ continuous}, f(a)f(b) < 0$$

Our goals is the construction of approximate solutions x_k (might be ambiguous, see Figure 13) with $\lim_{k\to\infty} x_k = \overline{x}$ with $\left| x_{k+1} - \overline{x} \right| \leq c \left| x_k - \overline{x} \right|^p$. p is called *convergence order*.

$p = 1, c < 1$.

Convergence for all $x_0 \in [a, b] \rightsquigarrow$ global convergence. Convergence only for $x_0 \in \mathcal{U}_\varepsilon(\overline{x}) \rightsquigarrow$ local convergence.

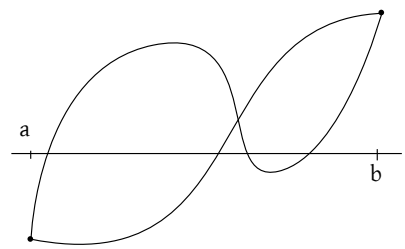


Figure 13: There might be multiple solutions for $f(x) = 0$ for $x \in [a, b]$

Bisection method

$f(x) = 0, x \in [a, b], f(x)$ continuous, $f(a)f(b) < 0$.

Algorithm:

1. $a_0 := a, b_0 := b$
2. For $k = 0, 1, 2, \ldots$
   (a) $x_k = \frac{1}{2}(a_k + b_k)$
   (b) $f(x_k) = 0 \implies \overline{x} = x_k$, then terminate
   (c) If $f(a_k)f(x_k) < 0$, $a_{k+1} = a_k, b_{k+1} = x_k$
   else $a_{k+1} = x_k, b_{k+1} = b_k$

$$\left|x_k - \overline{x}\right| \leq \frac{b_k - a_k}{2} \implies \left|x_k - \overline{x}\right| \leq \frac{1}{2^{k+1}} |b - a|$$

gives global convergence.

Example 12. *Let $x \in [1, 4]$, $f(x) = x^2 - 4$ and obviously $\overline{x} = 2$.*

k	a_k	b_k	x_k	
0	*1*	*4*	*2.5*	*0.5*
1	*1*	*2.5*	*1.75*	*0.25*
2	*1.75*	*2.5*	*2.125*	*0.125*
$\vdots$				

Example 13.

$$f(x) = \frac{x}{8}(63x^4 - 70x^2 + 15)$$

Let $[a,b] = [0.8, 1], \overline{x} = \frac{1}{21}\sqrt{245 + 14\sqrt{70}} \sim 0.906179\ldots$.

$$x_0 = 0.9, \left|x_0 - \overline{x}\right| \sim 0.006$$

$$x_1 = 0.95, \left|x_1 - \overline{x}\right| \sim 0.048\ldots$$

As we can see the error increases. So convergence is not monotone. So, what is our termination criterion? The desired convergence property would be:

$$\left|x_{k+1} - \overline{x}\right| < \left|x_k - \overline{x}\right|$$

Method of Successive Approximation

Determination of a root of $f(x) = 0, x \in [a,b]$. We look for fixed point $x = \varphi(x)$. Successive approximation takes the approach to define initial value x_0 and determines $x_{k+1} := \varphi(x_k)$. What about convergence?

Theorem 11 (Banach fixed point theorem)**.** *Let D be a self-mapping:*

$$D := [a,b] \qquad \varphi : [a,b] \to [a,b]$$

$$\left|\varphi(x) - \varphi(y)\right| \leq q\left|x - y\right| \forall x, y \in [a,b], q < 1 \text{ contraction}$$

Then the sequence $x_{k+1} = \varphi(x_k)$ *of approximate solution for every* $x_0 \in [a,b]$ *towards a unique solution* $\overline{x} = \varphi(\overline{x})$.

Remark. *The following error estimates hold:*

$$\overline{x} = \varphi(\overline{x}), x_{k+1} = \varphi(x_k)$$

$$\begin{aligned}
\left|x_{k+1} - \overline{x}\right| &= \left|\varphi(x_k) - \varphi(\overline{x})\right| \leq q\left|x_k - \overline{x}\right| \\
&= q\left|x_k \underbrace{-x_{k+1} + x_{k+1}}_{=0} - \overline{x}\right| \\
&\leq q\left|x_k - x_{k+1}\right| + q\left|x_{k+1} - \overline{x}\right| \\
\implies \left|x_{k+1} - \overline{x}\right| &\leq \frac{q}{1-q}\left|x_{k+1} - x_k\right|
\end{aligned}$$

is an a-posterior error estimate. Alternatively,

$$\begin{aligned}
\left|x_{k+1} - \overline{x}\right| &\leq q\left|x_k - \overline{x}\right| \\
&\leq q^2\left|x_{k-1} - \overline{x}\right| \\
&\leq \ldots \\
&\leq q^{k+1}\left|x_0 - \overline{x}\right| \\
&\leq q^k \underbrace{\left|x^1 - \overline{x}\right|}_{\leq \frac{q}{1-q}|x_1 - x_0|}
\end{aligned}$$

A-priori error estimate:

$$\left|x_{k+1} - \overline{x}\right| \leq \frac{q^{k+1}}{1-q} \left|x_1 - x_0\right|$$

Example 14. $[a, b] = [1, 4]$, $f(x) = x^2 - 4 = 0$.

$$\begin{aligned} x^2 &= 4 \\ 2x^2 &= 4 + x^2 \\ x &= \frac{1}{2}\left(x + \frac{4}{x^2}\right) \end{aligned}$$

$$\implies x_{k+1} = \frac{1}{2}\left(x_k + \frac{4}{x_k}\right) \qquad x_0 = 4$$

$\{x_{k+1}\}$ *is monotonically decreasing and bounded by below.*

$$\varphi(x) = \frac{1}{2}\left(x + \frac{4}{x}\right)$$

Contraction?

$$\left|\varphi(x) - \varphi(y)\right| \leq q\left|x - y\right| \overset{x \neq y}{\iff} \frac{\left|\varphi(x) - \varphi(y)\right|}{\left|x - y\right|} \leq q \qquad \forall x, y \in [2, 4], x \neq y$$

$$\max_{\eta \in [2,4]} \left|\varphi'(\eta)\right| = q$$

$$\begin{aligned} \varphi(x) &= \frac{1}{2}\left(x + \frac{4}{x}\right) \\ \varphi'(x) &= \frac{1}{2}\left(1 - \frac{4}{x^2}\right) \\ \implies q &= \frac{3}{8} < 1 \end{aligned}$$

Hence, Banach's Fixed Point Theorem provides linear convergence.

$$x_{k+1} = \frac{1}{2}\left(x_k + \frac{4}{x_k}\right)$$

$$x_0 = 4 \qquad \left|x_0 - \overline{x}\right| = 2$$

$$x_1 = \frac{5}{2} = 2.5 \qquad \left|x_1 - \overline{x}\right| = 0.5$$

$$x_2 = \frac{1}{2}\left(\frac{5}{2} + \frac{4}{\frac{5}{2}}\right) = \frac{41}{20} = 2.05 \qquad \left|x_2 - \overline{x}\right| = 0.05$$

$$x_3 = \frac{1}{2}\left(\frac{41}{20} + \frac{4 \cdot 20}{41}\right) = \frac{1}{2}\frac{41^2 + 1600}{820} \qquad \left|x_3 - \overline{x}\right| \approx 0.00061$$

Is this better than linear convergence?

Proof of higher convergence order.

$$\begin{aligned}
\left|x_{k+1}-\overline{x}\right| &= \left|\varphi(x_k)-\varphi(\overline{x})\right| \\
&= \left|\frac{1}{2}\left(x_k+\frac{4}{x_k}\right)-\frac{1}{2}\left(\overline{x}+\frac{4}{\overline{x}}\right)\right| \\
&= \frac{1}{2}\left|x_k-\overline{x}+\frac{4}{x_k}-\frac{4}{\overline{x}}\right| \\
&= \frac{1}{2}\left|x_k-\overline{x}+4\frac{\overline{x}-x_k}{x_k\overline{x}}\right| \\
&= \frac{1}{2}\left|x_k-\overline{x}\right|\underbrace{\left|1-\overbrace{\frac{4}{x_k\overline{x}}}^{=\overline{x}^2}\right|}_{=1-\frac{\overline{x}}{x_k}=\frac{1}{x_k}(x_k-\overline{x})}
\end{aligned}$$

$$\implies \left|x_{k+1}-\overline{x}\right| \leq \frac{1}{2}\frac{1}{x_k}\left|x_k-\overline{x}\right|^2$$

$p=2$ is squared convergence.

This is the Babylonian method of computing square roots. □

Recursion recurrence → Taylor

$$\begin{gathered}
f(x)=f(x_0)+(x-x_0)f'(\eta) \\
x_0 \rightsquigarrow x_k \qquad x \rightsquigarrow \overline{x} : f(\overline{x})=0 \\
0=f(\overline{x})=f(x_k)+(\overline{x}-x_k)f'(\eta) \\
\overline{x}=x_k-\frac{f(x_k)}{f'(\eta)}, f'(\eta)\neq 0
\end{gathered}$$

Approximation of $f'(\eta) \rightsquigarrow$ approximation method

$$f'(\eta)\sim\frac{f(b)-f(a)}{b-a} \implies x_{k+1}=x_k-\frac{b-a}{f(b)-f(a)}f(x_k)$$

This is the so-called *chord method*.

$$f'(\beta)\sim\frac{f(x_k)-f(x_{k-1})}{x_k-x_{k-1}} \qquad x_{k+1}=x_k-\frac{x_k-x_{k-1}}{f(x_k)-f(x_{k-1})}f(x_k)$$

This is the so-called *secant method*.

$$f(a)f(b)<0, f(x_k)f(x_{k-1})>0 \implies x_l : f(x_k)f(x_l)<0$$

$$f'(\eta) \approx \frac{f(x_k) - f(x_l)}{x_k - x_l} \qquad l := \operatorname{argmax}\left\{j : f(x_k)f(x_j) < 0\right\}$$

This is the so-called *Regula Falsi*

$$f'(x_k) \neq 0 \implies f'(\eta) \sim f'(x_k)$$
$$\implies x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

This is the so-called *Newton method*.

Theorem 12. *Let $f(x)$ be two times differentiable and in the neighborhood of zero value $\overline{x}$ it holds that*

$$\frac{1}{2}\left|\frac{f''(x)}{f'(\tilde{x})}\right| \leq M.$$

x_0, x_1 satisfy:

$$K = \max\left\{M\left|x_0 - \overline{x}\right|, \sqrt[p]{M\left|x_1 - \overline{x}\right|} < 1, p = \frac{1+\sqrt{5}}{2} \sim 1.618\right\}$$

$$\implies \left|x_{k+1} - \overline{x}\right| \leq \frac{1}{M}K^{p^{k+1}}$$

Secant method.

$$x_{k+1} = \varphi(x_k), \qquad \overline{x} = \varphi(\overline{x})$$
$$\varphi^{(n)}(\overline{x}) = 0 \implies \left|x^{k+1} - \overline{x}\right| \leq ?$$

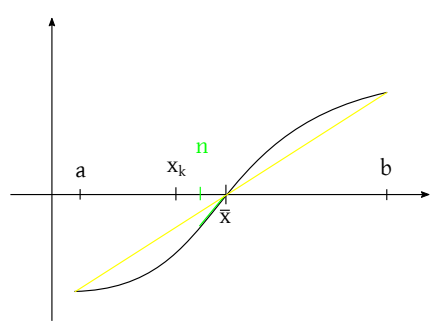


Figure 14: The green slope is approximated with the yellow slope in the chord method

This lecture took place on 2018/01/24.

Revision: Non-linear equations:

$$f(\overline{x}) = 0$$

$$x = \varphi(x) \qquad x_{k+1} = \varphi(x_k)$$

Theorem 13. *Let $D = [a, b]$. Let $\varphi(x)$ is p-times continuously differentiable in D. Furthermore we assume*

$$\varphi'(x) = \varphi''(x) = \ldots = \varphi^{(p-1)}(\overline{x}) = 0 \text{ in } \overline{x} = \varphi(\overline{x})$$

and $\varphi^{(p)}(\overline{x}) \neq 0$.

Then it holds that

$$\left|x_{k+1} - \overline{x}\right| \leq \frac{1}{p!} \max_{x \in \mathcal{U}_\delta(\overline{x})} \left|\varphi^{(p)}(x)\right| \left|x_k - \overline{x}\right|^p$$

where $\mathcal{U}_\delta$ defines a neighborhood.

Proof.

$$x_{k+1} = \varphi(x_k) = \varphi(\overline{x}) + \sum_{n=1}^{p-1} \frac{1}{n!}(x_k - \overline{x})^n \underbrace{\varphi^{(n)}(\overline{x})}_{=0} + \frac{1}{p!}\varphi^{(p)}(\eta)(x_k - \overline{x})^p$$

$$\implies x_{k+1} - \overline{x} = \frac{1}{p!}\varphi^{(p)}(\eta)(x_k - \overline{x})^p$$

$\varphi^{(p)}(\overline{x}) \neq 0$, $\varphi^{(p)}(x)$ is continuous $\implies \varphi^{(p)}(x) \neq 0$ in $\mathcal{U}_\delta(\overline{x})$, hence the assumption follows. □

Application of the Newton method:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} =: \varphi(x_k) \qquad \varphi(x) = x - \frac{f(x)}{f'(x)} \qquad f'(x) \neq 0 \text{ in } \mathcal{U}_\delta(\overline{x})$$

$$\varphi'(x) = 1 - \frac{f'(x)}{f'(x)} + \frac{f(x)f''(x)}{[f'(x)]^2} = \frac{f(x)f''(x)}{[f'(x)]^2}$$

$$\varphi'(\overline{x}) = \frac{f(\overline{x})f''(\overline{x})}{[f'(\overline{x})]^2} = 0$$

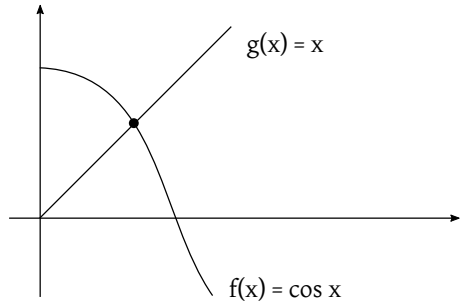
$$\varphi''(x) = \frac{f''(x)[f'(x)]^2 - 2f(x)[f''(x)]^2 + f(x)f'(x)f^{(3)}(x)}{[f'(x)]^3}$$

$$\varphi''(\overline{x}) = \frac{f''(\overline{x})}{f'(\overline{x})} \neq 0 \text{ in general}$$

$\implies p = 2$, hence

$$\left|x_{k+1} - \overline{x}\right| \leq c\left|x_k - \overline{x}\right|^2$$

Quadratic convergence of the Newton method.



Example 15.

Figure 15: Example intersecting $\cos(x)$ and x

$$x = \cos(x)$$
$$x_{k+1} = \cos(x_k)$$

$\varphi(x) = \cos(x)$; *contraction for* $x \in [0,1]$; *Banach fixed point theorem: convergence for* $x_0 \in [0,1]$; *Convergence for* $x_0 \in \mathbb{R}$.

Newton method:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$
$$f(x) = x - cos(x)$$
$$f'(x) = 1 + \sin(x) \qquad f'\left(\frac{3\pi}{2}\right) = 0$$

This example shows that we only achieve local convergence (even though quadratic convergence by Newton's method is given).

Example 16 (Babylonian method for computing the square root)**.**

$$x_{k+1} = \frac{1}{2}\left(x_k + \frac{a}{x_k}\right)$$
$$\varphi(x) = \frac{1}{2}\left(x + \frac{a}{x}\right)$$
$$\varphi'(x) = \frac{1}{2}\left(1 - \frac{a}{x^2}\right)$$
$$\overline{x} = \sqrt{a}$$
$$\varphi'(\sqrt{a}) = 0$$
$$\varphi''(x) = \frac{a}{x^3}$$
$$\varphi''(\sqrt{a}) = \frac{1}{\sqrt{a}} \neq 0$$

$p = 2$, quadratic convergence.

Example 17.

$$x^2 = a \qquad f(x) = x^2 - a \qquad f'(x) = 2x$$

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

Hence, the Babylonian method of computing square roots corresponds to the Newton method.

Non-linear equation systems:

$$F(\underline{x}) = 0 \qquad \underline{x} \in \mathbb{R}^n \qquad F(\underline{x}) = \left(f_i(\underline{x})\right)_{i=1}^n$$

$$f_i(x_1, \ldots, x_n) = 0$$

$$0 = f_i(\overline{\underline{x}}) = f_i(\underline{x}^k) + \sum_{j=1}^n \left(\overline{x}_j - x_j^k\right) \frac{\partial}{\partial x_j} f_i(\underline{x})\bigg|_{\underline{x}=\underline{x}^k} + \text{ remainder}$$

$$\iff 0 = f_i(\underline{x}^k) + \sum_{j=1}^n \left(x_j^{k+1} - x_j^k\right) \underbrace{\frac{\partial}{\partial x_j} f_i(\underline{x})\bigg|_{x=\underline{x}^k}}_{A_{ij}(\underline{x}^k)}$$

$$F(\underline{x}^k) + A(\underline{x}^k)\left(\underline{x}^{k+1} - \underline{x}^k\right) \overset{!}{=} \underline{0}$$

$$\underline{x}^{k+1} = \underline{x}^k - \left[A(\underline{x}^k)\right]^{-1} F(\underline{x}^k)$$

This lecture took place on 2018/01/29.

Today was the second partial exam of the practicals. No lecture.

This lecture took place on 2018/01/31.

Final conclusions

Approximation of functions

We considered the problem of approximation of functions. This problem has local and global solutions. We discussed two methods of interpolation and

projections. Approximation properties in a scale of function spaces (those spaces are called Sobolev-spaces[5]):

$$\|u - u_h\|_\tau \leq ch^{s-\tau} |u|_s \qquad 0 \leq \tau \leq s \leq p+1, \tau \leq 1$$

τ is bounded by the regularity of the base functions. Analogue error estimates also hold for $\tau < 0$ in case of projection methods (explicitly *no* interpolation!). Why is interpolation still popular? Interpolation is local and simple to compute[6], but continuity of the approximating function is required and stability is a big concern. In contrast, projection is more stable, but global[7].

Can we combine these approaches? This lead to the development of *Quasi-Interpolation*. You define a parameter:

$$R_b u(x) = \sum_{k=1}^{n} F_k(u) e_k(x)$$

This also works for higher dimensions. But the proof techniques become more difficult. Approximation property is part of computational calculus (dt. numerische Analysis) of discretization methods for Dgl (?).

Numerical integration

Next, we considered numerical integration. We discussed Gauss-Legendre in 1D. There are 3 approaches:

- Tensor product in $\mathbb{R}^n$
- multidimensional Gauss formula (Radon, 7 points)
- singular surface integrals

Linear Equation Systems

To solve linear equation systems, we discussed two direct methods: CG method and GMRES. These are just two of many methods, but especially the CG method is very fundamental. In "Elective Subject" courses, further variants of GMRES are discussed. Then we also discussed preconditioning and its application.

Non-linear equation systems

We discussed the Newton method.

[5] We explicitly did not define this space in the lecture.
[6] if one point changes, only one coefficient needs to be recomputed
[7] if one point changes, an entire linear equation system needs to be resolved

Eigenvalues problems

We did not cover this topic, but will be caught up in "Elective Subjects".

Further courses at University of Technology Graz:

1. Numerik 1 (Ordinary Differential Equations) [4th semester]
2. Numerik 2 (Ordinary Differential Equations), Partial Differential Equations [5th semester]
3. Numerik 3 (Ordinary Differential Equations) [6th semester]

Exams will be held orally and please look up the next exam dates online or request possible exam dates via email.