Numerical Computations Summary

Polynomial Interpolation

goal: given $\{(x_i, f_i)\}$, find $p \in P_n$ s.t. $p(x_i) = f_i$ (1)

application: extra-/interpol, int, diff

Theorem (Lagrange Interpol) x_i .. distinct $\Rightarrow \exists\, p \in P_n$ s.t.

$$p(x) = \sum_i f_i \cdot l_i(x), \qquad l_i(x) = \prod_{\substack{j=0 \\ j \neq i}} \frac{x - x_j}{x_i - x_j}$$

Proof:
1. $l_i \in P_n$
2. $l_i(x_j) = \delta_{ij}$
3. $1, 2 \Rightarrow p$ is a solution to the interp. problem (1)
4. p_1, p_2 .. solutions $\Rightarrow p := p_1 - p_2 \in P_n$, p has at least $n+1$ zeros, fund. theor. algebra $\Rightarrow p_1 \equiv p_2$ ∎

More efficient evaluation of $p(x)$: Neville-scheme

Theorem (Neville-scheme) given $\{(x_i, f_i)\}$, denote by $P_{jm} \in P_m$: find $p \in P_m$ s.t. $p(x_k) = f_k$ for $k \in \{j, \dots j+m\}$

$$\Rightarrow \begin{cases} P_{j0} = f_j \\ P_{jm} = \dfrac{(x - x_j)\, P_{j+1, m-1}(x) - (x - x_{j+m})\, P_{j, m-1}(x)}{x_{j+m} - x_j} =: \Pi, & m \geq 1 \end{cases}$$

Proof:
- $\Pi \in P_m$
- $\Pi(x_j) = P_{j, m-1}(x_j) = f_j$
- $\Pi(x_{j+m}) = P_{j+1, m-1}(x_{j+m}) = f_{j+m}$
- $i \in \{j+1, \dots j+m-1\}$

  $\Pi(x_i) = \dots f_i$

$\Big\}\ \#\ \Rightarrow \Pi = P_{j,m}$ ∎

Cost: $O(n^2)$ bzw. $O(\frac{n^2}{2})$

More efficient evaluation in $O(n)$:

Definition (divided Diff): $f[x_i] := f_i$

$$f[x_0, \dots x_k] := \frac{f[x_1, \dots x_k] - f[x_0, \dots x_{k-1}]}{x_k - x_0}$$

Definition (Newton Polyn.): $$p(x) = \sum_{j=0}^{n-1} d_j w_j \,, \qquad w_j := \prod_{i=0}^{j-1} (x - x_i) \qquad (2)$$

Theorem (Newton Polyn.): x_i .. distinct:

$$\Longrightarrow \quad d_i \equiv f[x_0, \dots x_i]$$

Proof: Neville-Theorem $\Longrightarrow$ leading coeff of $P_{j,k} := lc(P_{j,k}) = f[x_j, \dots x_{j+k}]$

then do induction on k

Remark: $$f[x_0, \dots x_k] \approx \frac{1}{k!} f^{(k)}(x_0)$$

Definition: (Horner scheme) rearrange (2) gives $O(n)$ evaluation:

$$p(x) = d_0 + d_1(x - x_0) + d_2(x - x_0)(x - x_1) + \dots$$

$$\Longleftrightarrow \quad p(x) = d_0 + (x - x_0)\Big[d_1 + (x - x_1)\big[d_2 + \dots\big]\Big]$$

Evaluation: $O(n)$, find coeffs: still $O(n^2)$

Remark:
Use Neville scheme for extrapolation, e.g. $u(x) = e^x$

Define $$D(h) := \begin{cases} u'(0) & h = 0 \\ \dfrac{u(0+h) - u(0)}{h} & \text{else} \end{cases}$$

Do a Neville scheme for $h_j = 2^{-j}$, $j \in \{0, 1, \dots 10\}$

$$\begin{array}{llll} & m_0 & m_1 & m_2 \; \dots \\ h_0 & D(h_0) = D_{00} & D_{01} & D_{02} \; \dots \\ h_1 & D_{10} & & \\ \vdots & D_{20} & & \\ & \vdots & & \end{array}$$

Theorem (Interp. error) $[a,b] \subset \mathbb{R}$, $x_i \in [a,b]$ distinct, $f \in C^{(n+1)}([a,b]) \Rightarrow \exists \xi \in [a,b]$ s.t.

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

Proof: 1. $g \in C^1,\ g(a)=g(b) \Rightarrow \exists \xi \in [a,b] : g'(\xi)=0$

2. for $x \in \{x_0, \dots x_n\} \Rightarrow w_{n+1}(x)=0 \Rightarrow p-f=0$

3. for $x \notin \{x_0, \dots x_n\}$.

Define $g(t) = f(t) - p(t) - K\, w_{n+1}(t)$, $\quad K := \dfrac{f(x)-p(x)}{w_{n+1}(x)}$

g has $n+2$ zeros : $x_0, \dots x_n$ and x

$g^{(n+1)}$ has 1 zero, $p^{(n+1)} \equiv 0$, $w_{n+1}^{(n+1)} = (n+1)!$

$$\Rightarrow 0 = g^{(n+1)}(\xi) = f^{n+1}(\xi) - \underbrace{p^{(n+1)}(\xi)}_{\equiv 0} - K \underbrace{w_{n+1}^{(n+1)}}_{=(n+1)!}$$

$$\Rightarrow K = \frac{f^{(n+1)}(\xi}{(n+1)!}$$

$\blacksquare$

Theorem (Interpol. err) $\quad f \in C^{n+1}([a,b])$, $h_i := q^i$, $x_0 \in [a,b]$

$p_{i,m} \in P_m$ interpolates f at $x_0 + h_{i+j}$, $j \in \{0, \dots m\} \Rightarrow \exists C >$ s.t.

$$|f(x_0) - p_{i,m}(x_0)| \le C \cdot h_i^{m+1}$$

Proof: use previous theorem $\Rightarrow \exists \xi$ st.

$$|f(x_0) - p_{i,m}(x_0)| \le \frac{1}{(m+1)!} |f^{(m+1)}(\xi)| \cdot \Big|\underbrace{\prod_j \left(x_0 - (\cancel{x_0} - h_{i+j})\right)}_{= w_{n+1}(x_0)}\Big| \le C\, h_i^{m+1}$$

$\blacksquare$

Extrapolation of func. with add. structure

$$D_{sym} := \frac{u(0+h) - u(0-h)}{2h} \overset{\text{Taylor}}{=} u'(0) + \frac{1}{3!} u^{(3)}(0) h^2 + \frac{1}{5!} u^{(5)}(0)\, h^4 + \dots$$

$\Rightarrow D_{sym}$ is a function of h^2

we interpolate $(h_i^2, D_{sym}(h_i))$, $\forall i \in \{0, \dots n\}$

$\Rightarrow$ because D_{sym} is symmetric $\Rightarrow (-h_{i+j}, D_{sym}(-h_{i+j})) = (-h_{i+j}, D_{sym}(h_{i+j}))$

$\Rightarrow$ error bound $C h_i^{2m}$

Theorem (Chebyshev points) $\quad$ choosing $x_i = \frac{a+b}{2} + \frac{b-a}{2} \cdot \cos\left(\pi \frac{2i+1}{2n+2}\right)$

yields $\Rightarrow \|w_{n+1}^{cheb}\|_\infty \le \|w_{n+1}\|_\infty$

Theorem (Chebyshev error bound)

Define Lebesgue const.

$\Lambda_n^{cheb} := \max_x \sum_i |\ell_i^{cheb}(x)|$ Lagrange polynom.

$I_n^{cheb} f$ ... interpolation polynomial of f

$\Rightarrow$ (i) $\|I_n^{cheb} f\|_\infty \leq \Lambda_n \|f\|_\infty$

(ii) $\|f - I_n^{cheb} f\|_\infty < (1+\Lambda_n) \min_{q \in P_n} \|f-q\|_\infty$

(iii) $\Lambda_n \leq \frac{2}{\pi} \ln(n+1) + 1$

Proof: (i) $\|I_n f\|_\infty = \max_x |(I_n f)(x)| = \max_x |\sum_i f(x_i) \cdot \ell_i(x)|$

$\leq \max_i |f(x_i)| \cdot \max_x \sum_i |\ell_i| \leq \|f\|_\infty \cdot \Lambda_n$

(ii) $\|f - I_n f\|_\infty = \|f - I_n f - \underbrace{(q - I_n q)}_{\equiv 0,\ q \in P_n}\|_\infty = \|f - q - I_n(f-q)\|_\infty$

$\leq \|f-q\|_\infty + \|I_n(f-q)\|_\infty$

$\overset{(i)}{\leq} \|f-q\|_\infty + \Lambda_n \|f-q\|_\infty = (1+\Lambda_n)\|f-q\|_\infty$

(iii) Literature ∎

Remark • Λ_n ... "how much worse Chebyshev interpol in comparison to best possible interpolation in $\|\cdot\|_\infty$ norm"

• Λ_n grows with $\log(n)$

• perturbations in $f(x_i^{cheb})$ have small impacts on error

Splines: Definition

partition $\Delta = \{a = x_0, x_1, \dots x_n = b\}$ on $[a,b] \subset \mathbb{R}$

step width $h_i = x_{i+1} - x_i$

spline space $S^{p,r}(\Delta) := \{u \in C^r([a,b]),\ u|_{I_i} \in P_p\ \forall i\}$

element $I_i := (x_i, x_{i+1})$

$s \in S^{p,r}(\Delta)$ is a spline if $s(x_i) = f_i\ \forall i$

Def: Lin. splines $p=1, r=0$: $s \in S^{1,0}$ has unique solution $s(x) = \sum_i f_i \varphi_i(x)$

with $\varphi_i(x_j) = \delta_{ij}$

Lemma (linear Spline error): $\|f-s\|_\infty \leq Ch^2 \|f''\|_\infty$

Def. Cubic Spline $\quad p=3,\ r=2$

$s \in S^{3,2}(\Delta)$ s.t. $s(x_i) = f_i\ ,\ \forall i \in \{0, \dots n\}$

these are $n+1$ equations

Lemma (Dim of $S^{p,r}(\Delta)$) $\quad \dim(\mathcal{P}_p) = p+1$

$\Rightarrow$ space of discont. polynomials : $\dim = n(p+1)$

$\left.\begin{array}{l} s \in C^r \\ n-1 \text{ interior points} \end{array}\right\} \Rightarrow (n-1)(r+1)$ conditions

$\Rightarrow \dim(S^{p,r}(\Delta)) = n(p+1) - (n-1)(r+1)$

for cubic spline : $\dim(S) = n+3 \Rightarrow$ need 2 more cond.

Def. Cubic splines

1. complete/clamped spline : $s'(x_0) = f'_0\ ,\quad s'(x_n) = f'_n$
2. periodic spline : $s'(x_0) = s'(x_n),\quad s''(x_0) = s''(x_n)$
3. natural spline : $s''(x_0) = s''(x_n) = 0$
4. „not-a-knot" : no jump at $s'''(x_0)$ or $s'''(x_n)$

Theorem (cubic Spline error)

if either (i) s ... complete/clamped
(ii) s ... periodic and $f_0 = f_n$
(iii) s ... „not-a-knot"

$\Rightarrow$ s is unique and $\quad \|f-s\|_\infty \leq Ch^4 \|f^{(4)}\|_\infty$
$\qquad \|f'-s'\|_\infty \leq Ch^3 \|f^{(4)}\|_\infty$

Theorem (energy minimization)

(i) complete $\quad s \in S^{3,2}$: $\|s''\|_{L^2} \leq \|y''\|_{L^2} \quad \forall y \in C_{compl.}$

$C_{compl.} = \{ y \in C^2 \mid y(x_i) = f_i,\ y'(x_0) = f'_0,\ y'(x_n) = f'_n \}$

(ii) natural $\quad s \in S^{3,2}$: $\|s''\|_{L^2} \leq \|y''\|_{L^2} \quad \forall y \in C_{nat}$

$C_{nat} = \{ \quad -\text{"}- \quad y''_0 = y''_n = 0 \}$

(iii) periodic $\quad s \in S^{3,2}$: $\|s''\|_{L^2} \leq \|y''\| \quad \forall y \in C_{per.}$

$C_{per} = \{ \quad -\text{"}- \quad y'_0 = y'_n\ ,\ y''_0 = y''_n \}$

Remark: in Elasticity theory: deflection y of spline is such that the energy $\frac{1}{2}\|y''\|^2_{L^2}$ is minimized

the prev. theorem shows splines that minimize this energy

Remark: $r \geq p \implies S^{p,r}(\Delta) = \mathcal{P}_p$

Hermite interpol:

Def. Trigonometric interpol. polyn. of f

$$p(x) = \sum_{j=-m}^{m} c_j e^{ijx} \quad \text{and} \quad p(x_k) \overset{!}{=} y_k \qquad (3)$$

Def. Fourier series of f

$$f(x) = \sum_{j=-\infty}^{\infty} f_j e^{ijx} \quad \text{with} \quad f_j = \frac{1}{2\pi}\int_0^{2\pi} f(x) e^{-ijx}\, dx$$

To approximate $f(x)$, use c_j instead of f_j

Modified Problem

$$(3) \implies e^{imx} p(x) = e^{imx} \sum_{j=-m}^{m} c_j e^{ijx} = \sum_{j'=0}^{2m} c_{j'-m} e^{ij'x} =: \tilde{p}(x)$$

and $\tilde{p}(x_k) \overset{!}{=} \tilde{y}_k := y_k e^{imx_k}$

or, with a new notation (!):

$$p(x) = \sum_{j=0}^{n-1} c_j e^{ijx}, \quad c_j \in \mathbb{C} \quad \text{and} \quad p(x_j) = y_j$$

Theorem: the problem has a unique sol.

Proof: $z_j := e^{ix_j}$, $j \in \{0, \dots, n-1\}$, Ansatz $p(x) = \sum_j c_j z^j(x)$

$$\implies \underbrace{\begin{pmatrix} z_0^0 & z_0^1 & \dots & z_0^{n-1} \\ \vdots & & & \vdots \\ z_{n-1}^0 & & \dots & z_{n-1}^{n-1} \end{pmatrix}}_{=:V} \begin{pmatrix} c_0 \\ \vdots \\ c_{n-1} \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_{n-1} \end{pmatrix}$$

$$\det(V) = \prod_{j \neq k} (z_k - z_j) \neq 0 \quad (\text{as } z_k \text{ are distinct})$$

$\blacksquare$

Theorem : Solution - the DFT (-Matrix)

From now on: uniform knot distr.: $x_j = \frac{2\pi j}{n}$, $e^{-\frac{2\pi i}{n}} =: w_n$

$\left(w_n^j = e^{-ix_j}\right)$

$p(x) = \sum_j c_j e^{ijx}$, $V_n := \left(w_n^{j\cdot k}\right)_{j,k=0,\dots n-1}$

$\Rightarrow$ (i) $\frac{1}{n} V_n \vec{y} = \vec{c}$

(ii) $\frac{1}{\sqrt{n}} V_n$ .. sym and unitary (i.e. $A^{-1} = \overline{A^T}$)

(iii) $\overline{V_n} = \left(w_n^{-j\cdot k}\right)_{j,k=0,\dots n-1}$

Proof: (iii) obvious

(ii) $\left(\vec{v}_0, \dots \vec{v}_{n-1}\right) := \frac{1}{\sqrt{n}} V_n$

- $\vec{v}_k^H \vec{v}_k = \frac{1}{n} \sum_j w_n^{-jk} w_n^{jk} = 1$
- $k \neq \ell$: $\vec{v}_k^H \vec{v}_\ell = \frac{1}{n} \sum_j w_n^{-jk} w_n^{\ell j} \overset{\text{geom. sequence}}{=} 0$

(i)

Definition DFT $\quad \mathcal{F}_n : \mathbb{C}^n \to \mathbb{C}^n$

$\vec{y} \longmapsto V_n \cdot \vec{y} = c$ is called DFT

cost: $\mathcal{O}(n^2)$

Lemma FFT $\quad n = 2m$, $w = e^{\frac{\pm 2\pi i}{n}}$, $\xi^2 := w^2$, $\ell \in \{0, \dots m-1\}$

$\Rightarrow a_k = \sum_j y_j w^{kj}$ can be split into

$$\begin{cases} a_{2\ell} = \sum_j^{m-1} g_j \xi^{j\ell}, & g_j = y_j + y_{j+m} \\ a_{2\ell+1} = \sum_j^{m-1} h_j \xi^{j\ell}, & h_j = (y_j - y_{j+m}) w^j \end{cases}$$

Proof: $\alpha_{2\ell} = \sum_j y_j w^{2\ell j} = \sum_{j=0}^{\frac{n}{2}-1} y_j w^{2\ell j} + y_{j+\frac{n}{2}} w^{2\ell(j+\frac{n}{2})} = \dots = \sum_j^{\frac{n}{2}-1} w^{2\ell j}(y_j + y_{j+\frac{n}{2}})$

$\alpha_{2\ell+1} = \sum_j y_j w^{(2\ell+1)j} = \dots \sum_{j=0}^{\frac{n}{2}-1} (y_j - y_{j+m}) w^j w^{2\ell j}$

This shows, computing $\mathcal{F}_n(\vec{y})$ can be reduced to computing $\mathcal{F}_{\frac{n}{2}}(\vec{g})$ and $\mathcal{F}_{\frac{n}{2}}(\vec{h})$!! Each of these have $\mathcal{O}((\frac{n}{2})^2)$!!

FFT: do that ~~rec~~ recursively !!

Lemma: Cost of FFT is $\mathcal{O}(n\log(n))$

Proof: $A(n)$ .. cost of DFT of n data points, $n =: 2^p$

$$\begin{aligned} A(n) &\leq 2A(\tfrac{n}{2}) + \underbrace{C\cdot n}_{\text{cost of computing } g,\,h} \\ &\leq 2A(2^{p-1}) + C 2^p \\ &\leq 2\left[2A(2^{p-2}) + C2^{p-1}\right] + C2^p \\ &\dots \\ &\leq 2^p A(2^0) + pC\cdot 2^p \leq n\log_2 n \cdot C' \end{aligned}$$

∎

Def. Convolution „$*$"

$$(f * g)_k := \sum_j f_{k-j}\, g_j$$

(f, g: n-periodic sequences)

Convolution Theorem

$$\mathcal{F}(f * g) = \hat{f}\cdot\hat{g}$$

... point-wise product of Fourier coeffs.

(No proof)

Fast convolution

naive conv.: $\mathcal{O}(n^2)$

using theorem before: $\mathcal{O}(n\log n)$

Example: Product of large numbers

$$x := \sum_j^n x_j b^j$$
$$y := \sum_j^n y_j b^j$$

$$\Rightarrow x\cdot y = \sum_j^{2n} z_j b^j \quad \text{with } z_j = \underbrace{\sum_k^j x_{j-k}\, y_k}_{\text{convolution!}}$$

Example: circulant matrix

$$C = \begin{pmatrix} c_0 & c_{n-1} & c_{n-2} & \dots & c_1 \\ c_1 & c_0 & c_{n-1} & & c_2 \\ \vdots & c_1 & c_0 & & \vdots \\ & \vdots & c_1 & & \\ c_{n-1} & \vdots & \vdots & & c_0 \end{pmatrix}, \quad \vec{c} := (c_0, \dots c_{n-1})^T \Rightarrow$$

$\vec{y} = C\vec{x}$ can be rewritten as $y_j = \sum \vec{c}_{j-k}\, x_k$