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ETH Lecture 401-0663-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

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URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE15.pdf

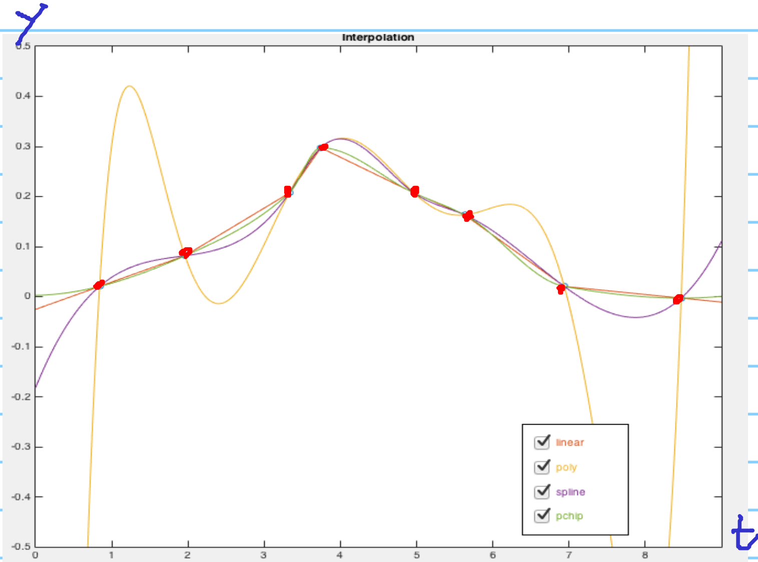
III. Data Interpolation in 1D

Given: data points $(t_i, y_i) \in \mathbb{R}$, $i = 0, \dots, n$,
(t_i: nodes, y_i: values)

Sought: interpolant $f: I \subset \mathbb{R} \to \mathbb{R}$

: $f(t_i) = y_i$, $i = 0, \dots, n$

[interpolation conditions]



Assumption: $t_0 < t_1 < \dots < t_n$ (not for coding!)
$I \subset [t_0, t_1]$

Application: empiric constitutive relations

For non-linear circuit element we measure (U_i, I_i)

Circuit simulation requires function $I = I(U)$, $U \to I(U)$ should be differentiable (Newton's method)

Our setting: interpolant f can be represented as a linear combination of basis function $b_j: I \to \mathbb{R}$

$$f(t) = \sum_{j=0}^{m} c_j \, b_j(t)$$

c_j: coefficients / parameter

b_j: may depend on t_i, must not depend on y_i

Example: $\{t_i\}$-piecewise linear interpolation

Piecewise linear interpolation

= connect data points (t_i, y_i), $i = 1, \dots, m$, $t_{i-1} < t_i$, by line segments

➤ interpolating polygon

Piecewise linear interpolant of data ▷

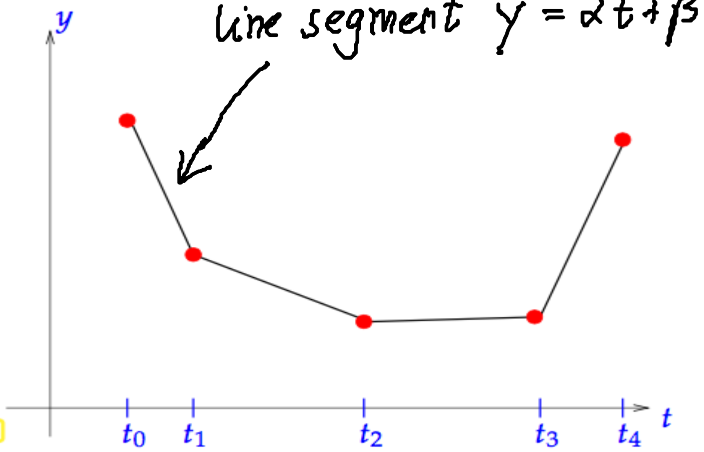
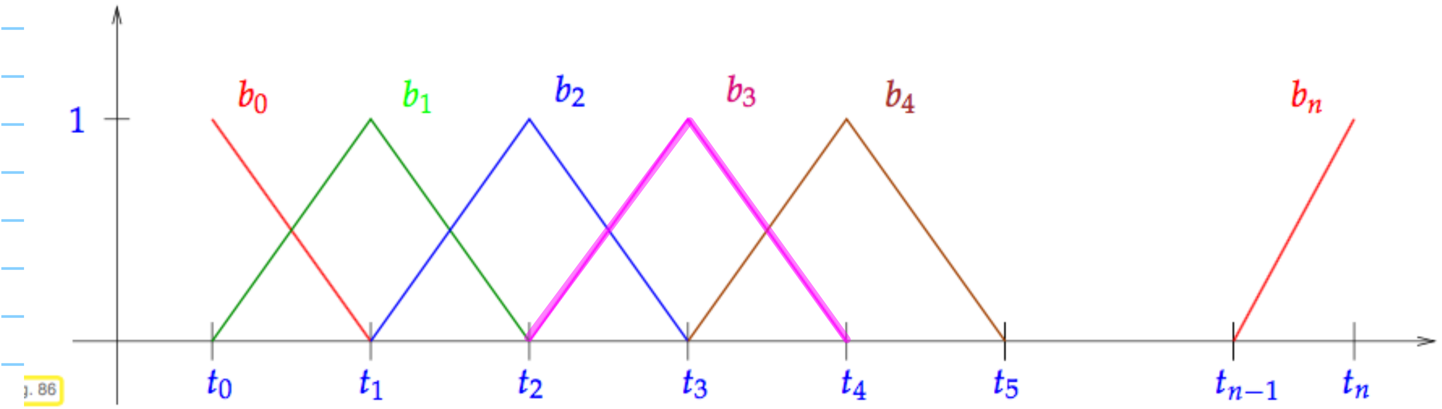


Fig. 85

② Basis functions for p.w. linear ip.: *"tent functions"*



(*) $\quad f(t) = \sum_{j=0}^{n} y_j b_j(t)$ p.w. linear ✓

& $\quad f(t_i) = y_i$, because $\underbrace{b_j(t_i) = \begin{cases} 1, & i=j \\ 0, & \text{else} \end{cases} = \delta_{ij}}$

→ cardinal basis for $\{t_i\}$

Linear interpolation: $\underbrace{\begin{cases} \mathbb{R}^{n+1} \longrightarrow C^0[t_0,t_n] \text{ [cont. fnct.]} \\ \mathbf{y} := [y_i]_{i=0}^{n} \longrightarrow f \text{ by } (*) \end{cases}}$

a linear mapping!

Definition 3.1.14. Linear interpolation operator

An interpolation operator $\mathsf{I} : \mathbb{R}^{n+1} \mapsto C^0([t_0, t_m])$ for the given nodes $t_0 < t_1 < \cdots < t_n$ is called linear, if

addition of functions

$$\mathsf{I}(c\mathbf{y} + \beta\mathbf{z}) = c\,\mathsf{I}(\mathbf{y}) + \beta\,\mathsf{I}(\mathbf{z}) \quad \forall \mathbf{y}, \mathbf{z} \in \mathbb{R}^{n+1},\ c, \beta \in \mathbb{R}\,. \tag{3.1.15}$$

Basis representation (□) + interpolation conditions

$$\sum_{j=0}^{m} c_j b_j(t_i) = y_i \quad , i = 0, \dots, n$$

$$\boxed{\mathbf{A}\mathbf{c} := \begin{bmatrix} b_0(t_0) & \dots & b_m(t_0) \\ \vdots & & \vdots \\ b_0(t_n) & \dots & b_m(t_n) \end{bmatrix} \begin{bmatrix} c_0 \\ \vdots \\ c_m \end{bmatrix} = \begin{bmatrix} y_0 \\ \vdots \\ y_n \end{bmatrix} =: \mathbf{y}}\,. \qquad (\diamond)$$

$\underbrace{f \text{ exists \& unique}}$ ⟺ LSE ($\diamond$) has unique solution

↳ Necessary: $m = n$

3.2. (Global) polynomial interpolation

3.2.1. Polynomials

$$\mathcal{P}_n := \{ t \to p(t) := \sum_{j=0}^{n} \alpha_j t^j,\ \alpha_j \in \mathbb{R} \}$$

↳ degree $\leq n$ polynomials: a vector space

$\dim \mathcal{P}_n = n+1$

monomial basis

Advantages of polynomials:
- smooth C^∞, easy to differentiate
- easy to evaluate *
- ↔ Taylor polynomials

* Horner scheme : "distributive evaluation"

$$p(t) = t(t(\cdots(\alpha_n t+\alpha_{n-1})+a_{n-2})\cdots)+\alpha_0$$

MATLAB-code 3.2.7: Horner scheme (polynomial in MATLAB format, see Rem. 3.2.4)

```
function y = polyval(p,x)
y = p(1); for i=2:length(p), y = x.*y+p(i); end
```

Effort : $O(n)$

3.2.2. Theory of polynomial interpolation

Lagrange polynomial interpolation problem*

Given the simple nodes $t_0,\dots,t_n$, $n \in \mathbb{N}$, $-\infty < t_0 < t_1 < \cdots < t_n < \infty$ and the values $y_0,\dots,y_n \in \mathbb{R}$ compute $p \in \mathcal{P}_n$ such that

$$p(t_j) = y_j \quad \text{for} \quad j = 0,\dots,n\,. \tag{3.2.9}$$

Lagrange polynomials:

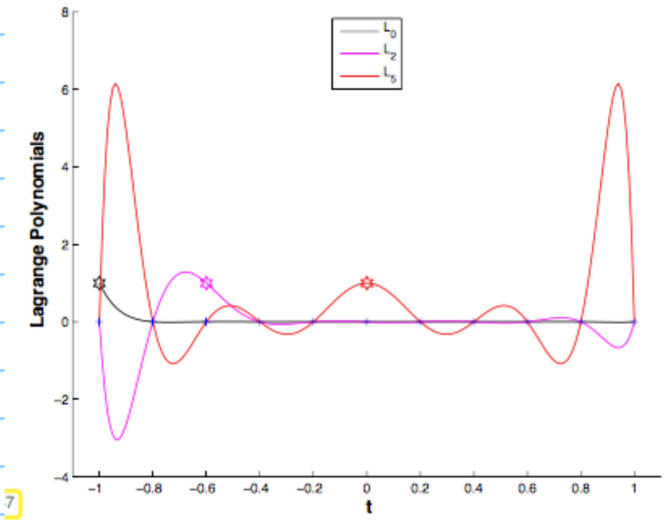
$$L_i(t) = \prod_{\substack{j=0\\ j\neq i}}^{n} \left(\frac{t-t_j}{t_i-t_j}\right) \in \mathcal{P}_n\,, \quad L_i(t_j) = \delta_{ij}$$

$\Downarrow$ cardinal basis of $\mathcal{P}_n$

$$p(t) = \sum_{j=0}^{n} y_j L_j(t) \;\to\; \text{existence} \quad (\heartsuit)$$

$\Downarrow$ uniqueness

* a linear mapping $\mathbb{R}^{n+1} \to \mathcal{P}_n$



◁ Lagrange polynomials for $n = 10$ on $[-1,1]$, equidistant nodes

Generalization : Hermite interpolation problem

Given $t_0,\dots,t_n$ & $y_0,\dots,y_n$: values
$c_0,\dots,c_n$: slopes

Find $p \in \mathcal{P}_{2n+1}$: $p(t_i) = y_i$, $p'(t_i) = c_i$

$\Downarrow$ existence & uniqueness

3.2.3. Algorithms

↳ for Lagr. IP through $(t_i,y_i)_{i=0}^{n}$

④ 3.2.3.1 Multiple evaluations


```
class PolyInterp {
  private:
  // various internal data describing p
  Eigen::VectorXd t;
  public:
    // Constructors taking node vector (t_0,...,t_n) as argument
  PolyInterp(const Eigen::VectorXd &_t);
  template <typename SeqContainer>
  PolyInterp(const SeqContainer &v);
  // Evaluation operator for data (y_0,...,y_n); computes
  // p(x_k) for x_k's passed in x
  Eigen::VectorXd eval(const Eigen::VectorXd &y,const Eigen::VectorXd
     &x) const;
};
```

PolyInterp(...) → called once

eval: many calls; x: long vector, size $N \gg n$

Attempt: ~~• Constructor computes monomial coeffs.~~
~~• eval → Horner scheme~~ } $O(n^3 + Nn)$

Attempt: • Constructor idle
• eval → use (♡) } $O(n + Nn^2)$

Solution : Barycentric formula

$$p(x) = \sum_{i=0}^{n} y_i L_i(x) = \sum_{i=0}^{n} y_i \prod_{j \neq i} \frac{(x-t_j)}{(t_i - t_j)}$$

$$= \prod_{j=0}^{n} (x-t_j) \sum_{i=0}^{n} y_i \frac{1}{x-t_i} \underbrace{\prod_{j \neq i} \frac{1}{(t_i - t_j)}}_{=:\ \lambda_i}$$

$$= \prod_{j=0}^{n} (x-t_j) \sum_{i=0}^{n} \frac{y_i \lambda_i}{x-t_i} = \frac{\sum_{i=0}^{n} \frac{\lambda_i}{x-t_i} y_i}{\sum_{i=0}^{n} \frac{\lambda_i}{x-t_i}}$$

$y_i = 1 \ \forall i \Rightarrow p \equiv 1$

$$1 = \prod_{j=0}^{n} (x-t_j) \sum_{i=0}^{n} \frac{\lambda_i}{x-t_i}$$

$$= \sum_{i=0}^{n} \frac{\lambda_i}{x-t_i} \prod_{j=0}^{n} (x-t_j)$$

$$\Rightarrow \prod_{j=0}^{n} (x-t_j) = \frac{1}{\sum_{i=0}^{n} \frac{\lambda_i}{x-t_i}}$$

λ_i depend only on t_i ⟹ Compute in constructor

In eval() : evaluate $\underline{\underline{}}$ with cost $O(n)$

▷ eval costs $O(Nn)$

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MATLAB-code 3.2.28: Evaluation of the interpolation polynomials with barycentric formula

```
function p = intpolyval(t,y,x)
% t:  row vector of nodes t_0,...,t_n
% y:  row vector of data y_0,...,y_n
% x:  row vector of evaluation points x_1,...,x_N
n = length(t); % number of interpolation nodes = degree of polynomial
  -1
N = length(x); % Number of evaluation points stored in x
% Precompute the weights λ_i with effort O(n^2)
for k = 1:n
  lambda(k) = 1 / prod(t(k) - t([1:k-1,k+1:n])); end;
for i = 1:N
% Compute quotient of weighted sums of λ_i/(t-t_i), effort O(n)
  z = (x(i)-t); j = find(z == 0);
  if (~isempty(j)), p(i) = y(j); % avoid division by zero
  else
    mu = lambda./z; p(i) = sum(mu.*y)/sum(mu);
  end
end
```

(lines 8–9: $\}\to$ Constructor; lines 10–16: $\}$ eval())

3.2.3.2 "Update-friendly" single evaluation

Given: data points $(t_i, y_i) \in \mathbb{R}^2$, $i = 0, \dots, n$

Lagrangian interp.: find $p \in \mathcal{P}_n$: $p(t_i) = y_i$, $i = 0, \dots, n$

$$p = \sum_{j=0}^{n} y_j L_j \quad [\text{in Lagrangian basis}]$$

```
double eval(const Eigen::VectorXd &t,const Eigen::VectorXd &y,
            double x);
```

↑ evaluation at a single point ("known in advance")

Algorithm: Aitken-Neville

- Partial Lagrange interpolants

$$p_{k,\ell} \in \mathcal{P}_{\ell-k} : \quad p(t_j) = y_j, \quad j = k, \dots, \ell$$

$\longrightarrow$ Recursion formula

$$p_{k,k} \equiv y_k, \quad k = 0, \dots, n$$

$$p_{k,\ell}(x) = \frac{1}{t_\ell - t_k}\underbrace{\{(x-t_k)\,p_{k+1,\ell}(x) - (x-t_\ell)\,p_{k,\ell-1}(x)\}}_{\text{satisfies i.c. for } (t_j, y_j),\ j = k, \dots, \ell}$$

↑ by uniqueness

$n =$	0	1	2	3
t_0	$y_0 =: p_{0,0}(x)$	$\to p_{0,1}(x)$	$\to p_{0,2}(x)$	$\to p_{0,3}(x)$
t_1	$y_1 =: p_{1,1}(x)$	$\to p_{1,2}(x)$	$\to p_{1,3}(x)$	
t_2	$y_2 =: p_{2,2}(x)$	$\to p_{2,3}(x)$		
t_3	$y_3 =: p_{3,3}(x)$			

$p_{0,n} \stackrel{!}{=} p$

⑥

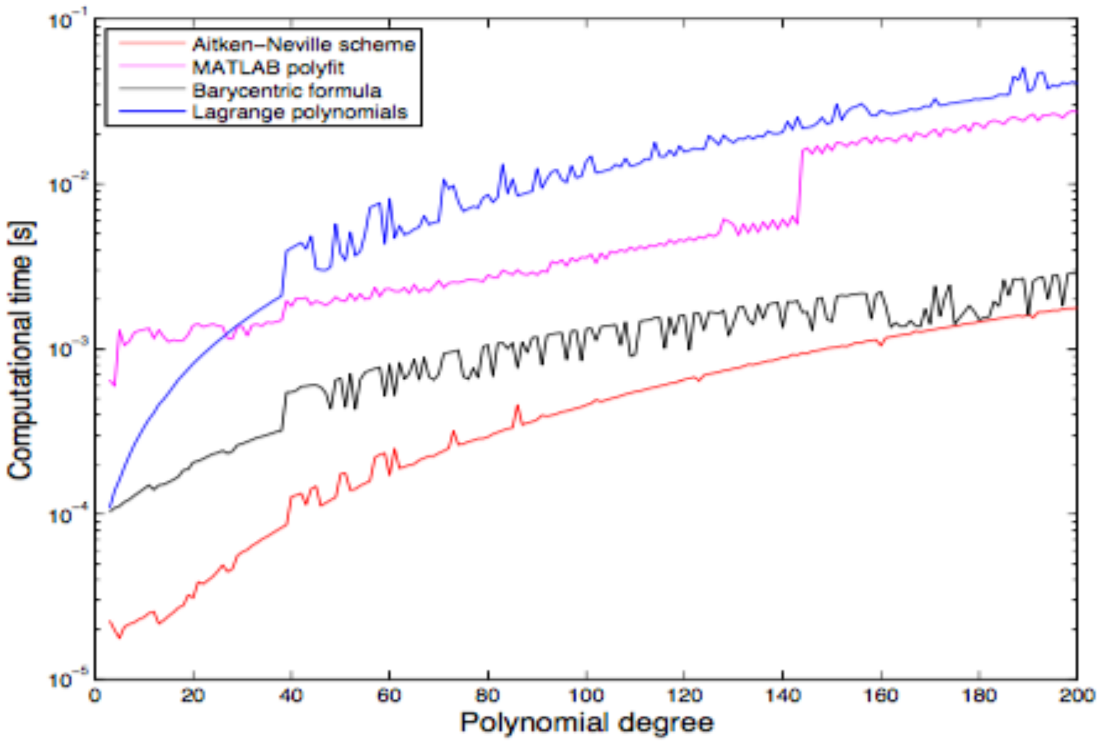
MATLAB-code 3.2.31: Aitken-Neville algorithm Effort : $O(n^2)$

```
function v = ANipoleval(t,y,x)
for i=1:length(y)
  for k=i-1:-1:1
    y(k) = y(k+1)+(y(k+1)-y(k))*(x-t(i))/(t(i)-t(k));
  end
end
v = y(1);
```

"update-friendly": A.N. scheme suitable for simultaneous evaluation & adding of data points

$$
\begin{array}{c|cccc}
n= & 0 & 1 & 2 & 3 \\
\hline
t_0 & y_0 =: p_{0,0}(x) & \to p_{0,1}(x) & \to p_{0,2}(x) & \to p_{0,3}(x) \\
 & & \nearrow & \nearrow & \nearrow \\
t_1 & y_1 =: p_{1,1}(x) & \to p_{1,2}(x) & \to p_{1,3}(x) & \\
 & & \nearrow & \nearrow & \\
t_2 & y_2 =: p_{2,2}(x) & \to p_{2,3}(x) & & \\
 & & \nearrow & & \\
t_3 & y_3 =: p_{3,3}(x) & & &
\end{array}
$$

```
class PolyEval {
  private:
    // evaluation point and various internal data describing the
       polynomials
  public:
    // Constructor taking the evaluation point as argument
    PolyEval(double x);
    // Add another data point and update internal information
    void addPoint(t,y);
    // Value of current interpolating polynomial at x
    double eval(void) const;
};
```



single point evaluation

NCSE15

3.2.3.3. Extrapolation to zero

Objective : Compute $\lim_{h\to 0} \Psi(h)$

↑ Smooth, but hard to evaluate* for $|h| \ll 1$.

Example : Difference quotient $\Psi(h) := \dfrac{f(x+h)-f(x)}{h}$

↳ * cancellation for $h < \sqrt{\text{EPS}}$

Idea: computing inaccessible limit by extrapolation to zero

0: Pick "rather large" $h_0, \dots, h_n$

① evaluation of $\psi(h_i)$ for different h_i, $i = 0, \dots, n$, $|t_i| > 0$.

② $\psi(0) \approx p(0)$ with interpolating polynomial $p \in \mathcal{P}_n$, $p(h_i) = \psi(h_i)$.

Apply to $\psi(h) := \dfrac{f(x+h) - f(x-h)}{2h}$

→ symmetric difference quotient: $\psi(-h) = \psi(h)$

Good setting for extrapolation

$f(x) = \arctan(x)$		$f(x) = \sqrt{x}$		$f(x) = \exp(x)$	
h	Relative error	h	Relative error	h	Relative error
2^{-1}	0.20786640808609	2^{-1}	0.09340033543136	2^{-1}	0.29744254140026
2^{-6}	0.00773341103991	2^{-6}	0.00352613693103	2^{-6}	0.00785334954789
2^{-11}	0.00024299312415	2^{-11}	0.00011094838842	2^{-11}	0.00024418036620
2^{-16}	0.00000759482296	2^{-16}	0.00000346787667	2^{-16}	0.00000762943394
2^{-21}	0.00000023712637	2^{-21}	0.00000010812198	2^{-21}	0.00000023835113
~~2^{-26}~~	~~0.00000001020730~~	~~2^{-26}~~	~~0.00000001923506~~	~~2^{-26}~~	~~0.00000000429331~~
2^{-31}	0.00000005960464	2^{-31}	0.00000001202188	2^{-31}	0.00000012467100
2^{-36}	0.00000679016113	2^{-36}	0.00000198842224	2^{-36}	0.00000495453865

Extrapolation: $h_0 = 1/2$, $h_1 = 1/4$, $h_2 = 1/8$, ...

Degree	Relative error	Degree	Relative error	Degree	Relative error
0	0.04262829970946	0	0.02849215135713	0	0.04219061098749
1	0.02044767428982	1	0.01527790811946	1	0.02129207652215
2	0.00051308519253	2	0.00061205284652	2	0.00011487434095
3	0.00004087236665	3	0.00004936258481	3	0.00000825582406
4	0.00000048930018	4	0.00000067201034	4	0.00000000589624
5	0.00000000746031	5	0.00000001253250	5	0.00000000009546
6	0.00000000001224	6	0.00000000004816	6	0.00000000000002
		7	0.00000000000021		

MATLAB-code 3.2.42: Numerical differentiation by extrapolation to zero

```
function d = diffex(f,x,h0,atol,rtol)
% f:  handle of to a function defined in a neighborhood of x ∈ ℝ,
% x:  point at which approximate derivative is desired,
% h0:  initial distance from x,
% tol:  relative target tolerance
h = h0;
% Aitken-Neville scheme, see Code 3.2.31 (x = 0!)

y(1) = (f(x+h0)-f(x-h0))/(2*h0);
for i=2:10
  h(i) = h(i-1)/2;
  y(i) = f(x+h(i))-f(x-h(i)))/h(i-1);
  for k=i-1:-1:1
    y(k) = y(k+1)-(y(k+1)-y(k))*h(i)/(h(i)-h(k));
  end
  % termination of extrapolation, when desired tolerance is achieved

  errest = abs(y(2)-y(1)); % error indicator
  if ((errest < rtol*abs(y(1))) || (errest < atol)), break; end %
end
d = y(1);
```

"Correction based termination" ⟹ error control !

(8) 3.2.3.4. Newton basis and divided differences

A.N. : x has to be known in advance

C++code 3.2.43: Polynomial evaluation

```
class PolyEval {
  private:
  // evaluation point and various internal data describing the
     polynomials
  public:
    // Idle Constructor
    PolyEval();
    // Add another data point and update internal information
    void addPoint(t,y);
    // Evaluation of current interpolating polynomial at x
    Eigen::VectorXd operator () (const Eigen::VectorXd &x) const;
};
```

"Update-friendly" Newton basis

$$N_0(t) \equiv 1\ , \quad N_k(t) = \prod_{\ell=0}^{k-1}(t-t_\ell) \in \mathcal{P}_k$$

↳ leading coefficient $= 1$

▷ $N_k(t_j) = 0\ , \quad j=0,\dots,k-1$

$$p = \sum_{j=0}^{n} a_j N_j\ , \quad p \triangleq \text{Lagrange interpolant}$$

I.C. ⇒

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & (t_1-t_0) & \ddots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 1 & (t_n-t_0) & \cdots & \prod_{i=0}^{n-1}(t_n-t_i) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}$$

triangular LSE

Structured way to perform forward elimination:

$a_{k,\ell} \triangleq$ leading coefficient of $p_{k,\ell}$

$$a_j = a_{0,j} \qquad \left[\, p_{0,\ell} = \sum_{j=0}^{\ell} a_j N_j \ ! \,\right]$$

A.N. recursion:

$$\begin{aligned} p_{k,k}(x) &\equiv y_k \quad \text{("constant polynomial")}\ , \quad k=0,\dots,n\ , \\ p_{k,\ell}(x) &= \frac{(x-t_k)p_{k+1,\ell}(x) - (x-t_\ell)p_{k,\ell-1}(x)}{t_\ell - t_k} \\ &= p_{k+1,\ell}(x) + \frac{x-t_\ell}{t_\ell - t_k}\, p_{k,\ell-1}(x)\ , \quad 0 \le k \le \ell \le n\ , \end{aligned} \tag{3.2.30}$$

$$a_{k,\ell} = \frac{1}{t_\ell - t_k}\left(1 \cdot a_{k+1,\ell} - 1 \cdot a_{k,\ell-1}\right)$$

$$a_{k,k} = y_k$$

Divided difference recursion

MATLAB-code 3.2.51: Divided differences, recursive implementation,

```
function y = divdiff(t,y)
n = length(y)-1;
if (n > 0)
  y(1:n) = divdiff(t(1:n),y(1:n));
  for j=0:n-1
    y(n+1) = (y(n+1)-y(j+1))/(t(n+1)-t(j+1));
  end
end
```

← "diagonal traversal"

Algorithm behind addPoint()

⑨ Implementation of ( ) : Horner scheme

```
function p = evaldivdiff(t,y,x)
dd=divdiff(t,y); % Compute divided differences, see Code 3.2.51
n = length(y)-1;
p=dd(n+1);
for j=n:-1:1, p = (x-t(j)).*p+dd(j); end
```

: Effort $O(n)$

$$p(x) = ((a_n(x-t_n)+a_{n-1})(x-t_{n-1})+a_{n-2})+\dots + a_0$$

3.2.4 : Polynomial Interpolation : Sensitivity

Given : Fixed nodes $t_0,\dots,t_n$ → set $\mathcal{T}$

Input : $y_0,\dots,y_n$ [might be perturbed : measured]

Output : $p \hat{=}$ Lagrange interpolant

Needed : norms on data space $\mathbb{R}^{n+1}$ → max norm. $\|y\|_\infty = \max_\ell |y_\ell|$

" result space $\mathcal{P}_n$ → max norm $\|p\|_\infty = \max_{t_0 \le x \le t_n} |p(x)|$

$$\|I_\mathcal{T}(y)\|_\infty = \left\|\sum_{j=0}^{n} y_j L_j\right\|_\infty$$
$$\le \max_x \sum_{j=0}^{n} |y_j|\,|L_j(x)|$$
$$\le \|y\|_\infty \left\|\sum_{j=0}^{n} |L_j|\right\|_\infty , \quad y \neq 0$$
$$\Rightarrow \quad \|I_\mathcal{T}\|_{\infty\to\infty} \le \left\|\sum_{j=0}^{n} |L_j|\right\|_\infty$$

Lemma 3.2.67. Absolute conditioning of polynomial interpolation

Given a mesh $\mathcal{T} \subset \mathbb{R}$ with generalized Lagrange polynomials L_i, $i = 0,\dots,n$, and fixed $I \subset \mathbb{R}$, the norm of the interpolation operator satisfies

$$\left[\ \|I_\mathcal{T}\|_{\infty\to\infty} := \sup_{\mathbf{y}\in\mathbb{R}^{n+1}\setminus\{0\}} \frac{\|I_\mathcal{T}(\mathbf{y})\|_{L^\infty(I)}}{\|\mathbf{y}\|_\infty} = \left\|\sum_{i=0}^{n} |L_i|\right\|_{L^\infty(I)}, \right] \tag{3.2.68}$$

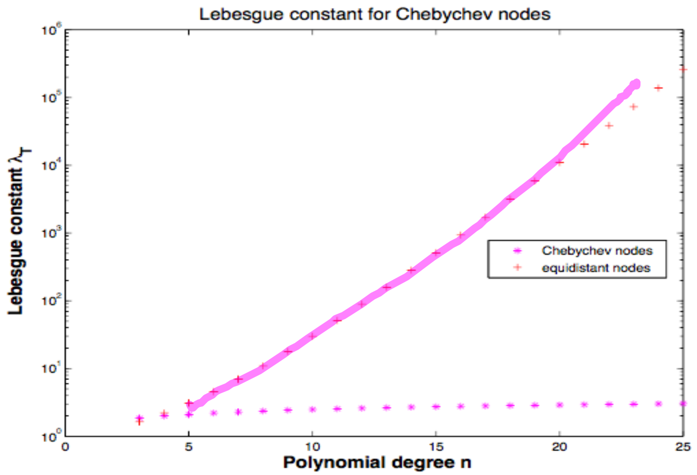
$$\|I_\mathcal{T}\|_{2\to2} := \sup_{\mathbf{y}\in\mathbb{R}^{n+1}\setminus\{0\}} \frac{\|I_\mathcal{T}(\mathbf{y})\|_{L^2(I)}}{\|\mathbf{y}\|_2} \le \left(\sum_{i=0}^{n} \|L_i\|^2_{L^2(I)}\right)^{\frac12}. \tag{3.2.69}$$

= Lebesgue constant (of $\mathcal{T}$) $\lambda_\mathcal{T}$

Note : Lagrange interpolation $I_\mathcal{T}$ is linear :

$L : X \to Y$ linear : $L(x+\delta x) = L(x) + L(\delta x)$

Amplification of perturbation measured by
$$\underbrace{\sup_{\delta x \in X\setminus\{0\}} \frac{\|L(\delta x)\|_Y}{\|\delta x\|_X}}_{\text{Operator norm, cf. matrix norm}} =: \|L\|_{X\to Y}$$



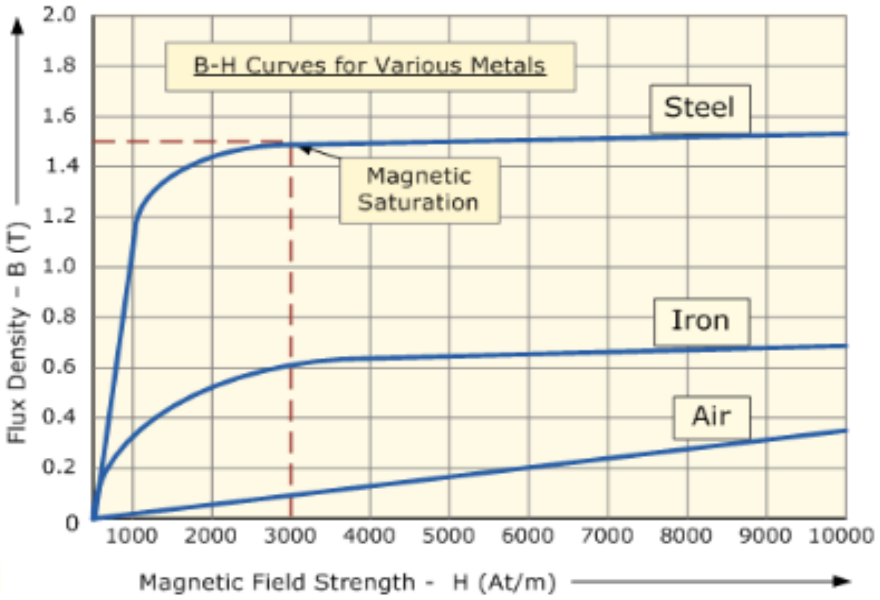
← $\lambda_\mathcal{T}$ for equidistant t_i in $[-1,1]$

$$\lambda_\mathcal{T} \ge C e^{n/2}$$

3.3. Shape preserving interpolation

Given: data points (t_i, y_i), $i = 0, \dots, n$; $t_0 < t_1 < \dots < t_n$

Seek: function $f : I \to \mathbb{R}$: $f(t_i) = y_i$



Magnetization curve

$H \longrightarrow B(H)$

- smooth
- monotonic
- concave

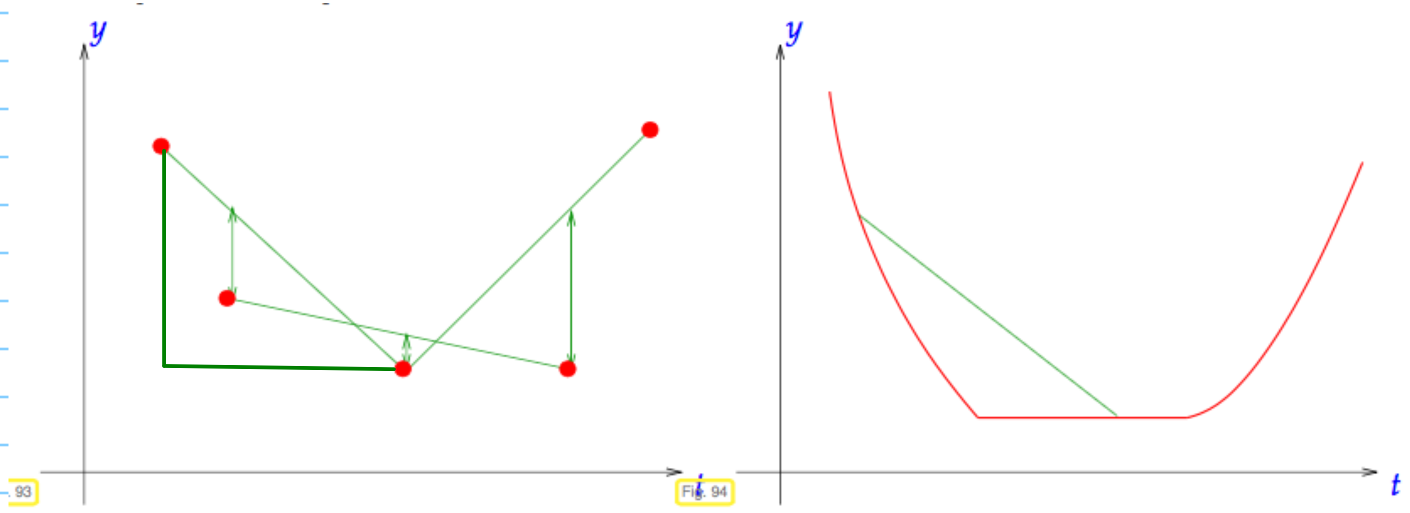
3.3.1. Shape properties of functions & data

- sign
- monotonicity

Definition 3.3.3. monotonic data

The data (t_i, y_i) are called monotonic when $y_i \geq y_{i-1}$ or $y_i \leq y_{i-1}$, $i = 1, \dots, n$.

- curvature



Convex data   Convex function

$$\Delta_j = \frac{y_j - y_{j-1}}{t_j - t_{j-1}} : \text{local slope}$$

f' increasing

Definition 3.3.4. Convex/concave data

The data $\{(t_i, y_i)\}_{i=0}^{n}$ are called convex (concave) if

$$\Delta_j \overset{(\geq)}{\leq} \Delta_{j+1}, \quad j = 1, \dots, n-1, \quad \Delta_j := \frac{y_j - y_{j-1}}{t_j - t_{j-1}}, \quad j = 1, \dots, n.$$

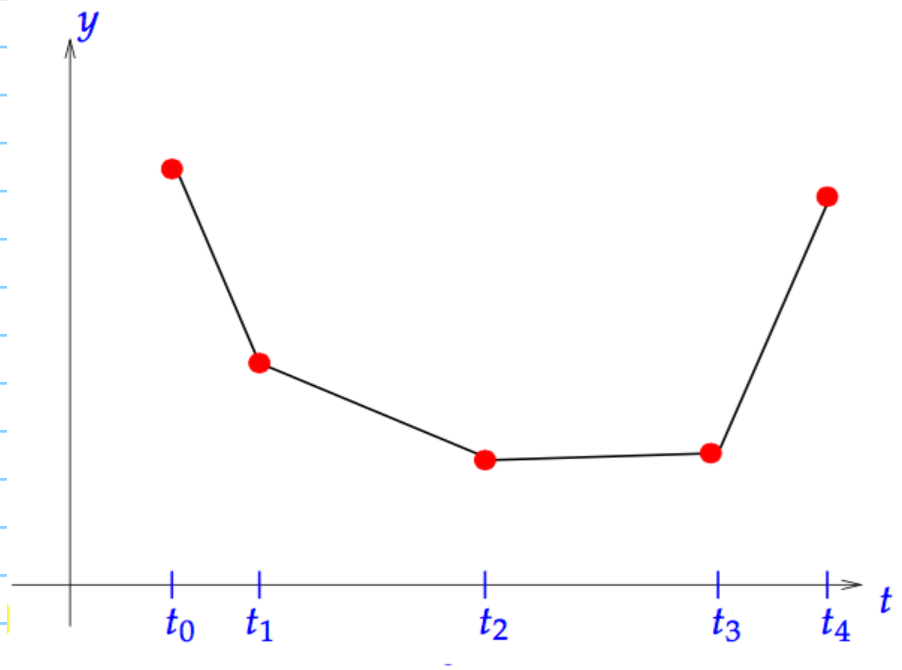
Shape preservation

(Local) Shape properties of data $\Longrightarrow$ shape property of interpolant

$\hookrightarrow$ holds on all $[t_{k-m}, t_k]$

⑪ Shape preservation for Lagrange IP ? NO WAY!

3.3.2. Piecewise linear interpolation



◁ Perfect local shape preservation!

Theorem 3.3.9. Local shape preservation by piecewise linear interpolation

Let $s \in C([t_0, t_n])$ be the piecewise linear interpolant of $(t_i, y_i) \in \mathbb{R}^2$, $i = 0, \dots, n$, for every subinterval $I = [t_j, t_k] \subset [t_0, t_n]$:

if $(t_i, y_i)|_I$ are positive/negative $\Rightarrow$ $s|_I$ is positive/negative,
if $(t_i, y_i)|_I$ are monotonic (increasing/decreasing) $\Rightarrow$ $s|_I$ is monotonic (increasing/decreasing),
if $(t_i, y_i)|_I$ are convex/concave $\Rightarrow$ $s|_I$ is convex/concave.

Remark: Locality of p.w. linear interpolation

$\hat{=}$ change of y_i affect interpolant only on $[t_{i-1}, t_{i+1}]$

Drawback: interpolant merely C^0 (kinks!)

3.4. (Piecewise) cubic Hermite interpolation

$\longrightarrow$ C^1-interpolants

3.4.1. Definition

Definition 3.4.1. Cubic Hermite polynomial interpolant

Given data points $(t_j, y_j) \in \mathbb{R} \times \mathbb{R}$, $j = 0, \dots, n$, with pairwise distinct ordered nodes t_j, and slopes $c_j \in \mathbb{R}$, the piecewise cubic Hermite interpolant $s : [t_0, t_n] \to \mathbb{R}$ is defined by the requirements

$$s_{|[t_{i-1}, t_i]} \in \mathcal{P}_3, \; i = 1, \dots, n \;, \quad \boxed{s(t_i) = y_i} \;, \quad \boxed{s'(t_i) = c_i} \;, \quad i = 0, \dots, n \,.$$

$\longrightarrow$ $s \in C^1$ continuity of s'

Express s locally through generalized cardinal basis functions

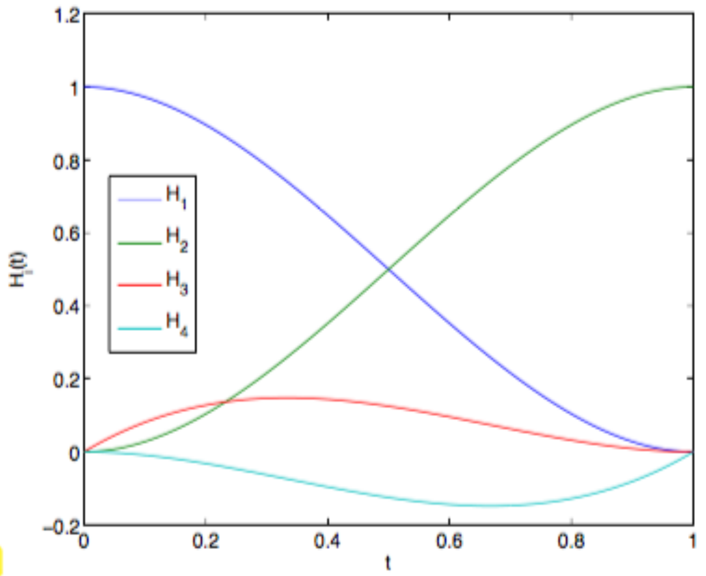
$$s(t) = y_{i-1} H_1(t) + y_i H_2(t) + c_{i-1} H_3(t) + c_i H_4(t)$$

for $t_{i-1} \leq t \leq t_i$

with

	$H(t_{i-1})$	$H(t_i)$	$H'(t_{i-1})$	$H'(t_i)$
H_1	1	0	0	0
H_2	0	1	0	0
H_3	0	0	1	0
H_4	0	0	0	1

$\longrightarrow$ 4x4 LSE for polynomial coefficients.



$$H_1(t) := \phi\left(\tfrac{t_i - t}{h_i}\right), \quad H_2(t) := \phi\left(\tfrac{t - t_{i-1}}{h_i}\right),$$
$$H_3(t) := -h_i\psi\left(\tfrac{t_i - t}{h_i}\right), \quad H_4(t) := h_i\psi\left(\tfrac{t - t_{i-1}}{h_i}\right),$$
$$h_i := t_i - t_{i-1} \;,$$
$$\phi(\tau) := 3\tau^2 - 2\tau^3 \;,$$
$$\psi(\tau) := \tau^3 - \tau^2 \,. \tag{3.4.5}$$

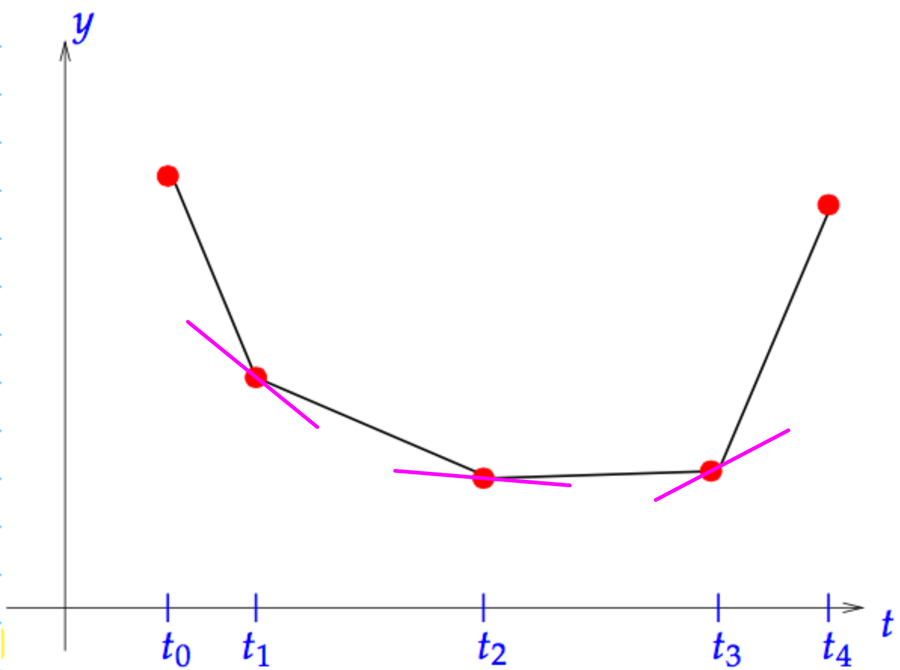
$$\tau := \frac{t - t_{i-1}}{t_i - t_{i-1}}$$

MATLAB-code 3.4.6: Local evaluation of cubic Hermite polynomial

```
function s=hermloceval(t,t1,t2,y1,y2,c1,c2)
% y1, y2: data values, c1, c2: slopes
h = t2-t1; t = (t-t1)/h;
a1 = y2-y1; a2 = a1-h*c1;
a3 = h*c2-a1-a2;
s = y1+(a1+(a2+a3*t).*(t-1)).*t;
```

Task: Find slopes from values : $c_i = c_i(y_0, \dots, y_n)$

Natural : local $c_i = c_i(y_{i-1}, y_i, y_{i+1})$



Idea :

c_i by local averaging of slopes

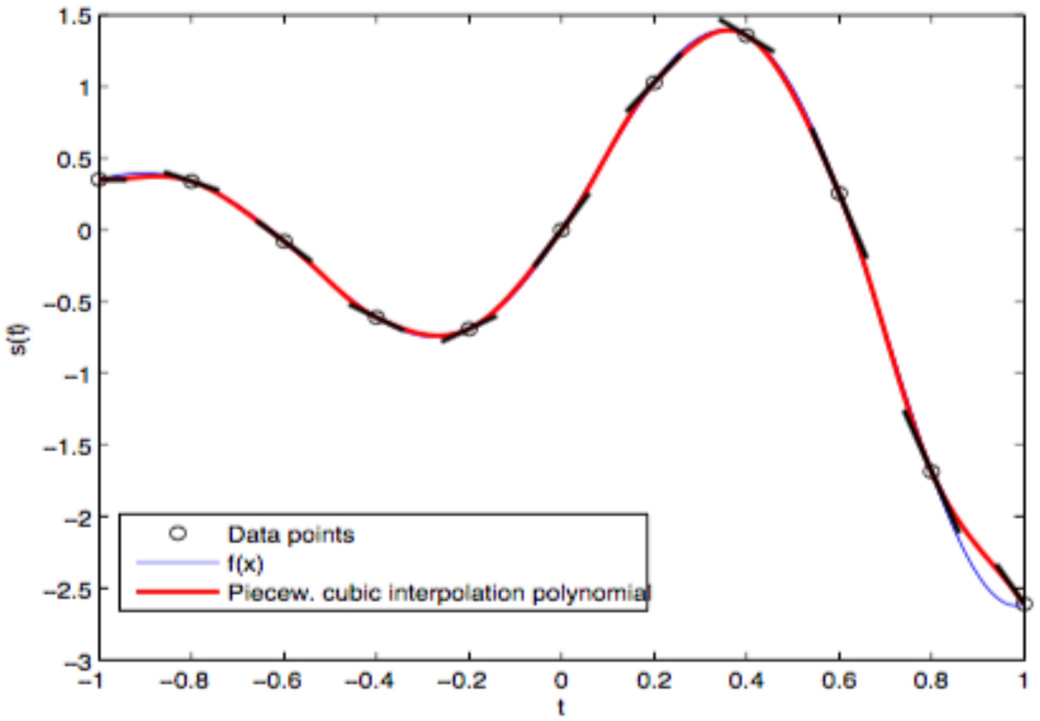
e.g. (generalized) arithmetic averaging :

$$c_i = \begin{cases} \Delta_1 & \text{, for } i = 0\,, \\ \Delta_n & \text{, for } i = n\,, \\ \underbrace{\frac{t_{i+1}-t_i}{t_{i+1}-t_{i-1}}\Delta_i + \frac{t_i - t_{i-1}}{t_{i+1}-t_{i-1}}\Delta_{i+1}} & \text{, if } 1 \le i < n\,. \end{cases} \quad , \quad \Delta_j := \frac{y_j - y_{j-1}}{t_j - t_{j-1}}, j = 1, \dots, n\,.$$

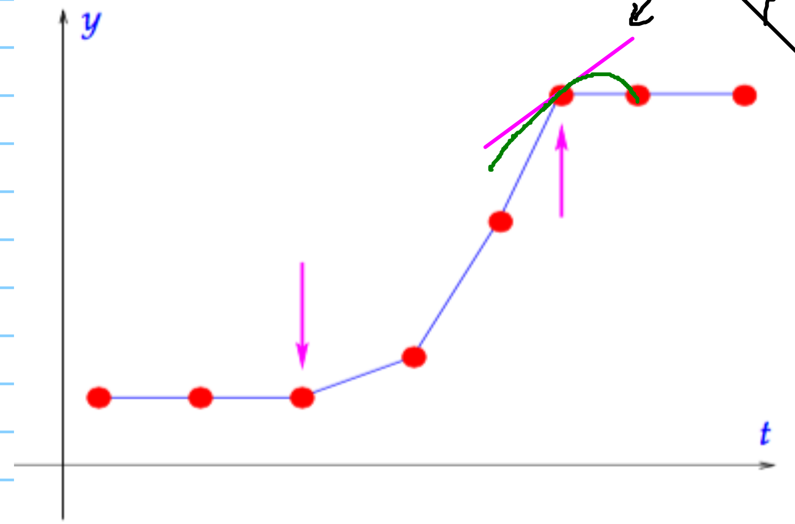
linear combination with non-negative coefficients adding up to 1.

$c_i = \frac{1}{2}(\Delta_i + \Delta_{i+1})$ for equispaced nodes !

Monotonicity preserving ? NO !



3.4.2. Local monotonicity preserving p.w. cubic Hermite intp.



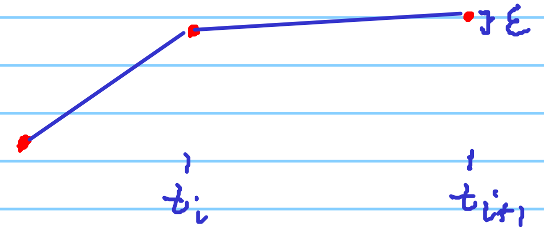
slope computed by arithmetic avg.

⇒ overshoot !

The only possible slope for the interpolant at the marked nodes is 0

▷ Use slope limiting

$$c_i = \begin{cases} 0 & \text{, if } \operatorname{sgn}(\Delta_i) \neq \operatorname{sgn}(\Delta_{i+1}) \,, \\ \text{some "average" of } \Delta_i, \Delta_{i+1} & \text{otherwise} \end{cases} \quad , \quad i = 1, \dots, n-1 \,.$$



⇒ If $\varepsilon \approx 0$, then $c_i \approx 0$

▷ $c_i \rightarrow 0$ as $\Delta_i \rightarrow 0$ or $\Delta_{i+1} \rightarrow 0$

Harmonic mean (weighted) : $c_i = \dfrac{w_i + w_{i+1}}{\frac{w_i}{\Delta_i} + \frac{w_{i+1}}{\Delta_{i+1}}}$, $w_i + w_{i+1} = 1$

$\operatorname{sgn}(\Delta_1) = \operatorname{sgn}(\Delta_2) \rightarrow$

$$c_i = \begin{cases} \Delta_1 & \text{, if } i = 0 \,, \\ \dfrac{3(h_{i+1}+h_i)}{\frac{2h_{i+1}+h_i}{\Delta_i} + \frac{2h_i + h_{i+1}}{\Delta_{i+1}}} & \text{, for } i \in \{1, \dots, n-1\} \,, \\ \Delta_n & \text{, if } i = n \,, \end{cases} \quad h_i := t_i - t_{i-1} \,. \tag{3.4.14}$$

otherwise use limiting

▷ C^1 interpolation scheme : MATLAB pchip

Theorem 3.4.18. Monotonicity preservation of limited cubic Hermite interpolation

The cubic Hermite interpolation polynomial with slopes as in Eq. (3.4.14) provides a local monotonicity-preserving C^1-interpolant.

Note: A non-linear (local) interpolation scheme

3.5. Splines

↳ Piecewise polynomial C^k-interpolants, $k \geq 2$ ($\to$ perceived as smooth)

Definition 3.5.1. Spline space → [21, Def. 8.1]

Given an interval $I := [a,b] \subset \mathbb{R}$ and a knot set/mesh $\mathcal{M} := \{a = t_0 < t_1 < \ldots < t_{n-1} < t_n = b\}$, the vector space $\mathcal{S}_{d,\mathcal{M}}$ of the spline functions of degree d (or order $d+1$) is defined by

$$\mathcal{S}_{d,\mathcal{M}} := \{s \in C^{d-1}(I) \colon s_j := s_{|[t_{j-1},t_j]} \in \mathcal{P}_d \; \forall j = 1,\ldots,n\} .$$

$d-1$-times continuously differentiable

locally polynomial of degree d

- $d = 0$: p.w. constant, discontinuous ("step function")
- $d = 1$: "polygon", $\mathcal{M}$-p.w. linear

Dimension of $\mathcal{S}_{d,\mathcal{M}}$: [counting argument]

$$\underbrace{n \cdot \dim \mathcal{P}_d}_{\text{dim. of } \mathcal{M}\text{-pw } \mathcal{P}_d} - \underbrace{(n-1) \cdot d}_{\#\text{ continuity constraint}} = \boxed{n + d = \dim \mathcal{S}_{\mathcal{M},d}}$$

Remark : $s \in \mathcal{S}_{d,\mathcal{M}} \Rightarrow s' \in \mathcal{S}_{d-1,\mathcal{M}}$

$\Rightarrow \int s \, dt \in \mathcal{S}_{d+1,\mathcal{M}}$

3.5.1 Cubic spline interpolation ($d = 3$)

Given : Knot set $\mathcal{M} = \{t_i\}_{i=0}^{n+1}$ + values $y_0, \ldots, y_n$

Find $s \in \mathcal{S}_{3,\mathcal{M}}$: $\underbrace{s(t_i) = y_i}_{n+1 \text{ conditions}}$ $\leftrightarrow$ $\dim \mathcal{S}_{3,\mathcal{M}} = n+3$

$\triangleright$ 2 degrees of freedom (d.o.f.) remain

Linear intp. $\Rightarrow$ LSE for expansion coefficient

Use same representation as for pchip !

(3.4.4) ▶

$$s_{|[t_{j-1},t_j]}(t) = \underset{y_{j-1}}{s(t_{j-1})} \cdot (1 - 3\tau^2 + 2\tau^3) + \underset{y_j}{s(t_j)} \cdot (3\tau^2 - 2\tau^3) + h_j \underset{c_{j-1}}{s'(t_{j-1})} \cdot (\tau - 2\tau^2 + \tau^3) + h_j \underset{c_j}{s'(t_j)} \cdot (-\tau^2 + \tau^3) , \tag{3.5.5}$$

C^1 already by construction $\Leftarrow$

with $h_j := t_j - t_{j-1}$, $\tau := (t - t_{j-1})/h_j$.

↑ unknown slopes c_j, $j = 0, \ldots, n$

Equations from $\underbrace{C^2\text{-continuity at internal knots}}$ t_j, $j = 1, \ldots, n-1$

$$s''_{|[t_{i-1},t_i]}(t_i) = s''_{|[t_i,t_{i+1}]}(t_i) \;, \quad i = 1, \ldots, n-1$$

$$s''_{|[t_{j-1},t_j]}(t_{j-1}) = -6 \cdot \underset{y_{j-1}}{s(t_{j-1})} h_j^{-2} + 6 \cdot \underset{y_j}{s(t_j)} h_j^{-2} - 4 \cdot h_j^{-1} \underset{c_{j-1}}{s'(t_{j-1})} - 2 \cdot h_j^{-1} \underset{c_j}{s'(t_j)} ,$$

$$s''_{|[t_{j-1},t_j]}(t_j) = 6 \cdot \underset{y_{j-1}}{s(t_{j-1})} h_j^{-2} + -6 \cdot \underset{y_j}{s(t_j)} h_j^{-2} + 2 \cdot h_j^{-1} \underset{c_{j-1}}{s'(t_{j-1})} + 4 \cdot h_j^{-1} \underset{c_j}{s'(t_j)} .$$

(15) Equate both sides: $j = 1, \dots, n-1$

$$\frac{1}{h_j}c_{j-1} + \left(\frac{2}{h_j}+\frac{2}{h_{j+1}}\right)c_j + \frac{1}{h_{j+1}}c_{j+1} = 3\left(\frac{y_j-y_{j-1}}{h_j^2}+\frac{y_{j+1}-y_j}{h_{j+1}^2}\right),$$

$$n-1\left\{\ \overbrace{\begin{bmatrix} b_0 & a_1 & b_1 & 0 & \cdots & \cdots & 0 \\ 0 & b_1 & a_2 & b_2 & & & \\ & 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & \ddots & \ddots & \\ & & & \ddots & a_{n-2} & b_{n-2} & 0 \\ 0 & \cdots & \cdots & 0 & b_{n-2} & a_{n-1} & b_{n-1} \end{bmatrix}}^{n+1}\right. \begin{bmatrix} c_0 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} 3\left(\frac{y_1-y_0}{h_1^2}+\frac{y_2-y_1}{h_2^2}\right) \\ \vdots \\ 3\left(\frac{y_{n-1}-y_{n-2}}{h_{n-1}^2}+\frac{y_n-y_{n-1}}{h_n^2}\right) \end{bmatrix}.$$

with

$$b_i := \frac{1}{h_{i+1}}, \quad i = 0,1,\dots,n-1,$$
$$a_i := \frac{2}{h_i}+\frac{2}{h_{i+1}}, \quad i = 0,1,\dots,n-1.$$
$$[\ b_i, a_i > 0\ ,\ a_i = 2(b_i + b_{i-1})\ ]$$

Fix missing constraint:

① Complete C.S.I.: prescribe $s'(t_0) = c_0$, $s'(t_n) = c_n$

[→ "drop" first & last column of A]

② Natural C.S.I: requires $s''(t_0) = s''(t_n) = 0$

→ two extra equations

→ $\frac{2}{h_1}c_0 + \frac{1}{h_1}c_1 = 3\frac{y_1-y_0}{h_1^2}$, $\frac{1}{h_n}c_{n-1} + \frac{2}{h_n}c_n = 3\frac{y_n-y_{n-1}}{h_n^2}$.

③ Periodic C.S.I: $s'(t_0) = s'(t_n)$, $s''(t_0) = s''(t_n)$: $c_0 = c_n$ + 1 equ.

→ $n \times n$ LSE

3.5.2. Properties of CSI

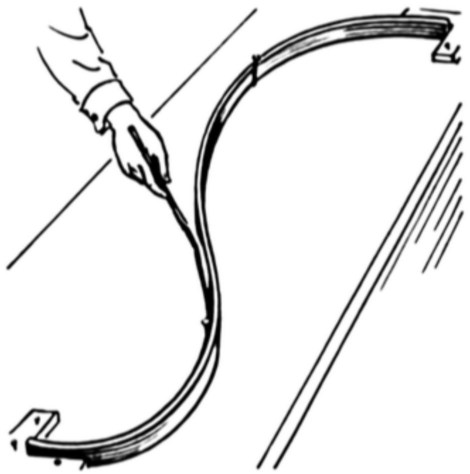
(i) Minimal "bending energy"

$$E_{bd}(f) = \int_a^b |f''(\tau)|^2\, d\tau$$

Theorem 3.5.14. Optimality of natural cubic spline interpolant

The natural cubic spline interpolant s minimizes the elastic curvature energy among all interpolating functions in $C^2([a,b])$, that is

$$E_{bd}(s) \le E_{bd}(f) \quad \forall f \in C^2([a,b]),\ f(t_i) = y_i,\ i = 0,\dots,n.$$



Proof: $d := f - s \in C^2$
$d(t_j) = 0$

$$\int_a^b d''(\tau)s''(\tau)\,d\tau = \sum_{j=1}^{n}\int_{t_{j-1}}^{t_j} d''(\tau)s''(\tau)\,d\tau$$
$$= \sum_{j=1}^{n} -\int_{t_{j-1}}^{t_j} d'(\tau)s'''(\tau)\,d\tau + \underbrace{\cancel{[d's'']_{t_{j-1}}^{t_j}}}_{=0}$$

telescopic sum

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$$= \sum_{j=1}^{n} \int_{t_{j-1}}^{t_j} d(\tau)\underbrace{s^{(iv)}(\tau)}_{=0}d\tau - \left[\underbrace{d}_{=0} s^{(iii)}\right]_{t_{j-1}}^{t_j} = 0$$

$$\int_a^b |f''|^2 - |s''|^2 d\tau = \int_a^b (f+s-2s)'' d'' d\tau = \int_a^b |d''|^2 d\tau \geq 0 \qquad \square$$

(ii) Monotonicity preservation :

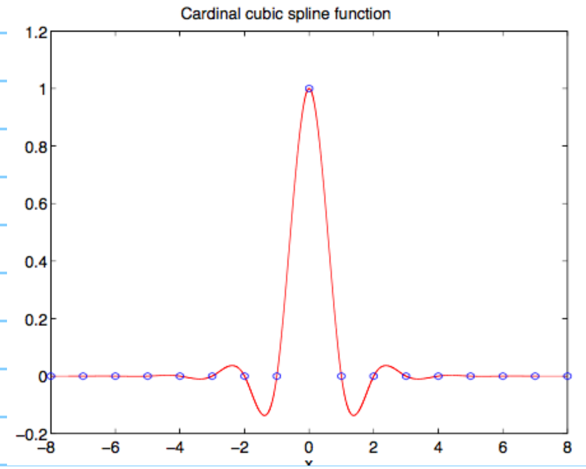
NO, because C.S.I. is a linear I.S.

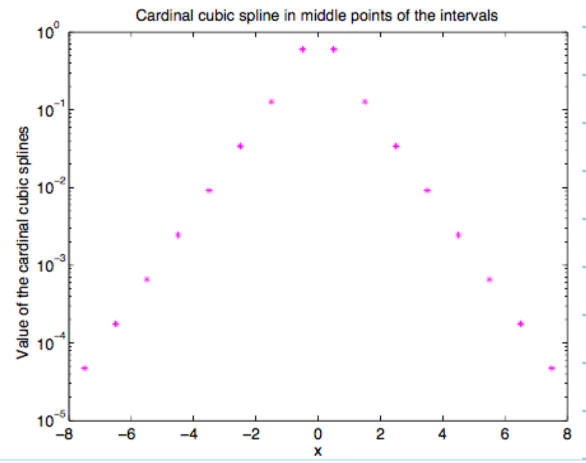
Theorem 3.4.17. Property of linear, monotonicity preserving interpolation into C^1

If, for fixed node set $\{t_j\}_{j=0}^n$, an interpolation scheme $\mathsf{I} : \mathbb{R}^{n+1} \to C^1(I)$ is linear as a mapping from data values to continuous functions on the interval covered by the nodes ($\to$ Def. 3.1.15), and monotonicity preserving, then $\mathsf{I}(\mathbf{y})'(t_j) = 0$ for all $\mathbf{y} \in \mathbb{R}^{n+1}$.

(iii) Locality : NO

C.S.I. linear $\Rightarrow$ Gauge locality by looking at cardinal interpolant $I_S e_j$





C.S.I. is "almost local" : cardinal interpolants decay exponentially