MAT 460 Numerical Differential Equations

Spring 2016

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Lecture 9

Topics : Error Formula for Polynomial-Interpolation, Hermite-Interpolation, Splines

Error formula I

Problem: Let $f : [a,b] \to \mathbb{R}$ be a function which is interpolated at the points

$$a \leq x_1 < x_2 < \ldots < x_{n+1} \leq b$$

by a polynomial p of degree $\leq n$.

Question: How good is the approximation of the function f by interpolation polynomial p?

More precise: How large is the maximal error

$$\max_{x\in[a,b]} |f(x) - p(x)| \quad ? \qquad (*)$$

For general f the error $(*)$ can be arbitrarily large. But if f is often enough differentiable we can find an estimate for the upper limit of $(*)$. Then

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \underbrace{(x-x_1)(x-x_2)\ldots(x-x_{n+1})}_{=:\omega_{n+1}(x)} \qquad \text{for a } \xi \in [a,b] \qquad (**)$$

From which we get the upper limit of $(*)$ as

$$\max_{x\in[a,b]} |f(x) - p(x)| \leq \frac{1}{(n+1)!} \max_{\xi\in[a,b]} |f^{(n+1)}(\xi)| \max_{x\in[a,b]} |\omega_{n+1}(x)|.$$

We prove the error formula $(**)$ on the following pages.

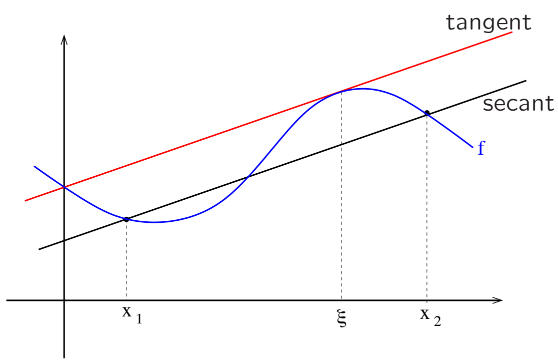
The error formula $(**)$ follows from the **generalized mean value theorem**, see next page. Recall the

mean value theorem of calculus:

Let $f : [a,\ b] \to \mathbb{R}$ be continuously differentiable, and let $a \leq x_1 < x_2 \leq b$.
Then a point $\xi \in [x_1, x_2]$ exist, such that

$$\underbrace{\frac{f(x_2) - f(x_1)}{x_2 - x_1}}_{=f[x_1,\, x_2]} = f'(\xi).$$

(Slope of secant is the same as slope of tangent at a point ξ in the interval)



Generalized mean value theorem:

Let $f : [a,b] \to \mathbb{R}$ be $(n+1)$-times differentiable and let $a \leq x_1 < x_2 < \ldots < x_{n+1} \leq b$.
Then a point $\xi \in [x_1, x_{n+1}]$ exist, such that

$$f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1}] = \frac{f^{(n)}(\xi)}{n!}.$$

Proof: Let p be the interpolation polynomial to the data $(x_j, f(x_j))$. Then

$$p(x) = q(x) + f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1}]\,(x-x_1)(x-x_2)\ldots(x-x_n).$$

with a polynomial q of $degree(q) \leq n-1$. Differentiating p n-times gives a constant, i. e.

$$p^{(n)}(x) = f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1}]\ n!. \qquad (*)$$

Consider the auxiliary function $\phi(x) = f(x) - p(x)$. ϕ has $n+1$ zeros $x_1, \ldots, x_{n+1}$. Between these zeros ϕ has local extrema (maxima or minima). This gives at least n zeros for the derivative ϕ'. Between the zeros ϕ' has local extrema. This gives at least $n-1$ zeros for the 2nd derivative, etc. The n-th derivative has at least one zero ξ. So we have

$$0 = \phi^{(n)}(\xi) = f^{(n)}(\xi) - f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1}]\ n!.$$

Lemma: Let p be the interpolation polynomial to $f : \mathbb{C} \to \mathbb{C}$ with the points $x_1, \ldots, x_{n+1} \in \mathbb{C}$. Then we have for all $x \in \mathbb{C}$:

$$f(x) = p(x) + \underbrace{f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1},\ x]\ (x - x_1)(x - x_2)\ldots(x - x_{n+1})}_{\text{remainder}},$$

Proof: The interpolation polynomial with the interpolation points $x_1, \ldots, x_{n+1}, x$ is

$$q(\tilde{x}) = p(\tilde{x}) + f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1},\ x]\ (\tilde{x} - x_1)(\tilde{x} - x_2)\ldots(\tilde{x} - x_{n+1})$$

By definition we have $f(x) = q(x)$.

Combining the generalized mean value theorem with this Lemma gives

$$\begin{aligned} f(x) &= p(x) + f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1},\ x]\ (x - x_1)(x - x_2)\ldots(x - x_{n+1}) \\ &= p(x) + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_1)(x - x_2)\ldots(x - x_{n+1})}_{\text{remainder}} \qquad (**) \end{aligned}$$

for a point ξ with

$$\min\{x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1},\ x\} \ \le \xi \le \max\{x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1},\ x\}.$$

This completes the proof of $(**)$.

Remark: The Taylor formula as the limit

We just proved that

$$f(x) \;=\; \underbrace{\sum_{j=0}^{n} f[x_1, \ldots x_{j+1}]\ (x - x_1)\ldots(x - x_j)}_{\text{interpolation polynomial } p(x)} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_1)(x - x_2)\ldots(x - x_{n+1})}_{\text{remainder}}$$

(The first summand ($j = 0$) ist $[x_1]f = f(x_1)$). Applying the generalized mean value theorem to each of the coefficients $f[x_1, \ldots x_{j+1}]$ gives

$$f(x) \;=\; \underbrace{\sum_{j=0}^{n} \frac{f^{(j)}(\xi_j)}{j!}(x - x_1)\ldots(x - x_j)}_{\text{interpolation polynomial } p(x)} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_1)(x - x_2)\ldots(x - x_{n+1})}_{\text{remainder}}$$

with ξ_j between x_1 and x_j. Now we can shrink the points x_j into a single point x_0 : $x_j \to x_0,\ \ j = 1, \ldots, n+1$. Then the ξ_j converge to x_0. The products $(x - x_1)\ldots(x - x_j)$ converge to $(x - x_0)^j$. And we get the Taylor formula

$$f(x) \;=\; \underbrace{\sum_{j=0}^{n} \frac{f^{(j)}(x_0)}{j!}(x - x_0)^j}_{\text{Taylor polynomial}} + \underbrace{\frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}}_{\text{remainder}}$$

with ξ between x_0 and x.

Error formula II

Consider the interpolation points $a \le x_1 < x_2 < \ldots < x_{n+1} \le b$.
For the interpolation error we showed that

$$\max_{x\in[a,b]} |f(x) - p(x)| \le \frac{1}{(n+1)!} \max_{\xi\in[a,b]} |f^{(n+1)}(\xi)| \ \max_{x\in[a,b]} |\omega_{n+1}(x)|.$$

where

$$\omega_{n+1}(x) = (x - x_1)(x - x_2)\ldots(x - x_{n+1})$$

We can show that for any choice of interpolation points:

$$2\left(\frac{b-a}{2}\right)^{n+1} \le \max_{x\in[a,b]} |\omega_{n+1}(x)| \le (b-a)^{n+1}$$

The maximum is smallest when

$$2\left(\frac{b-a}{2}\right)^{n+1} = \max_{x\in[a,b]} |\omega_{n+1}(x)|$$

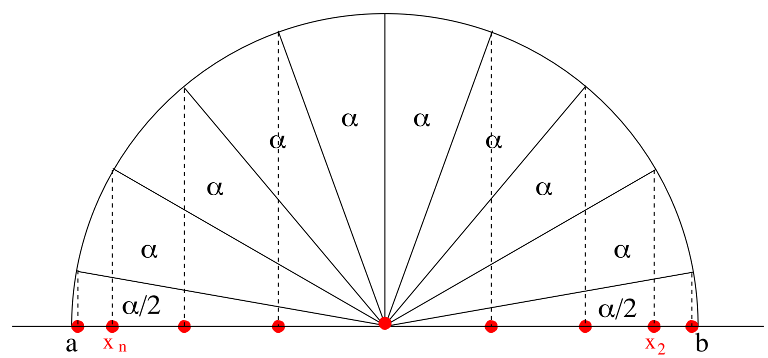
which is the case when the interpolation points are chosen as follows:

$$x_j = \frac{a+b}{2} + \frac{b-a}{2}\,\tau_{n+1,j}, \qquad \tau_{n+1,j} = \cos\left(\frac{2j-1}{2(n+1)}\pi\right), \qquad j = 1, \ldots, n+1.$$

This choice of interpolation points x_j are called **Chebyshev-interpolation points**.
The numbers $\tau_{n+1,j}$ are the zeros of the Chebyshev-polynomials. (See next slides.)

Illustration: Position of the Chebyshev-interpolation points

$$x_j = \frac{a+b}{2} + \frac{b-a}{2}\cos\left(\frac{2j-1}{2(n+1)}\pi\right), \qquad j = 1, \ldots, n+1.$$



● = Chebyshev-interpolation points $\qquad \alpha = \dfrac{\pi}{n+1}$

Chebyshev-polynomials

Using the addition theorem for cosines we prove that a polynomial $T_n(x)$ with integer coefficients and $degree(T_n) = n$ exist, such that

$$\cos(n\,\alpha) = T_n(\cos(\alpha)) \qquad (*)$$

Let $x \in [-1, 1]$, such that $\cos(\alpha) = x$. Then $\alpha = \arccos(x)$ if we plug this into $(*)$ we get

$$T_n(x) = \cos(n \arccos(x)).$$

Chebyshev-polynomials are computed using the recursion formula

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_{n+1}(x) = 2\,x\,T_n(x) - T_{n-1}(x)$$

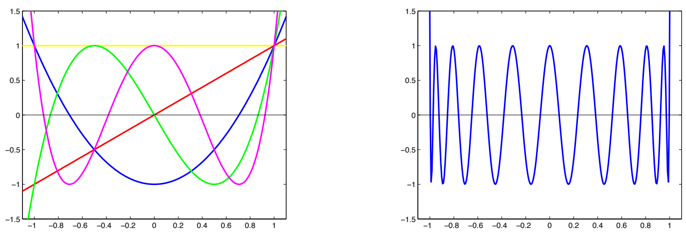
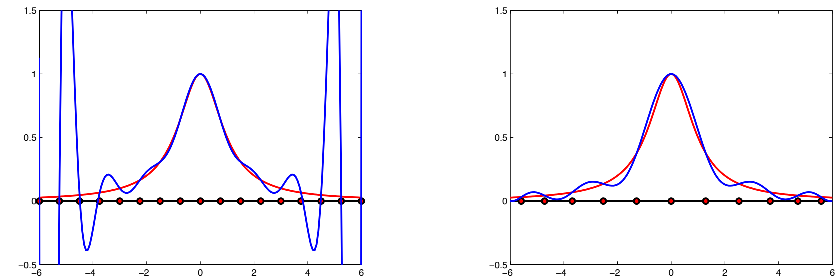


Figure left: Chebyshev-polynomials $T_0, \ldots, T_4$, Figure right: Chebyshev-polynomial T_{20}

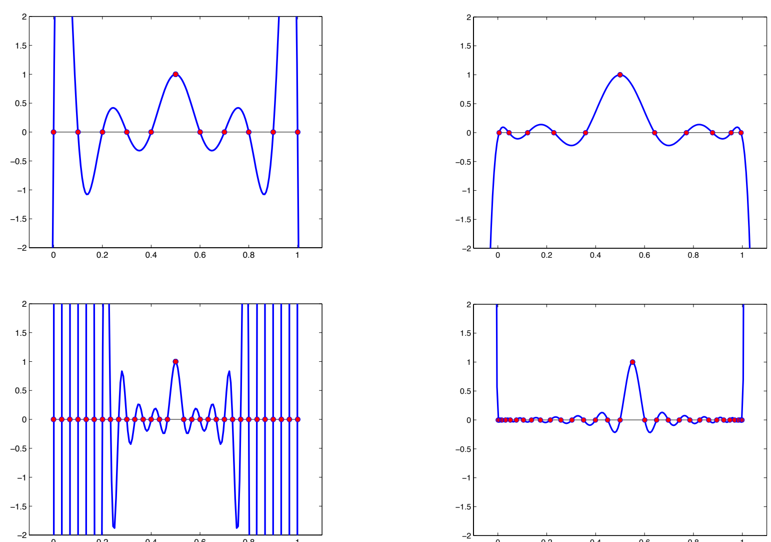
Interpolation example (from Runge):

Interpolation polynomial (blue) to the function $f(x) = \frac{1}{1+x^2}$ (red) with

17 equidistant interpolation points (left) and 17 Chebyshev-interpolation points (right)



Lagrange-basis polynomials w.r.t. equidistant (left) and Chebyshev-interpolation points (right)



Hermite-Interpolation

For Hermite-Interpolation besides function values also the derivatives have to be given at the interpolation points.

The Hermite-interpolation problem for polynomials is:

For given interpolation points $x_1, \ldots, x_r \in \mathbb{C}$ and at each point x_j a list of values

$$f_j = f_j^{(0)},\ f_j' = f_j^{(1)},\ \ldots, f_j^{(\mu_j - 1)} \in \mathbb{C}$$

find a polynomial p of $degree(p) \leq \mu_1 + \mu_2 + \ldots \mu_r - 1 =: n$, such that the derivatives of p satisfy

$$p^{(k)}(x_j) = f_j^{(k)}, \qquad k = 0, \ldots, \mu_{j-1}. \qquad (*)$$

We can show that the Hermite-interpolation problem has always a solution. If we make an ansatz of the form

$$p(x) = c_1\,\beta_1(x) + c_2\,\beta_2(x) + \ldots + c_{n+1}\,\beta_{n+1}(x)$$

with an arbitrary polynomial basis $\beta_j(x)$ of Π_n, then the equations $(*)$ are:

$$c_1\,\beta_1^{(k)}(x) + c_2\,\beta_2^{(k)}(x) + \ldots + c_{n+1}\,\beta_{n+1}^{(k)}(x) = f_j^{(k)} \qquad k = 0, \ldots, \mu_{j-1}$$

This is a linear equation system for the coefficients c_k, whose matrix is non-singular.

The simplest Hermite-Interpolation problem is: The Taylor-Polynomial

Problem: For a given function $f : U \to \mathbb{C}$, $U \subseteq \mathbb{R}$ oder $\mathbb{C}$, which is n-times differentiable at $x_0 \in U$,
find a polynomial p with $degree(p) \le n$, such that

$$p^{(k)}(x_0) = f^{(k)}(x_0), \qquad k = 0, \dots, n \qquad (*)$$

Solution: The unique solution is the Taylor-polynomial

$$\begin{aligned} p(x) &= f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x)}{2}(x - x_0)^2 + \ldots + \frac{f^{(k)}(x)}{n!}(x - x_0)^n \\ &= \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!}(x - x_0)^k. \end{aligned}$$

Explanation:

For the polynomial $\beta_k(x) := (x - x_0)^k$ we have

$$\beta_k'(x) = k\,(x - x_0)^{k-1}, \quad \beta_k''(x) = k(k-1)\,(x - x_0)^{k-2}, \quad \ldots \quad, \beta_k^{(k)}(x) = k!, \quad \beta_k^{(k+1)}(x) = 0.$$

From this it follows that

$$\beta_k^{(\ell)}(x_0) = \begin{cases} k! & \text{if } \ell = k \\ 0 & \text{otherwise} \end{cases} \qquad (**)$$

Substituting this into the ansatz $p(x) = c_0\,\beta_0(x) + c_1\,\beta_1(x) + \ldots + c_n\,\beta_n(x)$ gives:

$$f^{(k)}(x_0) \underset{(*)}{=} p^{(k)}(x_0) \underset{(**)}{=} c_k\,k! \qquad \Rightarrow c_k = f^{(k)}(x_0)/k!.$$

Divided differences for the Hermite-problem

To generalize the divided differences approach for Hermite-interpolation we allow that in the expression $f[x_1,\ x_2,\ \ldots,\ x_{n+1}]$ some or all x_j are equal. For the later we define

$$f\,\underbrace{[x_j,\ x_j,\ \ldots,\ x_j]}_{(n+1)-times} := \frac{f^{(n)}}{n!}. \qquad (*)$$

Then we write the Taylor polynomial with degree n at the point x_j as:

$$p(x) = \sum_{k=0}^{n} f\,\underbrace{[x_j,\ x_j,\ \ldots,\ x_j]}_{(k+1)-mal}\,(x - x_j)^k.$$

Divided differences where only some of the x_j are equal can be transformed to the case $(*)$ with the recursion formula

$$f[x_1,\ x_2,\ \ldots,\ x_n,\ x_{n+1}] = \frac{f[x_2,\ x_3,\ \ldots,\ x_n,\ \ x_{n+1}] - f[x_1,\ x_2,\ \ldots,\ x_n]}{x_{n+1} - x_1}, \quad \text{when } x_{n+1} \neq x_n$$

Example:

$$f[3,\ 3,\ 3,\ 7] \;=\; \frac{[3,\ 3,\ 7] - f[3,\ 3,\ 3]}{7 - 3} = \frac{f[3,\ 3,\ 7] - f''(3)/2}{7 - 3},$$

$$f[3,\ 3,\ 7] \;=\; \frac{f[3,\ 7] - f[3,\ 3]}{7 - 3} = \frac{\frac{f(7) - f(3)}{7 - 3} - f'(3)}{7 - 3}.$$

Divided differences for the Hermite-Problem II

With divided differences we can represent the solution of a Hermite-interpolation problem in Newtonian form. The most important case for applications we consider as an example:

Problem: Find a polynomial p of degree ≤ 3 (cubic polynomial), satisfying the following conditions:

$$p(x_1) = f_1, \quad p'(x_1) = s_1, \qquad p(x_2) = f_2, \quad p'(x_2) = s_2,$$

where $x_1, x_2, f_1, f_2, s_1, s_2 \in \mathbb{C}$ are prescribed and $x_1 \neq x_2$.

Solution: We make the ansatz

$$p(x) = f[x_1] + f[x_1,\ x_1]\ (x - x_1) + f[x_1,\ x_1,\ x_2]\ (x - x_1)^2 + f[x_1,\ x_1,\ x_2,\ x_2]\ (x - x_1)^2(x - x_2)$$

and compute

$$\begin{aligned} f[x_1,\ x_2] &= \frac{f_1 - f_2}{x_1 - x_2} \\ f[x_1,\ x_1,\ x_2] &= \frac{f[x_1,\ x_1] - f[x_1,\ x_2]}{x_1 - x_2} = \frac{s_1 - \frac{f_1 - f_2}{x_1 - x_2}}{x_1 - x_2} \\ f[x_1,\ x_1,\ x_2,\ x_2] &= \frac{f[x_1,\ x_1,\ x_2] - f[x_1,\ x_2,\ x_2]}{x_1 - x_2} \\ &= \frac{\frac{f[x_1, x_1] - f[x_1, x_2]}{x_1 - x_2} - \frac{f[x_1,\ x_2] - f[x_2,\ x_2]}{x_1 - x_2}}{x_1 - x_2} = \frac{s_1 + s_2 - 2\,\frac{f_1 - f_2}{x_1 - x_2}}{(x_1 - x_2)^2}. \end{aligned}$$

Hermite-basis polynomials

Consider again the problem from the last slide:

Problem: Find a polynomial p of degree ≤ 3 (cubic polynomial), which satisfies:

$$p(x_1) = f_1, \quad p'(x_1) = s_1, \qquad p(x_2) = f_2, \quad p'(x_2) = s_2. \qquad (*)$$

The solution p which we found on the last slide is not symmetric in the points x_1, x_2.
If we start out differently we can represent the solution symmetrically:

Define

$$\begin{aligned} \beta_1(x) &:= \frac{(x - x_2)^2(x - x_1)}{(x_2 - x_1)^2}, & \beta_3(x) &:= \frac{x - x_2 - \beta_1(x) - \beta_2(x)}{x_1 - x_2}, \\ \beta_2(x) &:= \frac{(x - x_1)^2(x - x_2)}{(x_2 - x_1)^2}, & \beta_4(x) &:= \frac{x - x_1 - \beta_1(x) - \beta_2(x)}{x_2 - x_1}. \end{aligned}$$

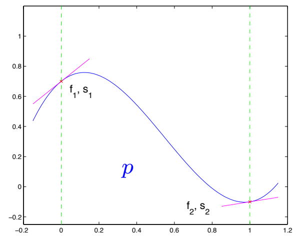
The polynomial p satisfying $(*)$ can be represented as

$$\begin{aligned} p(x) &= s_1\,\beta_1(x) + s_2\,\beta_2(x) + f_1\,\beta_3(x) + f_2\,\beta_4(x) \qquad (**) \\ &= (s_1 - m)\,\beta_1(x) + (s_2 - m)\,\beta_2(x) + f_1\,\frac{x - x_2}{x_1 - x_2} + f_2\,\frac{x - x_1}{x_2 - x_1}, \qquad m := \frac{f_2 - f_1}{x_2 - x_1}. \end{aligned}$$

Proof by computation (explanations are given in the lecture).

Advantage of the this representation: The coefficients in $(**)$ are the same as in $(*)$. Once we determined the β_k, nothing more needs to be done to solve $(*)$. The polynomials β_k are called **Hermite basis polynomials**.

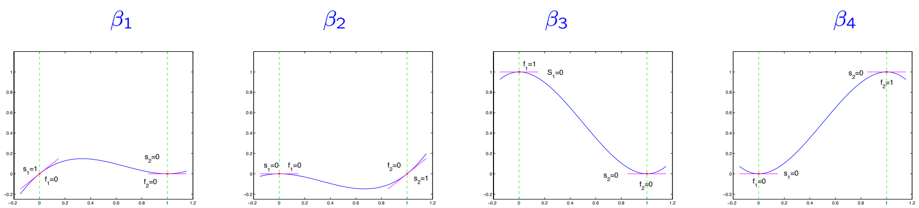
Illustration: a polynomial of degree 3 and Hermite-basis polynomials



Every polynomial p of $degree(p) \leq 3$ is a linear combination of the 4 Hermite-basis polynomials:

$$p(x) = s_1\,\beta_1(x) + s_2\,\beta_2(x) + f_1\,\beta_3(x) + f_2\,\beta_4(x).$$

The Hermite-basis polynomials for the interval $[0,1]$ are:



Spline-interpolation

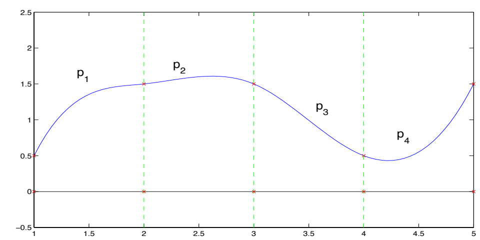
We saw that the interpolation of a function f with higher order polynomials often does not approximate the function f well. This is because higher degree polynomials tend to oscillate near the interpolation points at the boundary. We can get better approximations with splines. Splines are piecewise polynomials, which are connected smoothly at the interpolation points.

Definition: A spline of degree k with the interpolation points

$$a = x_1 < x_2 < \ldots < x_{n+1} = b$$

is a function $\sigma : [a,b] \to \mathbb{R}$ with the such that:

- σ is at least $(k-1)$-times continuous differentiable.
- In every interval $[x_j, x_{j+1}]$ is σ a polynomial function p_j with degree $\leq k$.



Cubic splines

The most important splines for applications are cubic splines.

Definition: A cubic spline with the interpolation points (knots)

$$a = x_1 < x_2 < \ldots < x_{n+1} = b$$

is a function $\sigma : [a,b] \to \mathbb{R}$ such that:

- σ is at least 2-times continuous differentiable.
- In each interval $[x_j, x_{j+1}]$ is σ a polynomial function p_j of degree ≤ 3.

The interpolation problem for cubic splines is:

Find to given knots f_j a cubic spline, such that

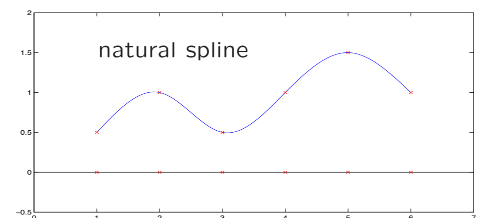
$$\sigma(x_j) = f_j, \qquad j = 1, \ldots, n+1.$$

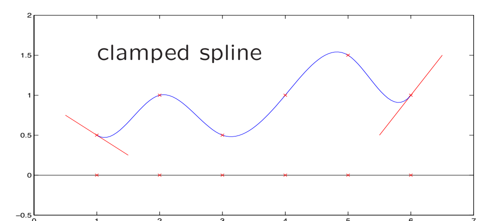
This problem has several solutions. To make the solution unique, we need to specify two boundary conditions. The most important splines are

1. $\sigma''(x_1) = \sigma''(x_{n+1}) = 0$ (natural spline)
2. $\sigma'(x_1) = s_1,\ \sigma'(x_{n+1}) = s_{n+1}$ (clamped spline)
   where $s_1, s_{n+1} \in \mathbb{R}$ are given.
3. $\sigma'(x_1) = \sigma'(x_{n+1}),\quad \sigma''(x_1) = \sigma''(x_{n+1})$ (periodic splines)

Comparison of natural and clamped cubic splines

The figures show splines with the same interpolation points.





Natural spline: 2nd derivatives are 0 at the boundary.

Clamped spline: 1st derivatives are prescribed at the boundary.

Two important features of splines

Splines have minimal total curvature

Let $\sigma : [a,b] \to \mathbb{R}$ a natural, clamped, or periodic cubic spline with the interpolation points $a = x_1, \dots, x_{n+1} = b$, and let $f : [a,b] \to \mathbb{R}$ be a 2-times continuous differentiable function, which has at all interpolation points the same values as σ and which satisfies the same boundary conditions. Then

$$\int_a^b \sigma''(x)^2 \, dx \le \int_a^b f''(x)^2 \, dx.$$

Error estimate

Let $\sigma : [a,b] \to \mathbb{R}$ be a cubic spline to the interpolation points $a = x_1, \dots, x_{n+1} = b$, and let $f : [a,b] \to \mathbb{R}$ be a 4-times continuous differentiable function, which has at all points the same values as σ and which has the same 1st derivatives at the boundary. Then

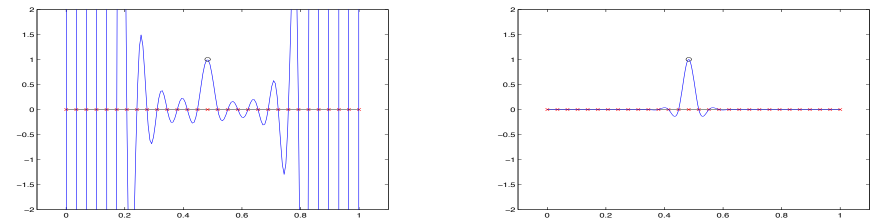
$$\max_{x \in [a,b]} |\sigma(x) - f(x)| \;\le\; \frac{5}{384} h^4 \max_{x \in [a,b]} |f^{(4)}(x)|,$$

where h is the maximal distance between two neighbor knots x_j.

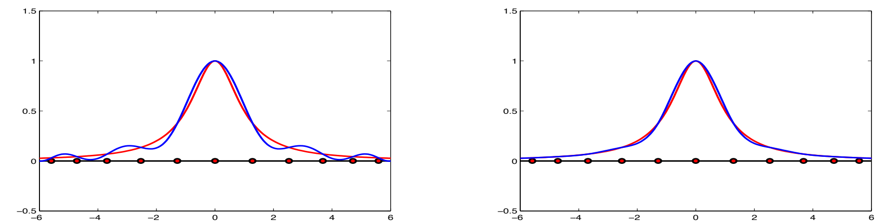
Note: Many error estimates are derived in the same way.

Comparison: Polynomial- and spline-interpolation

Left: Lagrange-basis polynomial. Right: Spline, which interpolates the same knots.



Left: Lagrange-interpolation of $f(x) = 1/(1+x^2)$ with Chebyshev-interpolation points.
Right: Spline-interpolation of $f(x) = 1/(1+x^2)$.



How to compute cubic splines?

A cubic spline σ with

$$\sigma(x_j) = f_j, \qquad \sigma'(x_j) = s_j, \qquad j = 1, \dots, n+1$$

is made of polynomials p_j with degree 3 and is represented by

$$\sigma(x) = p_j(x) = (s_j - m_j)\,\beta_{j,1}(x) + (s_{j+1} - m_j)\,\beta_{j,2}(x) + f_j \frac{x - x_{j+1}}{x_{j+1} - x_j} + f_{j+1} \frac{x - x_j}{x_{j+1} - x_j}, \qquad (*)$$

where $x \in [x_j, x_{j+1}]$, $m_j := \frac{f_{j+1} - f_j}{x_{j+1} - x_j}$ and $\beta_{j,1}, \beta_{j,2}(x)$ are the first 2 Hermite-basis polynomials in the interval $[x_j, x_{j+1}]$.

From the conditions that the σ are 2-times differentiable at the knots x_j

$$p''_{j-1}(x_j) = p''_j(x_j), \qquad j = 2, \dots, n$$

we get after some reordering the following linear equations for the slopes:

$$\lambda_j\, s_{j-1} + 2\, s_j + (1 - \lambda_j) s_{j+1} = 3\,(\lambda_j\, m_{j-1} + (1 - \lambda_j)\, m_j), \qquad \lambda_j = \frac{x_{j+1} - x_j}{x_{j+1} - x_{j-1}}.$$

Together with the boundary conditions this gives a linear equation system for all slopes s_j. After this is solved, the spline can be computed using $(*)$.

Details can be found in the (and any other good) numerical mathematics text book.