



LINMA2171 Numerical Analysis

SIMON DESMIDT

Academic year 2024-2025 - Q1



UCLouvain

Contents

1	Polynomials	2
1.1	Lagrange interpolation	2
1.2	Hermite interpolation	2
1.3	Neville's algorithm	3
1.4	Newton's interpolation formula	3
1.5	Linear algebra approach	3
1.6	Barycentric interpolation formula	4
1.7	Trigonometric interpolation	4
1.8	Rational interpolation	5
2	Splines	6
2.1	Definition	6
2.2	B-splines	6
2.3	Regression with splines	7
2.4	Interpolation by natural cubic splines	8

Polynomials

\mathcal{P}_n is the set of all real polynomials of degree at most n .

- The Runge phenomenon is the explosion of the polynomial near the boundary of the domain when the interpolation points are chosen to be equidistant. A solution to that is to put more points near the boundary and less in the middle of the domain, e.g. Chebyshev points.

1.1 Lagrange interpolation

Let x_0, \dots, x_n be distinct real numbers. The Lagrange polynomial L_k of degree n is such that it is equal to 0 for all $x_i, i \neq k$ and 1 for x_k . This serves as a base for the next interpolations. The general formula for the Lagrange polynomial is

$$L_k(x) = \prod_{i=0, i \neq k}^n \frac{x - x_i}{x_k - x_i} \quad k = 0, 1, \dots, n \quad (1.1)$$

- N.B.: we usually denote $L_k(x; x_0, \dots, x_n)$ or let $\chi = (x_0, \dots, x_n)$ and $L_k(x; \chi)$.

1.2 Hermite interpolation

Let x_0, \dots, x_n be distinct real numbers. Then, given two sets of real numbers (y_0, \dots, y_n) and (z_0, \dots, z_n) , there is a unique polynomial $p_{2n+1} \in \mathcal{P}_{2n+1}$ such that

$$p_{2n+1}(x_i) = y_i \quad p'_{2n+1}(x_i) = z_i \quad i = 0, \dots, n \quad (1.2)$$

The polynomial p_{2n+1} is termed the Hermite interpolation polynomial of degree at most $2n + 1$ for the data points $(x_0, y_0, z_0), \dots, (x_n, y_n, z_n)$. The expression is

$$p_{2n+1}(x) = \sum_{k=0}^n (H_k(x)y_k + K_k(x)z_k) \quad \begin{cases} H_k(x) = (L_k(x))^2(1 - 2L'_k(x_k)(x - x_k)) \\ K_k(x) = (L_k(x))^2(x - x_k) \end{cases} \quad (1.3)$$

where $L_k(x)$ is the Lagrange polynomial.

- The $H_k(x)$ are such that their derivative is zero for all x_i , and their value is zero for all x_i except x_k , where it is 1.

$$H_k(x_i) = \delta_{ik} \quad H'_k(x_i) = 0 \quad \forall i$$

- The $K_k(x)$ are such that their derivative is zero for all x_i except x_k where it is one, and their value is zero for all x_i .

$$K_k(x_i) = 0 \quad K'_k(x_i) = \delta_{ik} \quad \forall i$$

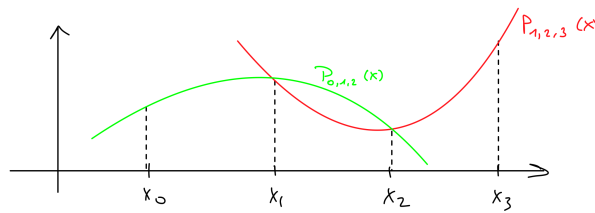
1.3 Neville's algorithm

Let us assume we are given a set of support points (x_i, y_i) , $i = 0, 1, \dots, n$, and p_n is their Lagrange interpolation polynomial. Let us now define the notation $P_{i_0 i_1 \dots i_k} \in \mathcal{P}_k$, the polynomial for which $P_{i_0 i_1 \dots i_k}(x_{i_j}) = y_{i_j}$ for all $j = 0, 1, \dots, k$. We work by recursion, with the following formula:

$$\begin{cases} P_i(x) = y_i \\ P_{i_0 i_1 \dots i_k} = \frac{(x - x_{i_0})P_{i_1 i_2 \dots i_k}(x) - (x - x_{i_k})P_{i_0 i_1 \dots i_{k-1}}(x)}{x_{i_k} - x_{i_0}} \end{cases} \quad (1.4)$$

Example:

Let us have four points $(x_0, y_0), \dots, (x_3, y_3)$. We want the polynomial interpolating all of them, using Neville's algorithm.



Here,

$$P_{0123}(x) = \frac{x - x_0}{x_3 - x_0} P_{123}(x) + \frac{x_3 - x}{x_3 - x_0} P_{012}(x) \quad (1.5)$$

1.4 Newton's interpolation formula

Newton's interpolation formula is used to evaluate polynomials with a computer, as it only needs to compute each operation $(x - x_i)$ one time. We write it like:

$$p_n(x) = ((\dots (y_{0\dots n}(x - x_n) + y_{0\dots n-1})(x - x_{n-1}) + y_{0\dots n-2})(x - x_{n-2}) + \dots) + y_0 \quad (1.6)$$

And the recursive formula is

$$P_{i_0 i_1 \dots i_k} = P_{i_0 i_1 \dots i_{k-1}}(x) + y_{i_0 i_1 \dots i_k}(x - x_{i_0})(x - x_{i_1}) \dots (x - x_{i_{k-1}}) \quad (1.7)$$

1.5 Linear algebra approach

Let (ϕ_0, \dots, ϕ_n) be a basis of \mathcal{P}_n , which is known to be an $(n + 1)$ -dimensional linear space. The interpolation polynomial can thus be expressed in a unique way in the basis:

$$p_n(x) = \sum_{i=0}^n a_i \phi_i(x) \quad (1.8)$$

and the coefficient are obtained by solving the linear system

$$\begin{bmatrix} \phi_0(x_0) & \phi_1(x_0) & \dots & \phi_n(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \dots & \phi_n(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \dots & \phi_n(x_n) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix} \quad (1.9)$$

This is called a Vandermonde matrix, and its determinant is

$$\det(V) = \prod_{0 \leq i < j \leq n} (x_j - x_i) \quad (1.10)$$

which is always non zero, as the x_i are disinct, and the system has one unique solution.

→ N.B.: the condition number¹ of such a matrix grows exponentially with n .

1.6 Barycentric interpolation formula

This formula is interesting, because it is numerically stable, contrary to the linear algebra method described before. We use the following notation, called the nodal polynomial:

$$\pi_{n+1}(x) = \prod_{i=0}^n (x - x_i) \quad (1.11)$$

We now define

$$\lambda_j = \frac{1}{\prod_{k \neq j} (x_j - x_k)} \quad (1.12)$$

The modified Lagrange formula is then

$$p_n(x) = \pi_{n+1}(x) \sum_{j=0}^n \frac{\lambda_j}{x - x_j} y_j \quad (1.13)$$

For the polynomial $p_n(x) = 1$, we have the following expression:

$$1 = \pi_{n+1}(x) \sum_{j=0}^n \frac{\lambda_j}{x - x_j}$$

and thus we generally prefer to use the equivalent formula for equation (1.13):

$$p_n(x) = \sum_{j=0}^n \frac{\lambda_j y_j}{x - x_j} / \sum_{j=0}^n \frac{\lambda_j}{x - x_j} \quad (1.14)$$

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

1.7 Trigonometric interpolation

Let us consider the evenly spaced points $x_j = \frac{2\pi j}{N}$, $j = 0, \dots, N$, on the interval $[0, 2\pi]$, and the interpolation values $f_0, \dots, f_N \in \mathbb{C}$, with $f_0 = f_N$. The trigonometric interpolation problem consists of finding β_k such that

$$p(x) = \sum_{k=0}^{N-1} \beta_k e^{ikx} \text{ such that } p(x_j) = f_j \quad j = 0, \dots, N-1 \quad (1.15)$$

¹It is a measure of the reaction of the system to a small perturbation

→ N.B.: the bound is $N - 1$ because the last condition $p(x_N) = f_N$ is satisfied when the others are (periodicity).

This is equivalent to the generalization to \mathbb{C} of the polynomial interpolation problem: if we denote $\omega := e^{ix}$, the complex polynomial is

$$P(\omega) = \sum_{k=0}^{N-1} \beta_k \omega^k \quad (1.16)$$

The Vandermonde matrix in the complex case is defined as in the real case. We denote it W .

Theorem: $W^*W = NI$ for a complex Vandermonde matrix in an interpolation problem.

From this, the solution to the interpolation problem is solved by multiplying both sides by W^* . We get

$$\beta = \frac{1}{N} W^* f \implies \beta_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-i2\pi k j / N} \quad k = 0, \dots, N-1 \quad (1.17)$$

And that is the discrete Fourier transform (DFT)

1.8 Rational interpolation

Let the interpolation points be $x_0 < x_1 < \dots < x_\sigma$, with the values $y_0, \dots, y_\sigma \in \mathbb{R}$. We define the polynomial

$$\Phi(x) = \frac{p_\mu(x)}{q_\nu(x)} \quad p_\mu \in \mathcal{P}_\mu, q_\nu \in \mathcal{P}_\nu \quad (1.18)$$

$$\text{such that } \Phi(x_i) = y_i \quad i = 0, \dots, \sigma \quad (1.19)$$

The interpolation polynomial can be written

$$\Phi(x) = \frac{\sum_{k=0}^{\mu} a_k x^k}{\sum_{k=0}^{\nu} b_k x^k} = \frac{\lambda p_\mu(x)}{q_\nu(x)} \quad (1.20)$$

The number of constraints, i.e. points needed for the interpolation is then $\sigma = \mu + \nu$. This implies that

If Φ is a solution to the equation (1.18), then p_μ, q_ν are solutions of

$$p_\mu(x_i) - y_i q_\nu(x_i) = 0 \quad i = 0, \dots, \mu + \nu \quad (1.21)$$

$$\left(\sum_{k=0}^{\mu} a_k x_i^k \right) - y_i \left(\sum_{k=0}^{\nu} b_k x_i^k \right) = 0 \quad (1.22)$$

The theorem of existence states that the equation (1.21) always has a non trivial solution, i.e. $(p_\mu, q_\nu) \neq (0, 0)$.

The theorem of uniqueness states that if Φ_1 and Φ_2 are non trivial solutions of (1.21), then they are equivalent, i.e. they differ only by a common polynomial factor in the numerator and denominator.

- p_μ, q_ν are relatively prime if they do not have zeros in common.

Given $\Phi = \frac{p_\mu}{q_\nu}$, let $\tilde{\Phi} = \frac{\tilde{p}_\mu}{\tilde{q}_\nu}$ be the equivalent expression for which \tilde{p}_μ and \tilde{q}_ν are relatively prime. Φ is the solution of (1.18) $\iff \tilde{p}_\mu(x_i) - y_i \tilde{q}_\nu(x_i) = 0, i = 0, \dots, \mu + \nu$.

Splines

2.1 Definition

Let $\mathcal{S} = \mathcal{S}(k) = \mathcal{S}(k; x_0, \dots, x_m) = \{s \in \mathcal{C}^{k-1}[a, b] : s|_{[x_{i-1}, x_i]} \in \mathcal{P}_k, i = 1, \dots, m\}$ denote the linear space of splines of degree $k \geq 1$, with knots $a = x_0 < x_1 < \dots < x_m = b$.

The conditions at the knots are the following:

$$s^{(j)}(x_i^-) = s^{(j)}(x_i^+) \quad j = 0, \dots, k-1 \quad (2.1)$$

$s^{(j)}$ denoting the j th derivative of the spline s . A basis of that set \mathcal{S} is

$$\{x^0, \dots, x^k, (x - x_1)_+^k, \dots, (x - x_{m-1})_+^k\} \quad (2.2)$$

where $(x - x_j)_+^k = (\max\{0, x - x_j\})^k$.

Theorem 2.1. The dimension of the linear space $\mathcal{S}(k; x_0, \dots, x_m)$ is $m + k$.

2.2 B-splines

The basis defined above is not well suited for computation, we will instead use the B-splines. These are functions ϕ such that

$$\phi(x) = 0 \quad \forall x \in [x_0, x_p] \cup [x_q, x_m] \quad (2.3)$$

with $0 < p < q < m$ and $q - p$ as small as possible. We will use ϕ of the form

$$\phi(x) = \sum_{j=p}^q d_j (x - x_j)_+^k, \quad a \leq x \leq b \quad (2.4)$$

where the parameters d_j satisfy

$$r_k(x) := \sum_{j=p}^q d_j (x - x_j)_+^k = 0, \quad x_q \leq x \leq b \quad (2.5)$$

Playing with arithmetics and algebra, we finally get the general formula for a B-spline:

$$B_p(x) = \sum_{j=p}^{p+k+1} \left(\prod_{l=p, l \neq j}^{p+k+1} \frac{1}{x_l - x_j} \right) (x - x_j)_+^k, \quad x \in \mathbb{R} \quad (2.6)$$

It belongs to \mathcal{S} and verifies the condition (2.3). It is well-defined for $(p = 0, \dots, m - k - 1)$ and thus gives $m - k$ B-splines. To define a basis of \mathcal{S} , we need $2k$ more functions. We are going to add k knots on the left of x_0 and on the right of x_m :

$$x_{-k} < x_{-k+1} < \dots, x_{-1} < x_0 = a < x_1 < \dots < x_m = b < x_{m+1} < \dots < x_{m+k} \quad (2.7)$$

and we will now define B_{-k}, \dots, B_{m-1} on these dots. We now have $m + k$ linearly independent functions, and thus a basis of \mathcal{S} .

Theorem 2.2. Let x_{-k}, \dots, x_{m+k} satisfy (2.7). Then, the $m + k$ functions $B_p, p = -k, \dots, m - 1$, given by (2.6) form a basis of the space $\mathcal{S}(k; x_0, x_m)$, with small support, meaning that B_p is null outside the interval (x_p, x_{p+k+1}) .

The recurrence formula for B-splines is the following, for $k > 1$:

$$\begin{cases} B_p^k(x) = \frac{(x - x_p)B_p^{k-1}(x) + (x_{p+k+1} - x)B_{p+1}^{k-1}(x)}{x_{p+k+1} - x_p} \\ B_p^0(x) = 1_{[x_p, x_{p+1})} \end{cases} \quad (2.8)$$

2.3 Regression with splines

Let B_{-k}, \dots, B_{m-1} be a basis of the linear space of splines $\mathcal{S}(k; u_0, \dots, u_m)$. We have a function $f \in \mathcal{C}[a, b]$ and sampling points w_0, \dots, w_q , assuming $q + 1 \geq k + m$. The goal of this section is to find a spline function $s \in \mathcal{S}$ that is the closest to the data points $(w_i, f(w_i)), i = 0, \dots, q$, i.e.

$$\arg \min_{s \in \mathcal{S}} \sum_{i=0}^q |f(w_i) - s(w_i)|^2 \quad (2.9)$$

Using $s = \sum_{j=-k}^{m-1} c_j B_j$, we must solve the system

$$\underbrace{\begin{bmatrix} B_{-k}(w_0) & \dots & B_{m-1}(w_0) \\ \vdots & \ddots & \vdots \\ B_{-k}(w_q) & \dots & B_{m-1}(w_q) \end{bmatrix}}_{=:A} \underbrace{\begin{bmatrix} c_{-k} \\ \vdots \\ c_{m-1} \end{bmatrix}}_{=:c} = \underbrace{\begin{bmatrix} f(w_0) \\ \vdots \\ f(w_q) \end{bmatrix}}_{=:F} \quad (2.10)$$

This is solved using the normal equations: $A^T A c = A^T F$.

Theorem 2.3. Under the above assumptions, the columns of A are linearly independent iff there exists a subset of $m + k$ sampling times $w_{i_{-k}} < \dots < w_{i_{m-1}}$ such that

$$u_p < w_{i_p} < u_{p+k+1} \quad p = -k, \dots, m - 1 \quad (2.11)$$

meaning that w_{i_p} must be in the support of B_p .

2.4 Interpolation by natural cubic splines

Let us define the set of cubic splines $\mathcal{S}(k = 3; \xi_0, \dots, \xi_m)$. The set of natural cubic splines with those knots is the set

$$\mathcal{S}_N(k = 3; \xi_0, \dots, \xi_m) = \{s \in \mathcal{C}^2[\xi_0, \xi_m] : s|_{[\xi_{i-1}, \xi_i]} \in \mathcal{P}_3, i = 1, \dots, m \text{ and } s''(\xi_0) = s''(\xi_m) = 0\} \quad (2.12)$$

For an arbitrary piece $[\xi_{i-1}, \xi_i]$, we have 4 conditions:

- $s|_{[\xi_{i-1}, \xi_i]}(\xi_{i-1}) = s_{i-1}$
- $s|_{[\xi_{i-1}, \xi_i]}(\xi_i) = s_i$
- $s''|_{[\xi_{i-1}, \xi_i]}(\xi_{i-1}) = \sigma_{i-1}$
- $s''|_{[\xi_{i-1}, \xi_i]}(\xi_i) = \sigma_i$

And we thus write

$$s|_{[\xi_{i-1}, \xi_i]} = s_{i-1}A(x) + s_iB(x) + \sigma_{i-1}C(x) + \sigma_iD(x) \quad (2.13)$$

where all functions are $\in \mathcal{P}_3$ and satisfy 4 conditions themselves:

$A(\xi_{i-1}) = 1$	$B(\xi_{i-1}) = 0$	$C(\xi_{i-1}) = 0$	$D(\xi_{i-1}) = 0$
$A(\xi_i) = 0$	$B(\xi_i) = 1$	$C(\xi_i) = 0$	$D(\xi_i) = 0$
$A''(\xi_{i-1}) = 0$	$B''(\xi_{i-1}) = 0$	$C''(\xi_{i-1}) = 1$	$D''(\xi_{i-1}) = 0$
$A''(\xi_i) = 0$	$B''(\xi_i) = 0$	$C''(\xi_i) = 0$	$D''(\xi_i) = 1$

Defining $h_i = \xi_i - \xi_{i-1}$, the final formula is

$$s(x) = \frac{(x - \xi_{i-1})s_i + (\xi_i - x)s_{i-1}}{h_i} \quad (2.14)$$

$$- \frac{1}{6}(x - \xi_{i-1})(\xi_i - x) \left[\left(1 + \frac{x - \xi_{i-1}}{h_i}\right) \sigma_i + \left(1 + \frac{\xi_i - x}{h_i}\right) \sigma_{i-1} \right] \quad x \in [\xi_{i-1}, \xi_i] \quad (2.15)$$

Now, we have the additional conditions that $s'(\xi_j^-) = s'(\xi_j^+)$, $j = 1, \dots, m-1$, which we write in the following matrix form:

$$Q^T s = R \sigma \quad (2.16)$$

where the matrices are:

$$Q^T = \begin{pmatrix} h_1^{-1} & -h_1^{-1} - h_2^{-1} & h_2^{-1} & 0 & \dots & 0 \\ 0 & h_2^{-1} & -h_2^{-1} - h_3^{-1} & h_3^{-1} & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & h_{m-1}^{-1} & -h_{m-1}^{-1} - h_m^{-1} & h_m^{-1} \end{pmatrix} \quad (2.17)$$

$$R = \begin{pmatrix} \frac{1}{3}(h_1 + h_2) & \frac{h_2}{6} & 0 & \dots & 0 \\ \frac{h_2}{6} & \frac{1}{3}(h_2 + h_3) & \frac{h_3}{6} & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \frac{h_{m-1}}{6} & \frac{1}{3}(h_{m-1} + h_m) \end{pmatrix} \quad (2.18)$$

Theorem 2.4. $s \in \mathcal{S}_N(k = 3; \xi_0, \dots, \xi_m)$ iff $Q^T s = R\sigma$.

Theorem 2.5. Consider ξ_0, \dots, ξ_m distinct and y_0, \dots, y_m . The interpolation at the knots

$$s \in \mathcal{S}_N(k = 3; \xi_0, \dots, \xi_m) \text{ such that } s(\xi_i) = y_i \quad i = 0, \dots, m \quad (2.19)$$

exists and is unique.

Theorem 2.6. Let s be a natural cubic spline. Then,

$$\int_{\xi_0}^{\xi_m} (s''(x))^2 dx = s^T K s \quad K = QR^{-1}Q^T \quad (2.20)$$

Theorem 2.7. Let s be the function in $\mathcal{S}_N(k = 3; \xi_0, \dots, \xi_m)$ such that $s(\xi_i) = y_i$, $i = 0, \dots, m$. Let v be any function in $H^2[a, b]$ that satisfies the same interpolation conditions. Then

$$\int_{\xi_0}^{\xi_m} (v''(x))^2 dx \geq \int_{\xi_0}^{\xi_m} (s''(x))^2 dx \quad (2.21)$$

with equality iff $v = s$.