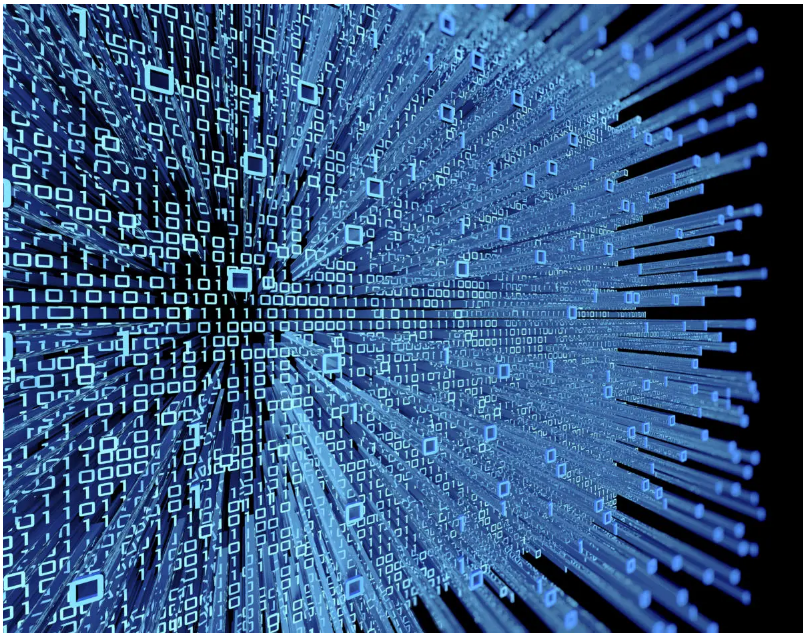

LINMA2171 Numerical Analysis

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Contents

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 $x_0, \ldots, x_n$ 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

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

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

1.2 Hermite interpolation

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

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

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

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

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.

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

- 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.

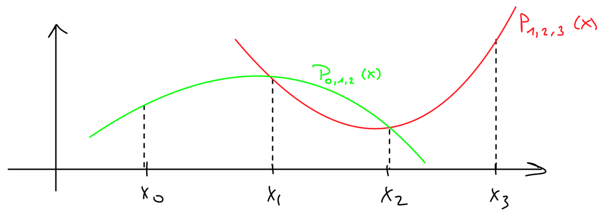
$$K_k(x_i) = 0 \qquad K'_k(x_i) = \delta_{ik} \qquad \forall i$$

1.3 Neville's algorithm

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

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

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



Here,

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

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:

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

And the recursive formula is

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

1.5 Linear algebra approach

Let $(\phi_0, \ldots, \phi_n)$ ba 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:

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

and the coefficient are obtained by solving the linear system

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

This is called a Vandermonde matrix, and its determinant is

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

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

→ N.B.: the condition number[1] 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:

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

We now define

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

The modified Lagrange formula is then

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

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):

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

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

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

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

[1]It 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

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

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

$$\beta = \frac{1}{N} W^* f \Longrightarrow \beta_k = \frac{1}{N} \sum_{j=0}^{N-1} f_j e^{-i2\pi kj/N} \qquad k = 0, \dots, N-1 \tag{1.17}$$

And that is the discrete Fourier transform (DFT)

1.8 Rational interpolation

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

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

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

The interpolation polynomial can be written

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

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

$$p_\mu(x_i) - y_i q_\nu(x_i) = 0 \qquad i = 0, \dots, \mu + \nu \tag{1.21}$$

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

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 $\tilde{p}_\mu$ and $\tilde{q}_\nu$ are relatively prime. Φ is the solution of (1.18) $\Longleftrightarrow \tilde{p}_\mu(x_i) - y_i \tilde{q}_\nu(x_i) = 0, i = 0, \dots, \mu + \nu$.

Splines

2.1 Definition

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

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

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

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

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

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

$$\phi(x) = 0 \qquad \forall x \in [x_0, x_p] \cup [x_q, x_m] \tag{2.3}$$

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

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

where the parameters d_j satisfy

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

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

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

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:

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

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 $k > 1$:

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

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.

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

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

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

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

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

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

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

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

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

And we thus write

$$s|_{[\xi_{i-1},\xi_i]} = s_{i-1}A(x) + s_i B(x) + \sigma_{i-1}C(x) + \sigma_i D(x) \tag{2.13}$$

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

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

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

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:

$$Q^T s = R\sigma \tag{2.16}$$

where the matrices are:

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

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

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

Theorem 2.5. Consider $\xi_0 \ldots, x_m$ distinct and $y_0, \ldots, y_m$. The interpolation at the knots

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

exists and is unique.

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

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

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

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

with equality iff $v = s$.

2.5 Smoothing splines

The problem studied in this section is

$$\arg \min_{s \in H^2[a,b]} F_\lambda(s) := \sum_{i=0}^{m} (y_i - s(x_i))^2 + \lambda \int_a^b (s''(x))^2 dx \tag{2.22}$$

where $a = x_0 < x_1 < \cdots < x_m = b$, $y_i \in \mathbb{R}$ are given and $\lambda > 0$ is a parameter. The first term is the data-attachment and the second is the roughness penalty.

Theorem 2.8. If $\hat{s}$ is a solution of (2.22), then $\hat{s} \in \mathcal{S}_N(k=3; x_0, \ldots, x_m)$.

To find the solution of (2.22), we can rewrite the function to minimize:

$$F_\lambda(s) = (y-s)^T(y-s) + \lambda s^T K s \tag{2.23}$$

This function is strictly convex and quadratic and thus s is the solution of the linear system

$$(I + \lambda K)s = y \tag{2.24}$$

Meaning that (2.22) has one and only one solution. The easiest way to compute s is

$$s = y - \lambda Q \sigma \tag{2.25}$$

- When $\lambda \to 0$, we get a simple interpolation problem and there is an infinity of solutions.
- When $\lambda \to \infty$, we find the linear regression solution.

2.6 Interpolation by natural splines

We define the linear space of natural splines as follows:

$$\mathcal{S}_N(2\kappa+1) = \{s \in \mathcal{S}(2\kappa+1) : s^{(j)}(a) = s^{(j)}(b) = 0, j = \kappa+1, \dots, 2\kappa\} \qquad \kappa \geq 1 \tag{2.26}$$

Provided that $m \geq \kappa$, the dimension of $\mathcal{S}_N(2\kappa+1)$ is $m+1$. Given a function $f \in \mathcal{C}[a,b]$, the set of interpolatory natural splines is

$$I_f\mathcal{S}_N(2\kappa+1) = \{s \in \mathcal{S}_N(2\kappa+1) : s(x_i) = f(x_i), i = 0, \dots, m\} \tag{2.27}$$

Theorem 2.9. If $m \geq \kappa$, then $I_f\mathcal{S}_N(2\kappa+1)$ is a singleton, meaning that the interpolating natural spline exists and is unique.

Theorem 2.10. Let $m \geq \kappa$ and let s ne the unique element of $I_f\mathcal{S}_N(2\kappa+1)$. Then, for all $v \in H^{\kappa+1}(a,b)$ that also interpolate f at $x_0, \dots, x_m$, it holds that

$$\|s^{(\kappa+1)}\|_2 \leq \|v^{(\kappa+1)}\|_2 \tag{2.28}$$

with equality iff $v = s$. In particular, the interpolating natural cubic spline, i.e. $\kappa = 1$, is the unique minimizer of the mean square acceleration under the interpolation conditions.

2.7 Error bounds of interpolation by natural splines

Theorem 2.11. Let s be the natural cubic spline interpolant of $f \in \mathcal{C}^4[a,b]$, where the interpolation is at equally spaced knots. Then,

$$\|(f-s)^{(r)}\|_\infty \leq C_r \|f^{(4)}\|_\infty h^{4-r} \qquad r = 0,1,2,3 \tag{2.29}$$

with $C_0 = 5/384, C_1 = 1/24, c_2 = 3/8, C_3 = 1$ and h the space between two knots. This means that the error between the interpolation and the function tends to 0 as the number of interpolation points goes to infinity.

2.8 Vector-valued splines

Vector-valued splines just work component-wise:

$$\mathbf{s}(x) = \sum_{j=-k}^{m-1} \mathbf{c}_j B_j(x) \tag{2.30}$$

where x and $B_j(x)$ are real and scalar, but $\mathbf{s}$ and $\mathbf{c}_j$ are in $\mathbb{R}^n$ for all j.
We deifne the Bernstein polynomials of degree n as

$$b_i^n(x) = \binom{n}{i} x^i (1-x)^{n-i} \qquad i = 0, \dots, n \tag{2.31}$$

They form a basis of $\mathcal{P}_n$ and a partition of unity, i.e. $\sum_{i=0}^n b_i^n(x) = 1$. We can thus write any polynomial piece $\mathbf{s}|_{[x_j, x_{j+1}]} \in \mathcal{P}_k$ in the Bernstein form:

$$\mathbf{s}|_{[x_j, x_{j+1}]} = \sum_{i=0}^k \mathbf{c}_i^j b_i^k \frac{x - x_j}{x_{j+1} - x_j} \tag{2.32}$$

aka the BÃl'zier curve on $[x_j, x_{j+1}]$ with control points $\mathbf{c}_0^j, \dots, \mathbf{c}_k^j$.

2.9 Thin plate splines

Thin plate splines consist of generalizing equation (2.22) to fit a function $s : \mathbb{R}^d \to \mathbb{R}$ to support points $(\mathbf{t}_i, z_i)$, $i = 0, \ldots, N$:

$$\arg_s \min F_\lambda(s) := \sum_{i=0}^{N} (z_i - s(\mathbf{t}_i))^2 + \lambda \sum_{i_1, i_2 = 1}^{d} \int_{\mathbb{R}^d} \left(\partial_{i_1, i_2} s(\mathbf{t})\right)^2 d\mathbf{t} \tag{2.33}$$

In the bivariate case, i.e. $d = 2$, we denote $\mathbf{t} = (x, y)$, and the equation reduces to

$$\arg_s \min F_\lambda(s) := \underbrace{\sum_{i=0}^{N} (z_i - s(x_i, y_i))^2}_{DA} + \lambda \underbrace{\int_{\mathbb{R}^2} \left(\frac{\partial^2 s}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2 s(x,y)}{\partial x \partial y}\right)^2 + \left(\frac{\partial^2 s}{\partial y^2}\right)^2 dxdy}_{PEN} \tag{2.34}$$

Definition 2.12. A function s is a thin plate spline on the data set $\mathbf{t}_0, \ldots, \mathbf{t}_N \in \mathbb{R}^2$ if it takes the form

$$s(\mathbf{t}) = \sum_{i=0}^{N} \delta_i \eta(\|\mathbf{t} - \mathbf{t}_i\|) + \sum_{j=1}^{3} a_j \phi_j(\mathbf{t}) \tag{2.35}$$

where δ_i, a_i are real numbers,

$$\eta_r = \begin{cases} \frac{1}{16\pi} r^2 \log(r^2) & \text{if } r > 0 \\ 0 & \text{if } r = 0 \end{cases} \tag{2.36}$$

and the ϕ_i simply denote the functions $\phi_1(x, y) = 1$, $\phi_2(x, y) = x$, $\phi_3(x, y) = y$.

If $\boldsymbol{\delta} = [\delta_0 \ldots \delta_N]^T$ satisfies $T\boldsymbol{\delta} = 0$, where

$$T = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ \mathbf{t}_0 & \mathbf{t}_1 & \ldots & \mathbf{t}_N \end{bmatrix} \tag{2.37}$$

then s is said to be a natural thin plate spline.

Theorem 2.13. Let s ba a thin plate spline. Then, $PEN(s)$ is finite iff s is a natural thin plate spline. If s is a natural thin plate spline, then $PEN(s) = \boldsymbol{\delta}^T E \boldsymbol{\delta}$, where $E_{ij} := \eta(\|\mathbf{t}_i - \mathbf{t}_j\|)$.

2.9.1 Interpolation by thin plate splines

Let $\mathbf{t}_0, \ldots, \mathbf{t}_m$ be non-collinear and let $\lambda \geq 0$. Then

$$\begin{bmatrix} E + \lambda I & T^T \\ T & 0 \end{bmatrix} \tag{2.38}$$

is nonsingular.

Theorem 2.14. Let $\mathbf{t}_0, \ldots, \mathbf{t}_N$ be distinct non-collinear points in $\mathbb{R}^2$. Given any values $z_0, \ldots, z_N$, there is one and only one natural thin plate spline s on the set $\mathbf{t}_0, \ldots, \mathbf{t}_N$ such that $s(\mathbf{t}_i) = z_i$ for all $i = 0, \ldots, N$.

2.9.2 Optimality of thin plate splines

Theorem 2.15. The natural thin plate spline interpolant uniquely minimizes PEN subject to the interpolation conditions $s(\mathbf{t}_i) = z_i$ for all i.

2.9.3 Thin plate spline smoother

Theorem 2.16. If $\hat{s}$ is a solution of the smoothing problem (2.33), then $\hat{s}$ admits the thin late spline form of 2.12 with the natural spline condition $T\boldsymbol{\delta} = 0$.

The objective function can be rewritten as

$$F_\lambda(s) = \begin{bmatrix}\boldsymbol{\delta}^T & \boldsymbol{a}^T\end{bmatrix} \underbrace{\begin{bmatrix} E^2 + \lambda E & ET^T \\ TE & TT^T \end{bmatrix}}_{= \begin{bmatrix} E & 0 \\ T & -\lambda I\end{bmatrix}\begin{bmatrix} E + \lambda I & T^T \\ T & 0\end{bmatrix}} \begin{bmatrix}\boldsymbol{\delta} \\ \boldsymbol{a}\end{bmatrix} - \begin{bmatrix}\boldsymbol{\delta}^T & \boldsymbol{a}^T\end{bmatrix}\begin{bmatrix} E \\ T\end{bmatrix}\boldsymbol{z} + \boldsymbol{z}^T\boldsymbol{z} \tag{2.39}$$

The unique solution of the minimization of the above function is

$$\begin{bmatrix} E + \lambda I & T^T \\ T & 0\end{bmatrix}\begin{bmatrix}\boldsymbol{\delta} \\ \boldsymbol{a}\end{bmatrix} = \begin{bmatrix}\boldsymbol{z} \\ 0\end{bmatrix} \tag{2.40}$$

2.10 Tensor product splines

In the last section, thin plate splines are not piecewise polynomials. If we want the admissible functions restrict to piecewise polynomials, we need other approaches, as the tensor product splines.

Definition 2.17. Tensor product Let $\mathcal{R}$ and $\mathcal{S}$ be two linear spaces of real-valued univariate functions. The tensor product of two functiuons $r \in \mathcal{R}$ and $s \in \mathcal{S}$ is $r \otimes s : \mathbb{R}^2 \to \mathbb{R} : (t_1, t_2) \to r(t_1)s(t_2)$. The tensor product of the two spaces is the linear space

$$\mathcal{R} \otimes \mathcal{S} = \left\{ \sum_{i,j} c_{ij} r_i \otimes s_j | c_{ij} \in \mathbb{R} \right\} \tag{2.41}$$

where $(r_1, \dots, r_{N_1})$ is a basis of $\mathcal{R}$ and $(s_1, \dots, s_{N_2})$ is a basis of $\mathcal{S}$.

Let us define the sets

$$\Delta = \{a = x_0 < x_1 < \cdots < x_m = b\} \tag{2.42}$$

$$\bar{\Delta} = \{\bar{a} = y_0 < y_1 < \cdots < y_{\bar{m}} = \bar{b}\} \tag{2.43}$$

and let $\mathcal{S}_k(\Delta) = \mathcal{S}(k; x_0, \dots, x_m)$, same for $\bar{\Delta}$. In this section, the set of admissible functions is

$$\mathcal{S}_k(\Delta) \otimes S_{\bar{k}}(\bar{\Delta}) \tag{2.44}$$

The functions of that set are called tensor product splines of degree $(k, \bar{k})$ and the points in $\Delta, \bar{\Delta}$ are the knots. The dimension of the space is $(m+k)(\bar{m}+\bar{k})$, and a basis is given by

$$B_{ij}^{k,\bar{k}}(x,y) := B_i^k(x) B_j^{\bar{k}}(y) \qquad i \in \{-k, \dots, m-1\}, j \in \{-\bar{k}, \dots, \bar{m}-1\} \tag{2.45}$$

where B functions are B-splines creating a basis of their respective $\mathcal{S}_k(\Delta), \mathcal{S}_{\bar{k}}(\bar{\Delta})$. Any admissible function can thus be uniquely written as a linear combination of those.

2.10.1 Matrix form

Any tensor-product spline s can be written in matrix form:

$$s(x,y) = \begin{bmatrix} B^k_{-k}(x) & \dots & B^k_{m-1}(x) \end{bmatrix} C \begin{bmatrix} B^{\bar{k}}_{-k}(y) \\ \vdots \\ B^{\bar{k}}_{\bar{m}-1}(y) \end{bmatrix} \qquad C = \begin{bmatrix} c_{-k,-\bar{k}} & \dots & c_{-k,\bar{m}-1} \\ \vdots & \ddots & \vdots \\ c_{m-1,-\bar{k}} & \dots & c_{m-1,\bar{m}-1} \end{bmatrix} \tag{2.46}$$

2.10.2 Interpolation and regression

Consider $t_1 < \cdots < t_n$ in $[a,b]$ and $\bar{t}_1 < \cdots < \bar{t}_{\bar{n}}$ in $\bar{a},\bar{b}$, and suppose that we are given real number $\{z_{ij}\}_{i=1,j=1}^{n,\bar{n}}$. The interpolation problem is to find a tensor product spline s such that

$$s(t_i,\bar{t}_j) = z_{ij} \quad i = 1,\dots,n, \quad j = 1,\dots,\bar{n} \tag{2.47}$$

In matrix form, this system of equations is

$$MC\bar{M}^T = Z = \begin{bmatrix} z_{1,1} & \dots & z_{1,\bar{n}} \\ \vdots & \ddots & \vdots \\ z_{n,1} & \dots & z_{n,\bar{n}} \end{bmatrix} \tag{2.48}$$

$$M = \begin{bmatrix} B^k_{-k}(t_1) & \dots & B^k_{m-1}(t_1) \\ \vdots & \ddots & \vdots \\ B^k_{-k}(t_n) & \dots & B^k_{m-1}(t_n) \end{bmatrix} \qquad \bar{M} = \begin{bmatrix} B^{\bar{k}}_{-k}(\bar{t}_1) & \dots & B^{\bar{k}}_{\bar{m}-1}(\bar{t}_1) \\ \vdots & \ddots & \vdots \\ B^{\bar{k}}_{-k}(\bar{t}_{\bar{n}}) & \dots & B^{\bar{k}}_{\bar{m}-1}(\bar{t}_{\bar{n}}) \end{bmatrix} \tag{2.49}$$

Solving this in the least square sense, the normal equations are

$$M^T MC\bar{M}^T\bar{M} = M^T Z\bar{M} \tag{2.50}$$