Splines

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March 8, 2005

Contents

Chapter 1

Piecewise Polynomial Representations

References:

- For a reference on splines, see "A practical guide to splines" by Carl de Boor.[1]
- A practical way to familiarise oneself with splines is to use the Matlab Spline Toolbox, which is in fact based on de Boor's book.

Context:

- Interpolation: Given the values of a function $f(x)$ (and possibly its derivatives) at discrete mesh points x_i, complete to an approximate "smooth" representation for all x.
  Various analytical representations can be used for $f(x)$ (polynomial, rational, trigonometric). Here one concentrates on polynomial-type representations.
- Finite Element Method.
- Shape functions for particle in cell (PIC)-type simulations.[2]

1.1 Splines

Origin of word spline: In construction, a spline is a thin wooden or metal strip used in the process of fairing, i.e. to draw smooth curves.

1.1.1 Spline Representation

Start considering problem of 1-Dim interpolation.

Assume the values $f_i = f(x_i)$ of a function $f(x)$ are given at mesh points x_i, $i = 1, \ldots, I$.

One wishes to approximate $f(x)$ by a piecewise polynomial of degree n over the mesh x_i, that is, for each interval $[x_i, x_{i+1}]$ one writes:

$$f(x) = P_i^n(x), \quad \text{for} \;\; x \in [x_i, x_{i+1}],$$

where the $P_i^n(x) = c_{i,0} + c_{i,1}x + \ldots + c_{i,n-1}x^{n-1} + c_{i,n}x^n$ are polynomials of degree n.

At first, to avoid the issue of more complex boundaries, one starts here by considering periodic boundaries so that $f(x_{i+I}) = f(x_i)$.

The coefficients $c_{i,n}$ of the polynomials $P_i^n(x)$ are determined by imposing a certain number of continuity conditions at the mesh points x_i. The coefficients $c_{i,n}$ represent $(n+1)I$ unknowns, for which one needs to find an equivalent number of equations. In any case, one imposes continuity of $f(x)$ on the grid:

$$P_{i-1}^n(x_i) = f_i = P_i^n(x_i), \quad i = 1, \ldots, I.$$

This provides $2I$ equations. Depending on the degree n of the polynomials considered, one may impose the additional continuity of d derivatives. For each considered derivative of order p one imposes:

$$\frac{d^p P_{i-1}^n}{dx^p}(x_i) = f_i^p = \frac{d^p P_i^n}{dx^p}(x_i), \quad i = 1, \ldots, I.$$

This provides $2I$ additional equations, but also I additional unknowns: the values f_i^p. By imposing continuity of d derivatives, one thus ends up with $(n+1)I + dI = (n+d+1)I$ unknowns and $2I(d+1)$ equations. Equating the number of equations with the number of unknowns leads to:

$$2I(d+1) = (n+d+1)I \quad \Longrightarrow \quad d = n-1, \tag{1.1}$$

i.e. when considering a piecewise polynomial representation of degree n, one imposes continuity up to the $(n-1)$th derivative (continuity C^{n-1}). Such a piecewise approximation of $f(x)$ is called the spline representation of degree n. An example of a linear $(n = 1)$ and cubic $(n = 3)$ spline representation of a periodic function $f(x)$ is given in Fig.1.1.

1.1.2 Spline Elements

For a given grid x_i, $i = 1, \ldots, I$, the space of piecewise polynomials of spline type form a vectorial space of dimension I. Each piecewise polynomial of this type can indeed be parametrised by the I independent values f_i.

Question: What is a practical choice of basis elements $B_i(x)$, $i = 1, \ldots, I$ for representing this space?

One possible choice is to consider the basis elements $B_i(x)$ for which $B_i(x_j) = \delta_{ij}$, where δ_{ij} is the Kroenecker function. As shown in Fig.1.2, when considering splines of degree higher than linear $(n > 1)$, these elements have a wide extent, in fact they are non-zero over the whole grid. This choice of basis functions is thus unpractical for most applications. Indeed, such elements would lead to full, instead of banded, matrices when applied for finite elements, and global instead of local operations when used for interpolation

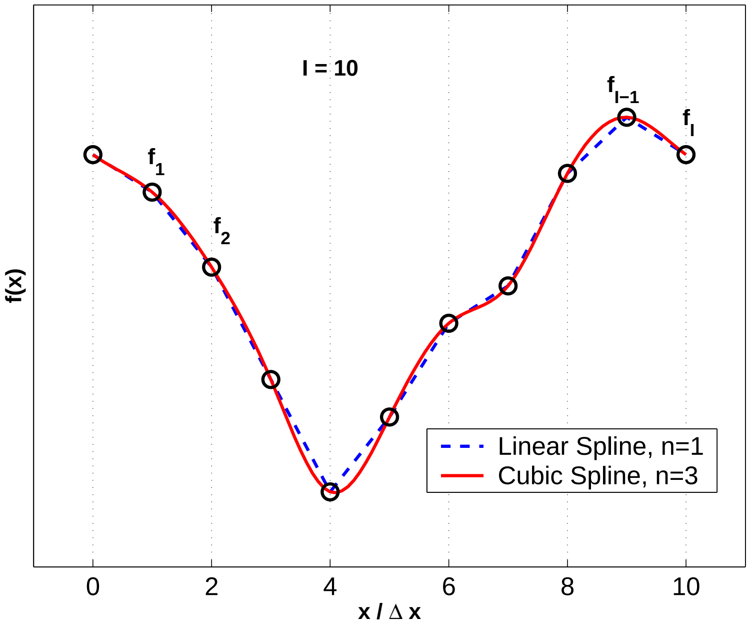

Figure 1.1: Example of linear ($n = 1$) and cubic ($n = 3$) spline representation passing through the data points $f_i = f(x_i)$ of a periodic function $f(x)$.

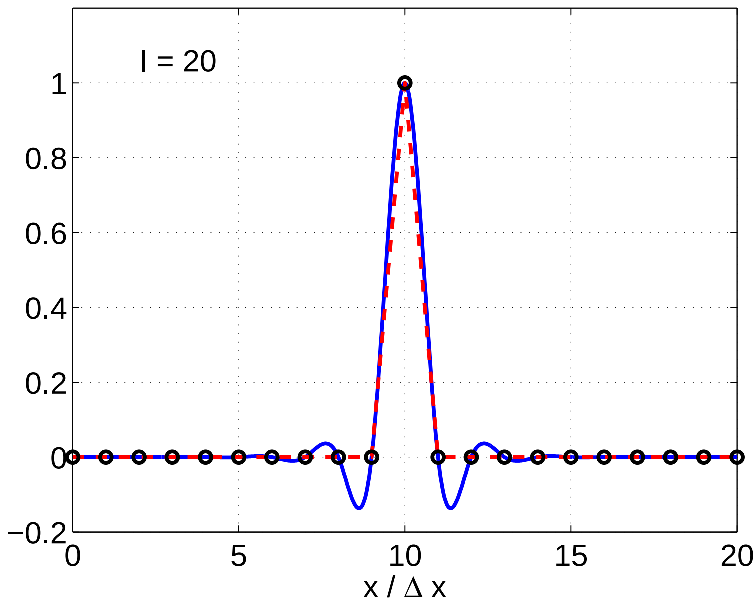

Figure 1.2: Spline basis elements $B_i(x)$ for which $B_i(x_j) = \delta_{ij}$, linear (dashed), and cubic (full)

evaluations. Note that Fig.1.2 also illustrates the problem of overshoot appearing when representing with splines of order $n > 1$ functions presenting strong variations (here the extreme case of a Dirac-type function).

A basis for splines of order n with minimum finite extent are given by the so-called spline elements $S_i^n(x)$. One restricts the discussion here to the case of an equidistant mesh, such that $\Delta x = x_i - x_{i-1}$, $i = 1, \ldots, I$. These spline elements $S_i^n(x)$ are chosen equivalent by translation:

$$S_i^n(x) = S^n(x - (x_i + \delta x^n)), \quad \text{for} \quad i = 1, \ldots, I, \tag{1.2}$$

where the spline shapes $S^n(x)$ of increasing order n, can be defined and generated iteratively from the spline $S^0(x)$ of order zero:

$$S^0(x) = 1, \quad \text{if} \quad |x/\Delta x| < 1/2, \tag{1.3}$$

$$S^0(x) = 0, \quad \text{else}, \tag{1.4}$$

$$S^{n+1}(x) = \frac{1}{\Delta x} \int dx' \, S^0(x') \, S^n(x - x'), \quad \text{for} \quad n \geq 0. \tag{1.5}$$

According to the above definition for the spline shapes $S^n(x)$, and so as to align the spline elements $S_i^n(x)$ onto the grid, one must define δx^n in Eq.(1.2) as follows:

$$\delta x^n = \Delta x/2, \qquad \text{if } n \text{ is even},$$

$$\delta x^n = 0, \qquad \text{if } n \text{ is odd}.$$

The spline shapes for $n = 0$ to 4 are shown in figure 1.3. Note that generating the shape function $S^n(x)$ is in fact equivalent to generating the probability distribution function of the sum of $n + 1$ independent random variables with equivalent, uniform distribution. By invoking the central limit theorem, one thus proves that the spline shapes $S^n(x)$ tend towards a Gaussian in the limit $n \to \infty$. This is illustrated in Fig.1.3 by comparing the spline shape $S^4(x)$ with the Gaussian of variance $5\,\sigma_0^2 = 5/12\Delta x^2$, where $\sigma_0^2 = \Delta x^2/12$ is the variance of $S^0(x)$.

1.1.3 Properties of Spline Shapes

The spline shapes $S^n(x)$ have a certain number of useful properties:

1. They are symmetric, i.e. $S^n(x) = S^n(-x)$.
2. The sum of all spline elements $S_i^n(x) = S^n(x - x_i)$ at any point x is unity:
$$\sum_i S^n(x - x_i) = 1. \tag{1.6}$$
3. They have unitary surface:
$$\frac{1}{\Delta x} \int dx \, S^n(x) = 1. \tag{1.7}$$

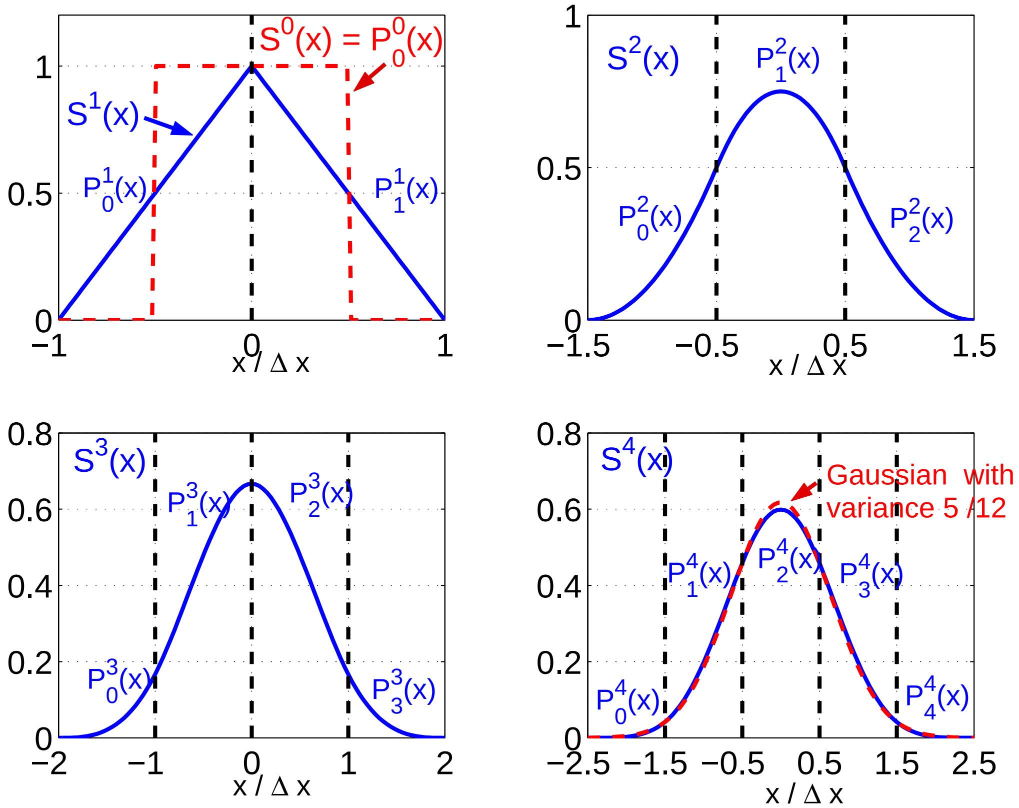

Figure 1.3: Spline shapes $S^n(x)$, and their polynomial components $P_k^n(x)$ of order n, for $n = 0, \ldots, 4$. The extent of the spline shape $S^n(x)$ is $n+1$, and its $P_i^n(x), i = 0, \ldots, n$ components form a basis for the polynomials of order n.

4. The derivative of the spline shape of order $n+1$ can be written in terms of the spline shape of order n:

$$\frac{d}{dx}S^{n+1}(x) = \frac{1}{\Delta x}\left[S^n(x+\frac{\Delta x}{2}) - S^n(x-\frac{\Delta x}{2})\right] \tag{1.8}$$

5. One also has the more general recurrence relation:

$$S^{n+m+1}(x) = \frac{1}{\Delta x}\int dx'\, S^m(x')\, S^n(x-x'), \quad \text{for } \ n,m \geq 0. \tag{1.9}$$

6. The Fourier transform of the spline shape in a periodic system of length $L = I\Delta x$:

$$\hat{S}^n(k) = \frac{1}{L}\int_0^L dx\, S^n(x)\exp(-\imath k\frac{2\pi}{L}x) = \frac{1}{I}\left[\frac{\sin(k\pi/I)}{k\pi/I}\right]^{n+1}. \tag{1.10}$$

All these properties can easily be proven by recurrence from the iterative relation defining the shape functions $S^n(x)$ given by Eqs.(1.3)-(1.5).

For example, the proof by recurrence of property 2 is as follows:
Trivial for $n = 0$.
The property is assumed true for n (recurrence hypothesis). One then needs to show that the property is true for $n+1$:

$$\begin{aligned}
\sum_i S^{n+1}(x-x_i) &= \sum_i \frac{1}{\Delta x}\int dx'\, S^0(x')\, S^n(x-x_i-x') \\
&= \frac{1}{\Delta x}\int dx'\, S^0(x')\, \sum_i S^n((x-x')-x_i) \\
&= \frac{1}{\Delta x}\int dx'\, S^0(x') = 1,
\end{aligned}$$

having first used Eq.(1.5), then the recurrence hypothesis, and finally property 3 for $n = 0$, which is trivial as well.

Proof by recurrence for property 4:
For $n = 1$ one clearly has $dS^1(x)/dx = (1/\Delta x)[S^0(x+\Delta x/2) - S^0(x-\Delta x/2)]$.
The property is assumed true for n (recurrence hypothesis). One then needs to show that the property is true for $n+1$:

$$\begin{aligned}
\frac{d}{dx}S^{n+1}(x) &= \frac{1}{\Delta x}\int dx'\, S^0(x')\,\frac{d}{dx}S^n(x-x') \\
&= \frac{1}{\Delta x}\int dx'\, S^0(x')\frac{1}{\Delta x}\left[S^{n-1}(x-x'+\frac{\Delta x}{2}) - S^{n-1}(x-x'-\frac{\Delta x}{2})\right] \\
&= \frac{1}{\Delta x}\left[\frac{1}{\Delta x}\int dx'\, S^0(x')\, S^{n-1}(x+\frac{\Delta x}{2}-x') - \frac{1}{\Delta x}\int dx'\, S^0(x')\, S^{n-1}(x-\frac{\Delta x}{2}-x')\right] \\
&= \frac{1}{\Delta x}\left[S^n(x+\frac{\Delta x}{2}) - S^n(x-\frac{\Delta x}{2})\right],
\end{aligned}$$

having again used Eq.(1.5), and the recurrence hypothesis.

Proof by recurrence on m for property 5:
The case $m = 0$ reduces to the iterative definition of the shape functions given by Eqs.(1.3)-(1.5).
The property is assumed true for m (recurrence hypothesis). One then needs to show that the property is true for $m+1$:

$$\begin{aligned}
\frac{1}{\Delta x}\int dx'\, S^{m+1}(x')\, S^n(x-x') &= \frac{1}{\Delta x}\int dx'\, S^n(x-x')\,\frac{1}{\Delta x}\int dx''\, S^0(x'')\, S^m(x'-x'') \\
&= \frac{1}{\Delta x}\int dx''\, S^0(x'')\,\frac{1}{\Delta x}\int dx'\, S^m(x'-x'')\, S^n(x-x') \\
&= \frac{1}{\Delta x}\int dx''\, S^0(x'')\,\frac{1}{\Delta x}\int dx'\, S^m(x')\, S^n((x-x'')-x') \\
&= \frac{1}{\Delta x}\int dx''\, S^0(x'')\, S^{n+m+1}(x-x'') \\
&= S^{n+m+2}(x),
\end{aligned}$$

having again used Eq.(1.5), changed variables $x'-x'' \to x'$, and invoked the recurrence hypothesis.

1.1.4 Algorithm for Generating Spline Shape Coefficients

From Eqs.(1.3)-(1.5) defining the spline shapes, it is straightforward to derive a generating algorithm for the coefficients of the corresponding piecewise polynomials. To derive this algorithm, one assumes here x normalised in units of Δx. The piecewise polynomial representation of the shape function of order n can be written:

$$S^n(x) = \sum_{k=0}^{n} P_k^n(x), \tag{1.11}$$

where $P_k^n(x)$ is a polynomial of order n on the interval $[x_k^n, x_{k+1}^n]$:

$$P_k^n(x) = \sum_{m=0}^{n} c_{k,m}^n (x - x_k^n)^m,$$

having defined $x_k^n = k - (n+1)/2$, and $P_k^n(x) = 0$ for $x \notin [x_k^n, x_{k+1}^n]$. Thus $c_{k,m}^n$ are the coefficients of the piecewise polynomial $P_k^n(x)$ with respect to the left hand boundary x_k^n of the corresponding interval. The $P_k^n(x)$ for the shape functions $S^n(x)$, $n = 0, \ldots, 4$ are pointed out in Fig.1.3.

The purpose here is to derive an algorithm which iteratively generates the coefficients $c_{k,m}^n$ for increasing n, starting from the single coefficient $c_{0,0}^0 = 1$ characterising the shape $S^0(x)$.

One starts by rewriting Eq.(1.5) as follows:

$$
\begin{aligned}
S^{n+1}(x) &= \int dx' \, S^0(x') \, S^n(x-x') = \int_{-1/2}^{1/2} dx' \, S^n(x-x') \\
&= \int_{x-1/2}^{x+1/2} dx' \, S^n(x').
\end{aligned} \tag{1.12}
$$

Inserting Eq.(1.11) into Eq.(1.12) thus leads to:

$$
S^{n+1}(x) = \sum_{k=0}^{n} \int_{x-1/2}^{x+1/2} dx' \, P_k^n(x') = \sum_{k=0}^{n+1} P_k^{n+1}(x).
$$

What remains to be done is to identify the contributions of each integral

$$
I_k^n(x) = \int_{x-1/2}^{x+1/2} dx' \, P_k^n(x'),
$$

to the various piecewise polynomials $P_k^{n+1}(x)$. In fact $I_k^n(x)$ only provides a contribution to $P_k^{n+1}(x)$ and $P_{k+1}^{n+1}(x)$ as appears clearly in the following. Indeed, when expliciting the integral $I_k^n(x)$ one needs to distinguish the case where the upper limit $x+1/2$ of the integral falls within the interval $[x_k^n, x_{k+1}^n]$ on which $P_k^n(x)$ is finite, from the case where the lower limit $x-1/2$ of the integral falls within the interval $[x_k^n, x_{k+1}^n]$:

1. $(x+1/2) \in [x_k^n, x_{k+1}^n] \Leftrightarrow x \in [x_k^{n+1}, x_{k+1}^{n+1}]$:

$$
\begin{aligned}
I_k^n(x) &= \int_{x_k^n}^{x+1/2} dx' \, P_k^n(x') = \sum_{m=0}^{n} c_{k,m}^n \int_{x_k^n}^{x+1/2} dx' (x'-x_k^n)^m \\
&= \sum_{m=0}^{n} \frac{c_{k,m}^n}{m+1} (x - x_k^{n+1})^{m+1},
\end{aligned} \tag{1.13}
$$

   which provides the contribution of $I_k^n(x)$ to $P_k^{n+1}(x)$.

2. $(x-1/2) \in [x_k^n, x_{k+1}^n] \Leftrightarrow x \in [x_{k+1}^{n+1}, x_{k+2}^{n+1}]$:

$$
\begin{aligned}
I_k^n(x) &= \int_{x-1/2}^{x_{k+1}^n} dx' \, P_k^n(x') = \sum_{m=0}^{n} c_{k,m}^n \int_{x-1/2}^{x_{k+1}^n} dx' (x'-x_k^n)^m \\
&= \sum_{m=0}^{n} \frac{c_{k,m}^n}{m+1} - \sum_{m=0}^{n} \frac{c_{k,m}^n}{m+1} (x - x_{k+1}^{n+1})^{m+1},
\end{aligned} \tag{1.14}
$$

   which provides the contribution of $I_k^n(x)$ to $P_{k+1}^{n+1}(x)$.

From Eqs. (1.13) and (1.14) one can thus finally derive the iterative relation for the coefficients $c_{k,m}^n$:

$$
c_{k,m}^{n+1} = \frac{1}{m} \left(c_{k,m-1}^n - c_{k-1,m-1}^n \right) + \delta_{m,0} \sum_{m'=1}^{n+1} \frac{c_{k-1,m'-1}^n}{m'}, \tag{1.15}
$$

assuming in the above relation any coefficient being zero if the index falls out of range.

The above algorithm thus clearly shows, by construction, that the shape functions $S^n(x)$ are indeed piecewise polynomials of degree n with an extent $n+1$ in units of Δx. Not incidentally, this extent corresponds to the dimension of the space of polynomials of degree n, as the set $\{P_k^n(x)\}_{k=0}^n$ must form a basis for this space. Furthermore, a direct consequence of property 4 is the proof that $S^n(x)$ is indeed $n-1$ continuously differentiable. These properties provide the actual proof that the shape functions are indeed appropriate for generating the basis elements $S_i^n(x) = S^n(x - x_i)$ for the space of piecewise polynomials of spline type.

By applying Eq.(1.15), one easily obtains the coefficients for the piecewise polynomials representing the spline shapes $S^n(x)$. The coefficients for $n = 1, \ldots, 3$ are given here, with the notation $\alpha_k^n = x - x_k^n$, where the indices on α are dropped in the following to lighten notations:

1. Linear spline $S^1(x)$:

$$P_0^1(x) = \alpha = 1 + x, \quad \text{for } x \in [-1, 0], \tag{1.16}$$
$$P_1^1(x) = 1 - \alpha = 1 - x, \quad \text{for } x \in [0, 1]. \tag{1.17}$$

2. Quadratic spline $S^2(x)$:

$$P_0^2(x) = \frac{1}{2}\alpha^2 = \frac{1}{2}(\frac{3}{2} + x)^2, \quad \text{for } x \in [-\frac{3}{2}, -\frac{1}{2}], \tag{1.18}$$
$$P_1^2(x) = \frac{1}{2} + \alpha - \alpha^2 = \frac{3}{4} - x^2, \quad \text{for } x \in [-\frac{1}{2}, \frac{1}{2}], \tag{1.19}$$
$$P_2^2(x) = \frac{1}{2} - \alpha + \frac{1}{2}\alpha^2 = \frac{1}{2}(\frac{3}{2} - x)^2, \quad \text{for } x \in [\frac{3}{2}, \frac{1}{2}]. \tag{1.20}$$

3. Cubic spline $S^3(x)$:

$$P_0^3(x) = \frac{1}{6}\alpha^3 = \frac{1}{6}(2 + x)^3, \quad \text{for } x \in [-2, -1], \tag{1.21}$$
$$P_1^3(x) = \frac{1}{6}\left(1 + 3\alpha + 3\alpha^2 - 3\alpha^3\right) = \frac{1}{6}\left(4 - 6x^2 - 3x^3\right), \quad \text{for } x \in [-1, 0], \tag{1.22}$$
$$P_2^3(x) = \frac{1}{6}\left(4 - 6\alpha^2 + 3\alpha^3\right) = \frac{1}{6}\left(4 - 6x^2 + 3x^3\right), \quad \text{for } x \in [0, 1], \tag{1.23}$$
$$P_3^3(x) = \frac{1}{6}\left(1 - 3\alpha + 3\alpha^2 - \alpha^3\right) = \frac{1}{6}(2 - x)^3, \quad \text{for } x \in [1, 2]. \tag{1.24}$$

1.1.5 Computing Spline Interpolation Coefficients

Returning to the problem defined in Sec.1.1.1 of 1-Dim interpolation, the spline representation of a function $f(x)$ defined on an equidistant grid x_i can thus be written in terms of the spline elements:

$$f(x) = \sum_i \tilde{f}_i \, S_i^n(x). \tag{1.25}$$

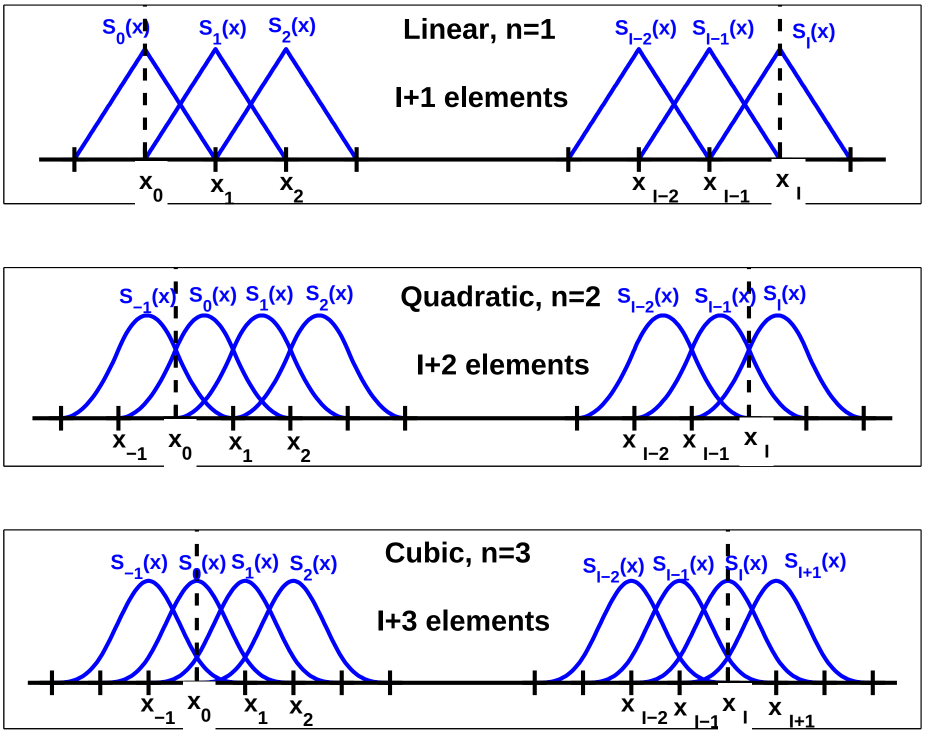

Figure 1.4: Spline elements $S_i^n(x)$ to be considered on a finite system for handling arbitrary boundaries.

The spline coefficients $\tilde{f}_i$ must be such that

$$\sum_j \tilde{f}_j\, S_j^n(x_i) = \sum_j \tilde{f}_j\; S^n((i-j)\Delta x - \delta x^n) = f_i = f(x_i). \tag{1.26}$$

which, at least in the case of periodic boundary conditions, provides I equations for the I unknowns $\tilde{f}_i$. This system of equations is a banded linear system with n diagonals (corresponding to the number of grid points for which $S^n(x_i - \delta x^n)$ is non-zero). For example, for $n = 3$ the tridiagonal system for the $\tilde{f}_i$ is of the form:

$$S^3(\Delta x)\,\tilde{f}_{i-1} + S^3(0)\,\tilde{f}_i + S^3(-\Delta x)\,\tilde{f}_{i+1} = \frac{1}{6}\tilde{f}_{i-1} + \frac{2}{3}\tilde{f}_i + \frac{1}{6}\tilde{f}_{i+1} = f_i. \tag{1.27}$$

1.1.6 Handling Boundary Conditions

To address the question of how to handle non-periodic boundaries when computing the spline representation of a function $f(x)$, let us consider a finite system with equidistant grid $\{x_i\}_{i=0}^{I}$, where x_0 and x_I are the left and right hand boundaries respectively. To easily handle arbitrary boundary conditions, it is usually convenient to extend the grid x_i

for $i < 0$ on the left hand side of the system, and for $i > I$ on the right hand side, so as to consider all spline elements $S_i^n(x)$ which at least partially overlap the interval of interest $[x_0, x_I]$, as shown in Fig.1.4 for $n = 1, 2$ and 3. This requires considering ceil($(n-1)/2$) additional elements to the left of the system, and floor($(n-1)/2$) to the right, resulting in $n-1$ additional elements to the number $I+1$ of elements centred on the grid points in the interval $[x_0, x_I]$. The $I+1$ equations given by Eq.(1.26) must therefore be supplemented by $n-1$ additional equations.

In the case of cubic splines ($n = 3$), one must therefore impose 2 additional conditions on the boundary. Typical boundary conditions are:

1. Complete: Match the first derivative $df(x)/dx$ at x_0 and x_I to given values f_0' and f_I', or estimate f_0' and f_I' using the slope of the cubic that matches the first four grid values of $f(x)$ at each end (i.e. estimate f_0' and f_I' using Lagrange interpolation of degree 3).

2. Natural: Impose the second derivative $d^2f(x)/dx^2$ to be zero at x_0 and x_I.

3. Not-a-knot: Make the third derivative $d^3f(x)/dx^3$ continuous at x_1 and x_{I-1}.

For example, for $n = 3$ and natural boundaries the additional equation from the left hand boundary is given by

$$\Delta x^2 \left[\frac{d^2S^3}{dx^2}(\Delta x)\, \tilde{f}_{-1} + \frac{d^2S^3}{dx^2}(0)\, \tilde{f}_0 + \frac{d^2S^3}{dx^2}(-\Delta x)\, \tilde{f}_1 \right] = \tilde{f}_{-1} - 2\tilde{f}_0 + \tilde{f}_1 = 0. \qquad (1.28)$$

and in the same way for the right hand boundary:

$$\tilde{f}_{I-1} - 2\tilde{f}_I + \tilde{f}_{I+1} = 0.$$

In some cases, in particular for imposing boundary conditions in the context of the finite element method, it may however be more convenient to work with a transformed set of spline elements $\hat{S}_i^n(x)$ which directly incorporates the boundary conditions. The transformation from the elements S_i^n to the elements $\hat{S}_i^n$ in fact only involves the elements overlapping the boundaries x_0 and x_I, and is simply obtained by inserting the boundary equation into the spline representation given by Eq.(1.25). This is illustrated here for a natural left hand boundary in the case of cubic splines by combining Eqs. (1.25) and (1.28):

$$\begin{aligned}
f(x) &= \sum_{i=-1}^{\cdots} \tilde{f}_i\, S_i^3(x) \\
&= (2\tilde{f}_0 - \tilde{f}_1) S_{-1}^3(x) + \tilde{f}_0\, S_0^3(x) + \tilde{f}_1\, S_1^3(x) + \tilde{f}_2\, S_2^3(x) + \ldots \\
&= \tilde{f}_0 \left[S_0^3(x) + 2S_{-1}^3(x) \right] + \tilde{f}_1 \left[S_1^3(x) - S_{-1}^3(x) \right] + \tilde{f}_2\, S_2^3(x) + \ldots \\
&= \tilde{f}_0\, \hat{S}_0^3(x) + \tilde{f}_1\, \hat{S}_1^3(x) + \tilde{f}_2\, S_2^3(x) + \ldots \\
&= \sum_{i=0}^{\cdots} \tilde{f}_i\, \hat{S}_i^3(x),
\end{aligned}$$

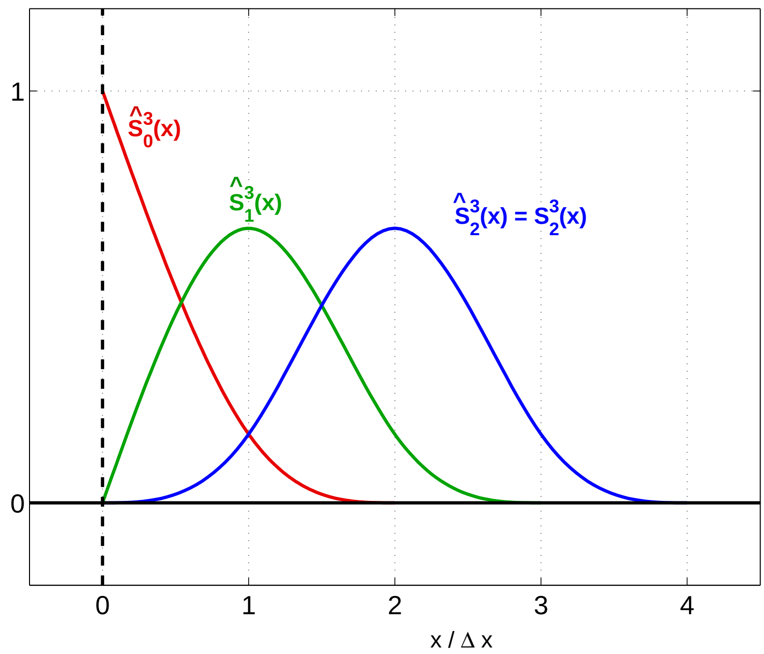

Figure 1.5: Cubic spline elements $\hat{S}^3_i(x)$ incorporating natural boundaries for the left hand edge.

so that the corresponding spline transformation is determined by

$$\begin{aligned}
\hat{S}^3_0(x) &= S^3_0(x) + 2S^3_{-1}(x), \\
\hat{S}^3_1(x) &= S^3_1(x) - S^3_{-1}(x), \\
\hat{S}^3_i(x) &= S^3_i(x) \quad \text{for} \quad i > 1.
\end{aligned}$$

The splines $\hat{S}^n_i$ for this case are shown in figure 1.5. Note that the elements $\hat{S}^n_i(x)$ now directly contain the condition of zero derivative at the edge, and that there is therefore no more need for an additional element $\hat{S}^n_{-1}$.

1.1.7 Derivative of Spline Representation

One considers the spline representation of order n of a function $f(x)$:

$$f(x) = \sum_i \tilde{f}_i \, S^n_i(x) = \sum_i \tilde{f}_i \, S^n(x - (x_i + \delta x^n)).$$

Making use of property 4 (Sec.1.1.3) of the spline shapes and assuming $n \geq 1$, one can express the derivative of $f(x)$ as a spline representation of order $n-1$, as follows:

$$\begin{aligned}
\frac{df(x)}{dx} &= \sum_i \tilde{f}_i \frac{dS^n}{dx}(x - (x_i + \delta x^n)) \\
&= \sum_i \tilde{f}_i \frac{1}{\Delta x} \left[S^{n-1}(x - (x_i - \frac{\Delta x}{2} + \delta x^n)) - S^{n-1}(x - (x_i + \frac{\Delta x}{2} + \delta x^n)) \right]
\end{aligned}$$

$$
\begin{aligned}
&= \sum_i \frac{\tilde{f}_i - \tilde{f}_{i-1}}{\Delta x} S^{n-1}(x - (x_i - \frac{\Delta x}{2} + \delta x^n)) \\
&= \sum_i \tilde{f}'_i \, S_i^{n-1}(x),
\end{aligned} \tag{1.29}
$$

having identified the coefficients $\tilde{f}'_i$ as follows:

$$
\begin{aligned}
\tilde{f}'_i &= \frac{\tilde{f}_i - \tilde{f}_{i-1}}{\Delta x}, \quad \text{if } n \text{ even}, \\
\tilde{f}'_i &= \frac{\tilde{f}_{i+1} - \tilde{f}_i}{\Delta x}, \quad \text{if } n \text{ odd}.
\end{aligned}
$$

In the same way, assuming $n \geq 2$, one can obtain the expression for the second order derivative:

$$
\begin{aligned}
\frac{d^2 f(x)}{dx^2} &= \sum_i \frac{\tilde{f}_{i+1} + \tilde{f}_{i-1} - 2\tilde{f}_i}{\Delta x^2} S^{n-2}(x - (x_i + \delta x^n)) \\
&= \sum_i \tilde{f}''_i \, S_i^{n-2}(x),
\end{aligned}
$$

having identified:

$$
\tilde{f}''_i = \frac{\tilde{f}_{i+1} + \tilde{f}_{i-1} - 2\tilde{f}_i}{\Delta x^2}.
$$

1.1.8 Spline Elements on a Non-Equidistant Mesh

To be completed ...

1.1.9 Spline Representation in Higher Dimension

The generalisation of the spline representation to multiple dimensions is straightforward by considering the linear space spanned by the tensorial product of the 1-Dim spline elements relative to each direction.

For example, the spline representation of degree n for the function of two variables $f(x, y)$ is of the form:

$$
f(x, y) = \sum_{i,j} \tilde{f}_{ij} \, S_i^n(x) \, S_j^n(y), \tag{1.30}
$$

where $S_i^n(x)$ and $S_j^n(y)$ are the 1-Dim spline elements of degree n (as defined in Sec.1.1.2) relative to equidistant grids $\{x_i\}_{i=0}^I$ and $\{y_j\}_{j=0}^J$ along the directions x and y respectively. The spline elements $S_{ij}^n(x, y) = S_i^n(x) \, S_j^n(y)$ indeed form a basis for the vectorial space of 2-Dim piecewise polynomials in x and y of degree n with C^{n-1} continuity across all grid cell boundaries. More exactly, C^{n-1} continuity implies that $\partial^{p_x} \partial^{p_y} f(x, y)/\partial x^{p_x} \partial y^{p_y}$ is continuous for all $p_x, p_y = 0, n-1$. For illustration, the 2-Dim spline shapes $S^n(x)S^n(y)$ of degree $n = 1$ and 3 are plotted in Fig.1.6.

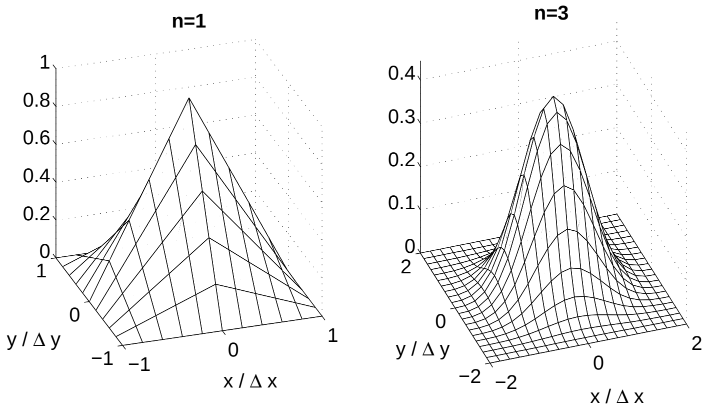

Figure 1.6: 2-Dim spline elements of degree $n = 1$ and $n = 3$.

In the case of interpolation, where the values $f_{ij} = f(x_i, y_j)$ of the function on the grid are known, the spline coefficients $\tilde{f}_{ij}$ are computed by solving the system of equations:

$$\sum_{i',j'} \tilde{f}_{i'j'}\, S^n_{i'}(x_i)\, S^n_{j'}(y_j) = f_{ij}, \tag{1.31}$$

with possibly additional boundary equations as required. A convenient way for solving Eq.(1.31) is to rewrite this system of equations for the $\tilde{f}_{ij}$ as follows:

$$\sum_{i'} \left[\sum_{j'} \tilde{f}_{i'j'}\, S^n_{j'}(y_j) \right] S^n_{i'}(x_i) = \sum_{i'} F_{i'j}\, S^n_{i'}(x_i) = f_{ij}, \tag{1.32}$$

having defined

$$F_{ij} = \sum_{j'} \tilde{f}_{ij'}\, S^n_{j'}(y_j). \tag{1.33}$$

Equation (1.32) provides a system of equations for the coefficients F_{ij}, where j appears as a parameter. For each j this system is thus first solved with appropriate boundary conditions in the x direction. Once the values F_{ij} have been determined in this way, equation (1.33) provides a system of equations for the actual spline coefficients $\tilde{f}_{ij}$, where this time it is the index i which appears as a parameter. Thus, in a second step, Eq.(1.33) is solved for each i this time accounting for appropriate boundaries in the y direction.

The generalisation of the above discussion to dimensions higher than 2 is quite obvious.

Note furthermore, that using hybrid elements, i.e. formed of spline elements of different order for each direction, can be of interest in some applications.

1.1.10 Illustration: Solving the 1-Dim Poisson Equation with FEM

As an illustration of applying a spline representation in the context of the finite element method (FEM), one considers here the case of the 1-Dim Poisson equation with periodic boundaries:

$$\frac{d^2\phi}{dx^2}(x) = -\rho(x). \tag{1.34}$$

Assuming the order n spline representation of the source term ρ is known on an equidistant grid $\{x_i\}_{i=0}^{I-1}$:

$$\rho = \sum_i \tilde{\rho}_i \, S_i^n(x),$$

the goal is to find the order n spline representation for the potential ϕ:

$$\phi = \sum_i \tilde{\phi}_i \, S_i^n(x).$$

One proceeds with the FEM approach by projection Eq.1.34 onto a test function $S_i^n(x)$ $[(1/\Delta x) \int dx \, S_i^n(x) \ldots]$, so that after integration by parts and having invoked the periodicity one obtains:

$$\sum_j \left[\frac{1}{\Delta x} \int dx \, \frac{dS_i^n(x)}{dx} \frac{dS_j^n(x)}{dx} \right] \tilde{\phi}_j = \sum_j \left[\frac{1}{\Delta x} \int dx \, S_i^n(x) \, S_j^n(x) \right] \tilde{\rho}_j,$$

which can be written in matrix form as follows:

$$D^n \, \tilde{\phi} = M^n \, \tilde{\rho}. \tag{1.35}$$

The "mass" matrix M^n can be expressed in terms of higher order spline values:

$$\begin{aligned} M_{ij}^n = M_{j-i}^n &= \frac{1}{\Delta x} \int dx \, S^n(x - (x_i + \delta x^n)) \, S^n(x - (x_j + \delta x^n)) \\ &= \frac{1}{\Delta x} \int dx \, S^n(x) \, S^n((j-i)\Delta x - x), \\ &= S^{2n+1}((j-i)\Delta x), \end{aligned} \tag{1.36}$$

having made use of property 1 and 5 of the spline shapes (see Sec.1.1.3). A similar derivation applies to the differential matrix D^n:

$$\begin{aligned} D_{ij}^n = D_{j-i}^n &= \frac{1}{\Delta x} \int dx \, \frac{dS^n}{dx}(x - (x_i + \delta x^n)) \, \frac{dS^n}{dx}(x - (x_j + \delta x^n)) \\ &= \frac{1}{\Delta x} \int dx \, \frac{dS^n}{dx}(x) \, \frac{dS^n}{dx}(x - (j-i)\Delta x) \\ &= \frac{1}{\Delta x^3} \int dx \, \left[S^{n-1}(x + \frac{\Delta x}{2}) - S^{n-1}(x - \frac{\Delta x}{2}) \right] \times \\ &\qquad \left[S^{n-1}(x - (j-i)\Delta x + \frac{\Delta x}{2}) - S^{n-1}(x - (j-i)\Delta x - \frac{\Delta x}{2}) \right] \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\Delta x^3}\Big[2\int dx\, S^{n-1}(x)\, S^{n-1}((j-i)\Delta x - x) \\
&\qquad - \int dx\, S^{n-1}(x)\, S^{n-1}((j-i+1)\Delta x - x) \\
&\qquad - \int dx\, S^{n-1}(x)\, S^{n-1}((j-i-1)\Delta x - x)\Big] \\
&= \frac{1}{\Delta x^2}\Big[2S^{2n-1}((j-i)\Delta x) - S^{2n-1}((j-i+1)\Delta x) - S^{2n-1}((j-i-1)\Delta x)\Big] \\
&= \frac{1}{\Delta x^2}\left(2M^{n-1}_{j-i} - M^{n-1}_{j-i+1} - M^{n-1}_{j-i-1}\right), \qquad (1.37)
\end{aligned}
$$

having in this case made use of property 4 of the spline shapes as well.

As a result of the translational invariance of the system, it is naturally convenient to solve Eq.(1.34) in Fourier space. For this purpose, one considers the discrete Fourier transform (DFT) $\hat{\tilde{\rho}}_k$ and $\hat{\tilde{\phi}}_k$ of the spline coefficients $\tilde{\rho}_i$ and $\tilde{\phi}_i$ respectively. For example, for ϕ:

$$
\tilde{\phi}_i = \sum_{k=0}^{I-1} \hat{\tilde{\phi}}_k \exp(\imath\frac{2\pi}{I}ik) \quad \Longleftrightarrow \quad \hat{\tilde{\phi}}_k = \frac{1}{I}\sum_{i=0}^{I-1} \tilde{\phi}_i \exp(-\imath\frac{2\pi}{I}ik)
$$

Carrying out the DFT on equation (1.35) then leads to:

$$
\hat{D}^n_k\, \hat{\tilde{\phi}}_k = \hat{M}^n_k\, \hat{\tilde{\rho}}_k \quad \Longrightarrow \quad \hat{\tilde{\phi}}_k = \frac{\hat{M}^n_k}{\hat{D}^n_k}\, \hat{\tilde{\rho}}_k. \qquad (1.38)
$$

Relations for the DFTs $\hat{M}^n_k$ and $\hat{D}^n_k$ of the matrices M^n_k and D^n_k are obtained from Eqs.(1.36) and (1.37):

$$
\begin{aligned}
\hat{M}^n_k &= \frac{1}{I}\sum_{i=0}^{I-1} M^n_i \exp(-\imath\frac{2\pi}{I}ik) = \frac{1}{I}\sum_{i=-n}^{n} S^{2n+1}(i\Delta x)\exp(-\imath\frac{2\pi}{I}ik) \\
&= \frac{1}{I}\left[S^{2n+1}(0) + 2\sum_{i=1}^{n} S^{2n+1}(i\Delta x)\cos(\frac{2\pi}{I}ik)\right] \\
&= \frac{1}{I}\left[1 - 4\sum_{i=1}^{n} S^{2n+1}(i\Delta x)\sin^2(\frac{ik\pi}{I})\right], \qquad (1.39) \\
\hat{D}^n_k &= \frac{2}{\Delta x^2}\left[1 - \cos(\frac{2\pi}{I}k)\right]\hat{M}^{n-1}_k = \frac{4}{\Delta x^2}\sin^2(\frac{k\pi}{I})\,\hat{M}^{n-1}_k, \qquad (1.40)
\end{aligned}
$$

having invoked property 2 of the spline shapes for deriving the relation for $\hat{M}^n_k$. As expected, the ratio $\hat{D}^n_k/\hat{M}^n_k$ appearing in Eq.(1.38) thus obviously tends towards $(k2\pi/L)^2$ for all n in the limit $k/I \ll 1$, with $L = I\Delta x$ the length of the system.

From Eq.(1.39) one can thus easily explicit $\hat{M}^n_k$ for the first n values:

$$
\hat{M}^0_k = \frac{1}{I},
$$

$$\begin{aligned}
\hat{M}_k^1 &= \frac{1}{I}\left[1 - \frac{2}{3}\sin^2(\frac{k\pi}{I})\right], \\
\hat{M}_k^2 &= \frac{1}{I}\left[1 - \frac{13}{15}\sin^2(\frac{k\pi}{I}) - \frac{1}{30}\sin^2(\frac{2k\pi}{I})\right], \\
\hat{M}_k^3 &= \frac{1}{I}\left[1 - \frac{397}{420}\sin^2(\frac{k\pi}{I}) - \frac{2}{21}\sin^2(\frac{2k\pi}{I}) - \frac{1}{1260}\sin^2(\frac{3k\pi}{I})\right].
\end{aligned}$$

The solution to the Poisson equation in Fourier space for linear elements, for example, would thus read:

$$\hat{\tilde{\phi}}_k = \left(\frac{\Delta x}{2}\right)^2 \frac{1 - \frac{2}{3}\sin^2(\frac{k\pi}{I})}{\sin^2(\frac{k\pi}{I})}\ \hat{\tilde{\rho}}_k,$$

and for cubic elements:

$$\hat{\tilde{\phi}}_k = \left(\frac{\Delta x}{2}\right)^2 \frac{1 - \frac{397}{420}\sin^2(\frac{k\pi}{I}) - \frac{2}{21}\sin^2(\frac{2k\pi}{I}) - \frac{1}{1260}\sin^2(\frac{3k\pi}{I})}{\sin^2(\frac{k\pi}{I})\left[1 - \frac{13}{15}\sin^2(\frac{k\pi}{I}) - \frac{1}{30}\sin^2(\frac{2k\pi}{I})\right]}\ \hat{\tilde{\rho}}_k,$$

As $\hat{M}_0^n = 1$ and $\hat{D}_0^n = 0$ for all n, Eq. (1.38) naturally reflects the solvability condition for the Poisson equation in a periodic system:

$$0 = \hat{\tilde{\rho}}_0 = \frac{1}{I}\sum_{i=0}^{I-1}\tilde{\rho}_i = \frac{1}{L}\int dx\,\tilde{\rho}_i\,S_i^n(x) = \frac{1}{L}\int dx\,\rho(x),$$

having used property 3 of the spline shapes.

1.2 Hermite Splines

1.2.1 Hermite Spline Representation

Let us come back to the 1-Dim interpolation problem.

In some cases, not only the values $f_i = f(x_i)$ of the function $f(x)$ are known on the grid x_i, but also the values $f_i' = df/dx(x_i)$ of its first derivative, or possibly even the values $f_i^p = d^p f(x_i)/dx^p$, $p > 1$ of its higher derivatives. When computing a piecewise polynomial representation of $f(x)$ for all x, one naturally wants to take account of this additional information.

Thus, assuming the values of $f(x)$ and D of its derivatives are known on the grid, what is the degree n of the piecewise polynomial which is uniquely determined by imposing C^D continuity on the grid? For each grid interval $[x_i, x_{i+1}]$ there are $n+1$ unknowns corresponding to the coefficients of the polynomial, and $2(D+1)$ equations obtained by imposing the continuity of $f(x)$ and its D derivatives on the left and right hand edge x_i and x_{i+1} respectively. Equating the number of conditions to the number of unknowns simply leads to:

$$2(D+1) = n+1 \quad\Longrightarrow\quad n = 2D+1. \tag{1.41}$$

The piecewise polynomial representation obtained in this way is the so-called Hermite spline representation of $f(x)$.

Note, that to ensure C^D continuity for $D > 1$, the Hermite representation requires a higher n polynomial representation than using standard splines. For example, cubic Hermite splines ensure only C^1 continuity, while standard cubic splines ensure C^2 continuity.

One can imagine generalising both the standard spline representation (Sec.1.1) and the Hermite spline representation, by imposing here the continuity of d additional derivatives. This would lead to $n = 2D + d + 1$, which clearly generalises both Eq. (1.1) and (1.41).

1.2.2 Cubic Hermite Elements

In the following, one limits the discussion to the case of cubic Hermite representation of a function $f(x)$, assuming the values $f_i = f(x_i)$ and $f'_i = df/dx(x_i)$ are known on an equidistant grid x_i. The cubic Hermite representation of $f(x)$ can then be written:

$$f(x) = \sum_i \left[f_i \, H_i(x) + f'_i \, G_i(x) \right], \tag{1.42}$$

where the cubic piecewise polynomials $H_i(x)$ and $G_i(x)$ are the Hermite elements defined as follows:

- The elements of both sets $\{H_i(x)\}$ and $\{G_i(x)\}$ are equivalent by translation:

$$H_i(x) = H(x - x_i), \qquad G_i(x) = G(x - x_i),$$

- The two cubic Hermite shape functions $H(x)$ and $G(x)$ are cubic piecewise polynomials of extent $2\Delta x$ on the interval $[-\Delta x, \Delta x]$, uniquely determined by the conditions:

$$H(-\Delta x) = 0, \quad H(0) = 1, \quad H(\Delta x) = 0, \tag{1.43}$$

$$dH/dx(-\Delta x) = 0, \quad dH/dx(0) = 0, \quad dH/dx(\Delta x) = 0, \tag{1.44}$$

$$G(-\Delta x) = 0, \quad G(0) = 0, \quad G(\Delta x) = 0, \tag{1.45}$$

$$dG/dx(-\Delta x) = 0, \quad dG/dx(0) = 1, \quad dG/dx(\Delta x) = 0. \tag{1.46}$$

  Conditions (1.43)-(1.46) clearly justify the validity of Eq.(1.42) and lead to the explicit relations:

$$H(x) = \begin{cases} P_1(x/\Delta x + 1), & \text{for } x \in [-\Delta x, 0], \\ P_2(x/\Delta x), & \text{for } x \in [0, \Delta x], \end{cases} \tag{1.47}$$

$$G(x)/\Delta x = \begin{cases} P_3(x/\Delta x + 1), & \text{for } x \in [-\Delta x, 0], \\ P_4(x/\Delta x), & \text{for } x \in [0, \Delta x], \end{cases} , \tag{1.48}$$

  with

$$P_1(\alpha) = 3\alpha^2 - 2\alpha^3, \tag{1.49}$$

$$P_2(\alpha) = 1 - 3\alpha^2 + 2\alpha^3, \tag{1.50}$$

$$P_3(\alpha) = -\alpha^2 + \alpha^3, \tag{1.51}$$

$$P_4(\alpha) = \alpha - 2\alpha^2 + \alpha^3. \tag{1.52}$$

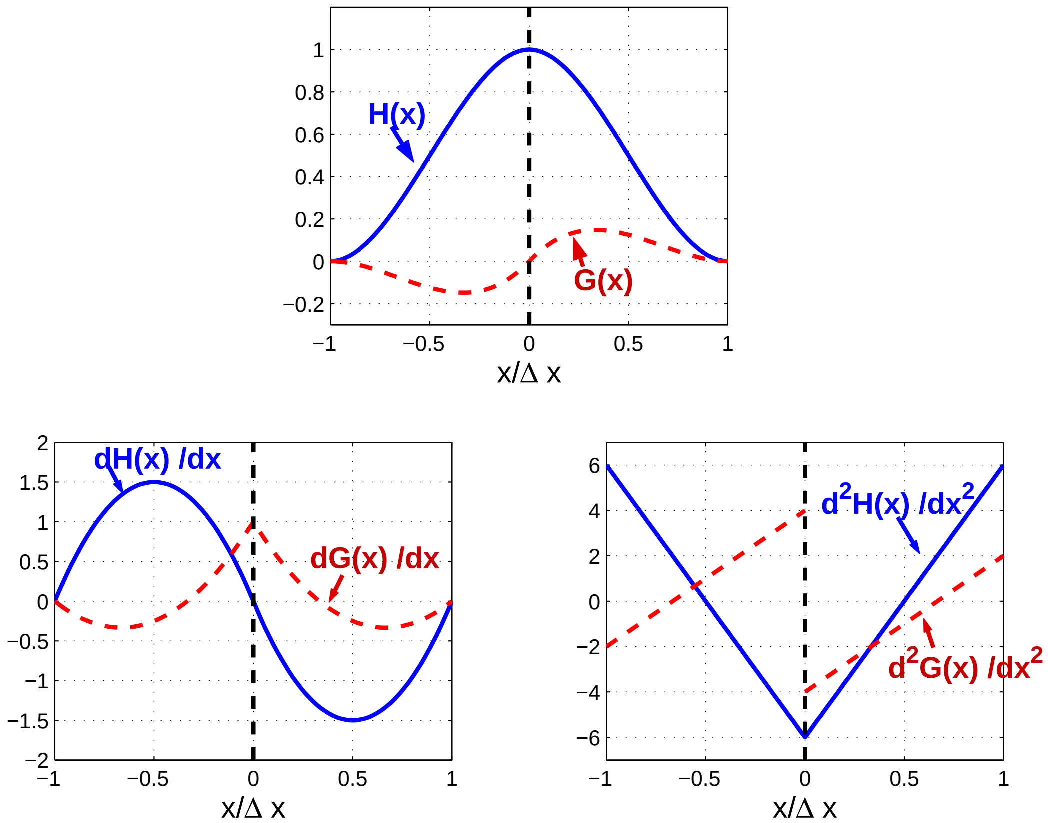

Figure 1.7: Cubic Hermite elements $H(x)$ and $G(x)$, as well as their first and second derivatives.

The shape functions $H(x)$ and $G(x)$, as well as their first and second derivatives, are plotted in Fig.1.7. Note that $H(x)$ and $G(x)$ are indeed C^1 continuous, but present discontinuities on the grid in their second derivatives.

The shape functions $H(x)$ and $G(x)$ have the following additional properties:

- Symmetry:

$$H(x) = H(-x), \qquad G(x) = -G(-x).$$

- Integral:

$$\int dx\, H(x) = \Delta x, \qquad \int dx\, G(x) = 0.$$

- The sum of all Hermite spline elements $H_i(x) = H(x - x_i)$ at any point x is unity:

$$\sum_i H(x - x_i) = 1.$$

In the context of interpolation, note that contrary to the standard spline representation in terms of the spline elements $S_i(x)$ as given in Eq.(1.25), the coefficients of the Hermite representation (1.42) are conveniently given by the known data values f_i and f_i', without the need for solving any system of equations.

1.2.3 Relation between Standard and Hermite Cubic Representation

When considering the standard cubic spline representation, the cubic Hermite relation (1.42) can actually be used as an alternative to the decomposition (1.25) in terms of the standard spline elements $S_i(x)$. In this case, only the values $f_i = f(x_i)$ are known, and the values of the derivative $f'_i = df/dx(x_i)$ on the grid are unknowns, which need to be determined by imposing continuity of the second derivative on the grid:

$$\lim_{x\to x_i-} \frac{d^2 f}{dx^2}(x) = \lim_{x\to x_i+} \frac{d^2 f}{dx^2}(x), \qquad \text{with } f(x) \text{ given by Eq.(1.42)}$$

$$\Longleftrightarrow \quad \lim_{x\to x_i-} \left[f_{i-1}H''_{i-1}(x) + f'_{i-1}G''_{i-1}(x) + f_iH''_i(x) + f'_iG''_i(x)\right]$$
$$= \lim_{x\to x_i+} \left[f_iH''_i(x) + f'_iG''_i(x) + f_{i+1}H''_{i+1}(x) + f'_{i+1}G''_{i+1}(x)\right]$$

$$\Longleftrightarrow \quad f_{i-1}P''_2(1) + \Delta x f'_{i-1}P''_4(1) + f_iP''_1(1) + \Delta x f'_iP''_3(1)$$
$$= f_iP''_2(0) + \Delta x f'_iP''_4(0) + f_{i+1}P''_1(0) + \Delta x f'_{i+1}P''_3(0)$$

$$\Longleftrightarrow \quad \frac{1}{6}f'_{i-1} + \frac{2}{3}f'_i + \frac{1}{6}f'_{i+1} = \frac{f_{i+1} - f_{i-1}}{2\Delta x}, \qquad (1.53)$$

which leads to a tridiagonal system for the f'_i similar to the tridiagonal system given by Eq. (1.27) for the standard spline coefficients $\tilde{f}_i$. In fact, comparing Eqs. (1.53) and (1.27) leads to the relation:

$$f'_i = \frac{df}{dx}(x_i) = \frac{\tilde{f}_{i+1} - \tilde{f}_{i-1}}{2\Delta x},$$

which could naturally also have been obtained directly from Eq.(1.29).

1.2.4 Cubic Hermite Representation in Higher Dimension

As in the case of standard splines, the generalisation of the Hermite spline representation to multiple dimensions is simply obtained by considering the space spaned by the tensorial product of the 1-Dim Hermite elements. Thus, for a function of two variables $f(x,y)$ characterised by its values $f_{ij} = f(x_i, y_j)$ as well as its partial derivatives $\partial_x f_{ij} = \partial f/\partial x(x_i, y_j)$, $\partial_y f_{ij} = \partial f/\partial y(x_i, y_j)$, and $\partial^2_{xy} f_{ij} = \partial^2 f/\partial x \partial y(x_i, y_j)$ on an equidistant grid x_i and y_i, the cubic Hermite representation reads:

$$f(x,y) = \sum_{i,j} \left[f_{ij}\, H_i(x)H_j(y) + \partial_x f_{ij}\, G_i(x)H_j(y) + \partial_y f_{ij}\, H_i(x)G_j(y) + \partial^2_{xy} f_{ij}\, G_i(x)G_j(y)\right],$$

where $\{H_i(x), G_i(x)\}$, and $\{H_j(y), G_j(y)\}$, are the 1-Dim cubic Hermite spline elements [as defined by Eqs.(1.47)-(1.52)] relative to the grids x_i and y_j respectively.

The 2-Dim cubic Hermite spline shapes $H(x)\,H(y)$, $G(x)\,H(y)$, $H(x)\,G(y)$, and $G(x)\,G(y)$

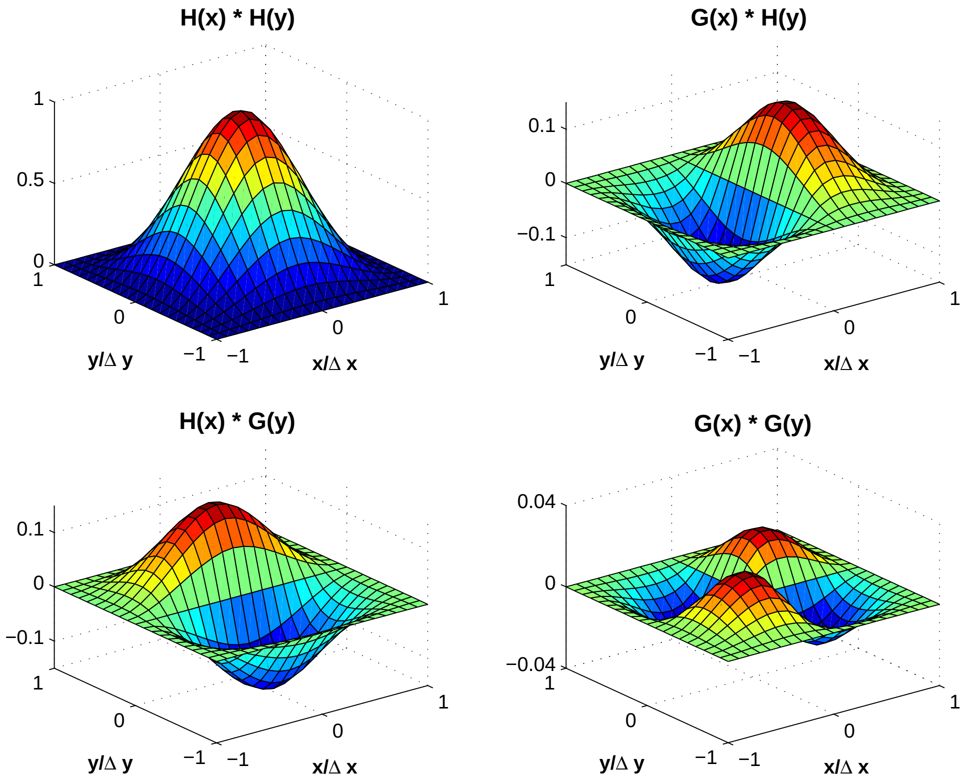

Figure 1.8: 2-Dim Hermite elements.

are shown in Fig.1.8. The partial derivatives $\partial/\partial x$ and $\partial^2/\partial x\partial y$ of these 2-Dim shape functions are shown in Fig.1.9 and Fig.1.10 respectively. These shape functions clearly generate a basis for the space of 2-Dim piecewise cubic polynomials in x and y with C^1 continuity across all cell boundaries. More exactly, C^1 continuity implies that the partial derivatives $\partial^{p_x}\partial^{p_y} f(x,y)/\partial x^{p_x}\partial y^{p_y}$ are continuous for all $p_x, p_y = 0, 1$.

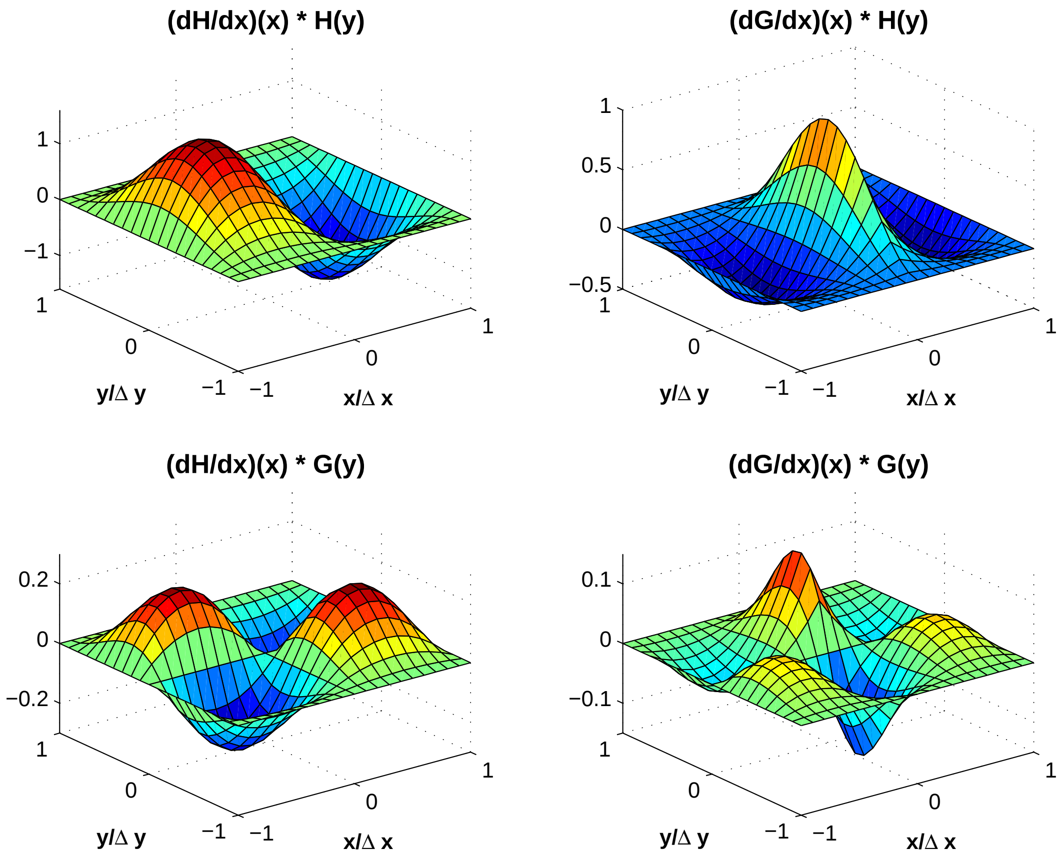

Figure 1.9: First order partial derivative in x of 2-Dim Hermite elements.

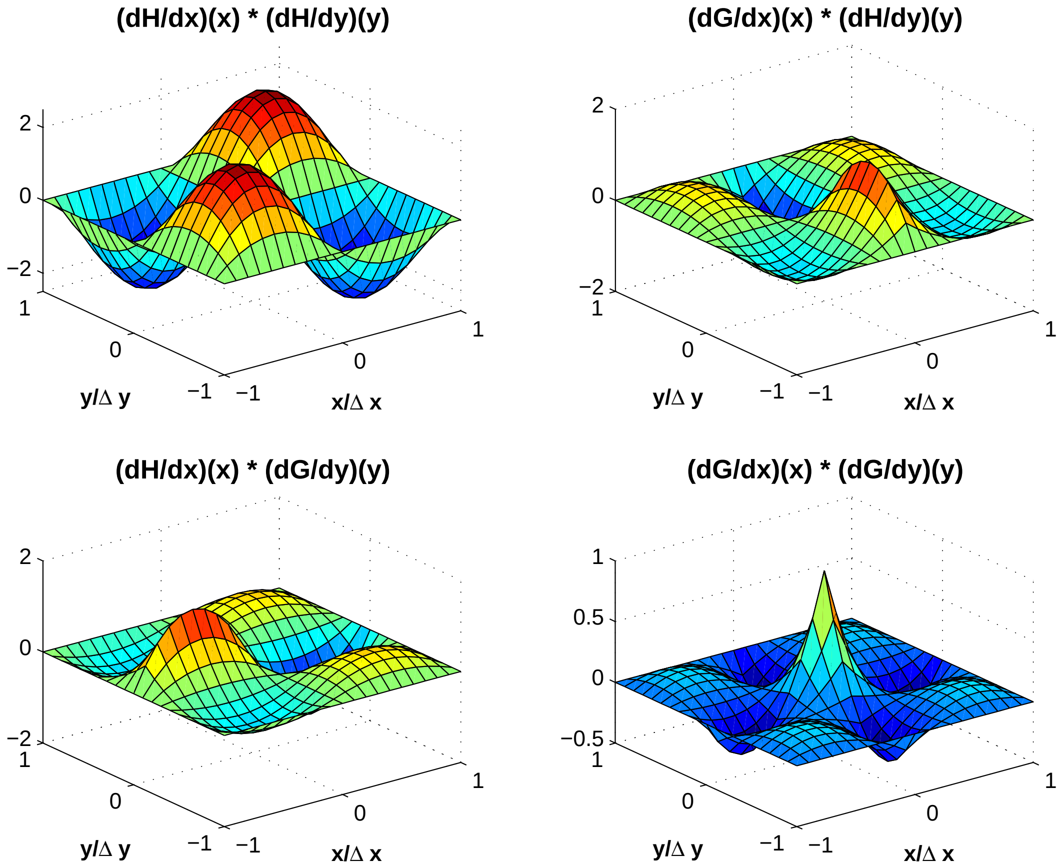

Figure 1.10: Second order partial derivative $\partial^2/\partial x \partial y$ of 2-Dim Hermite elements.

Bibliography

[1] C. de Boor, *A practical guide to splines, Applied mathematical sciences; vol. 27* (Springer, New York, 2001).

[2] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation* (Institute of Physics Publishing, London, 1998).