15
Interpolating Functions and Unfolding Problems

15.1 INTERPOLATING FUNCTIONS

Often we have a set of \( n \) data points \((z_i, y_i), i = 1, \ldots, n\), and want to find a function which matches the measured points and smoothly interpolates between them. For example, we might have measured the distortions on a lens at a series of different angles away from the axis and wish to find a smooth curve to represent the distortions as a function of angle.

One choice is to use an expansion of orthonormal functions. This method can work quite well if we fit using the regularized chi-square method described in Section 14.3.

Another choice is the use of spline functions and we will discuss these in the next sections.

15.2 SPLINE FUNCTIONS

A spline function, \( y = S(z) \), of \( k \)th degree is a \( k - 1 \) differentiable function coinciding on every subinterval \((z_i, z_{i+1})\) with a polynomial of degree \( k \).[18] The set of abscissa points, \( z_i \), are called "knots." At every knot, the definition requires that the values of the polynomials of the adjacent intervals and their first \( k - 1 \) derivatives must match.

Because of the endpoint effects, the coefficients of the polynomials are not completely fixed. At the inner knots, there are \((n - 2) \times k\) conditions from matching the polynomial and derivative values at the knots. There are \( n \) further conditions for matching the polynomials to the values \( y_i \) at the knots. Since a polynomial of \( k \)th degree has \( k + 1 \) coefficients, we have \((n - 2)k + n\) conditions and \((n - 1)(k + 1)\) coefficients to determine. We lack \( k - 1 \) conditions.

Cubic splines are among the most commonly used splines and we will concentrate on them for now. For cubic splines, we lack two conditions. There are several standard choices to determine them:

(a) \( S''(z_1) = 0; \quad S''(z_n) = 0 \). Natural spline.
(b) \( S'(z_1) = y'_1; \ S'(z_n) = y'_n. \) Complete spline. (This choice requires known values for the initial and final first derivatives.)

(c) \( S''(z_1) = y''_1; \ S''(z_n) = y''_n. \) (This choice requires known values for the initial and final second derivatives.)

(d) \( S'''(z) \) continuous across \( z_2 \) and \( z_{n-1}. \) Not-a-knot condition.

The last condition is called the not-a-knot condition because it forces the polynomials for the first two regions and for the last two regions to each be identical. Thus, there is no change in polynomial across the second or the penultimate knot.

Recall that we have used

\[
\frac{b}{a} \int [G''(z)]^2 \, dz
\]

as a measure of the curvature of a function. Using this measure, it can be shown that the natural spline gives the function interpolating the \( z_i, y_i \) with the least possible curvature. (This same function approximately minimizes the strain energy in a curved elastic bar,

\[
\frac{b}{a} \int \frac{[G''(z)]^2}{[1 + G'(z)]^{5/2}} \, dz \quad (15.1)
\]

This is the origin of the name "spline function.")

Smoothness, i.e., lack of curvature, is not the sole criterion, however. If the derivatives are known at the beginning and at the end, conditions (b) or (c) can lead to improved accuracy. If the points, \( z_i, y_i \) are points on a smooth function \( y = G(z), \) then, for the not-a-knot choice, it can be shown that for the \( p \)th derivative of the function,

\[
|G^p(z) - S^p(z)| < B, \quad B \propto (\text{knot spacing})^{4-p}, \quad p = 0, 1, 2, 3 \quad (15.2)
\]

The natural spline condition produces an error proportional to \((\text{knot spacing})^2\) near the ends of the interval. This goes to zero more slowly than the \((\text{knot spacing})^4\) of the first term above \((p = 0)\) as the knot spacing decreases. The not-a-knot condition avoids this problem and is recommended as a general condition.