Appendix D
Some statistical concepts

The statistical concepts used in this book are very elementary and can be found in any book on probability theory or random variables (e.g., Papoulis 1965).

A random variable is a variable that takes on values at random and can be thought of as a function of the outcomes of some random experiment. Consider the state variable s as a random variable. The expectation or expected value of s is defined as the sum of all values the variable might take, each weighted by the probability with which the value is taken. Suppose s can take on all values between $-\infty$ and ∞. Then, the expectation value of s is given by

$$\langle s\rangle = \int_{-\infty}^{\infty} sp(s)\, ds \tag{D1}$$

where $p(s)$ is called the density or probability density function of s. $p(s)$ is the probability that the value of s lies in the infinitesimal interval between s and $s + ds$, and it satisfies

$$p(s) \geq 0 \qquad \text{and} \qquad \int_{-\infty}^{\infty} p(s)\, ds = 1 \tag{D2}$$

The function $dp(s)/ds$ is called the distribution function and is a monotonically increasing function of s; $\eta = \langle s\rangle$, the expectation of s, is also known as the mean value or first moment of s.

If $f(s)$ is an arbitrary function of s, then,

$$\langle f(s)\rangle = \int_{-\infty}^{\infty} f(s)p(s)\, ds \tag{D3}$$

Suppose $f(s) = (s - \eta)^j$, where j is an integer and $\eta = \langle s\rangle$ is the expected value of s. Then,

$$\langle (s-\eta)^j\rangle = \int_{-\infty}^{\infty} (s-\eta)^j p(s)\, ds \tag{D4}$$

is defined as the jth moment of s around its expected value η. The second moment ($j=2$) defines the variance of s,

$$\sigma_s^2 = \langle (s-\eta)^2 \rangle \tag{D5}$$

σ_s is the standard deviation of s and is a measure of the dispersion of s about η.

An important specific form of the probability distribution is the normal distribution. The normal probability density function is given by

$$p(s) = \frac{1}{\sigma_s\sqrt{2\pi}} \exp\left[-\frac{(s-\eta)^2}{2\sigma_s^2}\right] \tag{D6}$$

where σ_s is the standard deviation defined in (D5) and η the mean value defined in (D1).

The expectation operator commutes with the addition operator. Thus, if s and q are two random variables,

$$\langle s+q \rangle = \langle s \rangle + \langle q \rangle \tag{D7}$$

as can be verified from the definition (D1). The expectation operator does *not*, in general, commute with the multiplication operator. For example, consider the covariance of the two variables s and q, defined by

$$\mathrm{cov}(s,q) = \langle [s-\langle s\rangle][q-\langle q\rangle] \rangle = \langle sq \rangle - \langle s\rangle\langle q\rangle \tag{D8}$$

The variables s and q are said to be independent or uncorrelated if $\langle sq\rangle = \langle s\rangle\langle q\rangle$. In the uncorrelated case, the expectation and multiplication operators *do* commute. Note that

$$\mathrm{cov}(s,s) = \langle s^2 \rangle - \langle s \rangle^2 = \sigma_s^2 \tag{D9}$$

is the variance of s.

The correlation coefficient ρ_{sq} can be defined as

$$\rho_{sq} = \rho_{qs} = \frac{\langle [s-\langle s\rangle][q-\langle q\rangle] \rangle}{\sigma_s\sigma_q} \tag{D10}$$

where σ_s and σ_q are defined by (D5). Applications of (D1) and Schwartz's inequality demonstrates that

$$\langle [s-\langle s\rangle][q-\langle q\rangle] \rangle^2 \le \langle [s-\langle s\rangle]^2 \rangle \langle [q-\langle q\rangle]^2 \rangle \tag{D11}$$

and $-1 \le \rho_{sq} \le 1$. If s and q are independent, then $\rho_{sq}=0$. If s is a linear function of q, $\rho_{sq} = \pm 1$.

Now consider the case when s and q are functions of $\mathbf{r}$, with $\mathbf{r}=(x,y,z)$ being a three-dimensional spatial coordinate. Suppose s and q are defined at the spatial locations $\mathbf{r}_i$, $1 \le i \le I$. Define $\underline{s}$ and $\underline{q}$ to be the column vectors of length I with elements $s(\mathbf{r}_i)$ and $q(\mathbf{r}_i)$, respectively. Now form the expectation value of the *outer product* of $\underline{s} - \langle \underline{s} \rangle$ and $\underline{q} - \langle \underline{q} \rangle$:

$$\underline{\underline{C}}_{sq} = \langle [\underline{s} - \langle \underline{s}\rangle][\underline{q} - \langle \underline{q}\rangle]^{\mathrm{T}} \rangle$$

where $\underline{\underline{C}}_{sq}$ is a real, square $I \times I$ *covariance matrix* and T indicates matrix transpose.

The double underlining for matrices and single underlining for column vectors is the usual convention adopted in this book. An arbitrary element of $\underline{\underline{C}}_{sq}$ is given by

$$C_{sq}(\mathbf{r}_i, \mathbf{r}_j) = \text{cov}[s(\mathbf{r}_i), q(\mathbf{r}_j)] = \langle [s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle][q(\mathbf{r}_j) - \langle q(\mathbf{r}_j)\rangle]\rangle \tag{D12}$$

By analogy with (D10), it is possible to define a *correlation matrix* $\underline{\underline{\rho}}_{sq}$ with elements $\rho_{sq}(\mathbf{r}_i, \mathbf{r}_j)$ given by

$$\rho_{sq}(\mathbf{r}_i, \mathbf{r}_j) = \frac{\langle [s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle][q(\mathbf{r}_j) - \langle q(\mathbf{r}_j)\rangle]\rangle}{\sigma_s(\mathbf{r}_i)\sigma_q(\mathbf{r}_j)} \tag{D13}$$

where

$$\sigma_s^2(\mathbf{r}_i) = \langle [s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle]^2\rangle \qquad \text{and} \qquad \sigma_q^2(\mathbf{r}_j) = \langle [q(\mathbf{r}_j) - \langle q(\mathbf{r}_j)\rangle]^2\rangle$$

$\rho_{sq}(\mathbf{r}_i, \mathbf{r}_j)$ can be related to $C_{sq}(\mathbf{r}_i, \mathbf{r}_j)$ and $\underline{\underline{\rho}}_{sq}$ to $\underline{\underline{C}}_{sq}$ as follows:

$$\rho_{sq}(\mathbf{r}_i, \mathbf{r}_j) = C_{sq}(\mathbf{r}_i, \mathbf{r}_j)/\sigma_s(\mathbf{r}_i)\sigma_q(\mathbf{r}_j) \tag{D14}$$

and

$$\underline{\underline{C}}_{sq} = \underline{\underline{\sigma}}_s \underline{\underline{\rho}}_{sq}$$

where $\underline{\underline{\sigma}}_s$ is the diagonal matrix with elements $\sigma_s(\mathbf{r}_i)$ and $\underline{\underline{\sigma}}_q$ is the diagonal matrix with elements $\sigma_q(\mathbf{r}_i)$. From (D11), $-1 \le \rho_{sq}(\mathbf{r}_i, \mathbf{r}_j) \le 1$.

In the special case $q = s$, $\underline{\underline{C}}_{ss}$ is symmetric and known as an autocovariance matrix. $\underline{\underline{C}}_{ss}$ is also positive semidefinite (2.3.12). This can be seen as follows. Suppose $\underline{z}$ is an arbitrary column vector with elements z_i, $1 \le i \le I$ (not all $z_i = 0$). Then,

$$\begin{aligned}
\underline{z}^{\mathrm{T}} \underline{\underline{C}}_{ss} \underline{z} &= \sum_{i=1}^{I} \sum_{j=1}^{I} C_{ss}(\mathbf{r}_i, \mathbf{r}_j) z_i z_j \\
&= \sum_{i=1}^{I} \sum_{j=1}^{I} z_i z_j \langle [s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle][s(\mathbf{r}_j) - \langle s(\mathbf{r}_j)\rangle]\rangle \\
&= \left\langle \left[\sum_{i=1}^{I} z_i \{s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle\} \right]^2 \right\rangle \ge 0
\end{aligned}$$

From (2.3.15), the eigenvalues of $\underline{\underline{C}}_{ss}$ must be real and nonnegative. A zero eigenvalue of $\underline{\underline{C}}_{ss}$ occurs when any row is a linear combination of other rows. This happens if two spatial locations $\mathbf{r}_i$ and $\mathbf{r}_j$ coincide. Thus, if all spatial locations $\mathbf{r}_i$ are distinct, then $\underline{\underline{C}}_{ss}$ is strictly positive definite and all its eigenvalues are strictly positive. Clearly, the same is true for the correlation matrix $\underline{\underline{\rho}}_{ss}$.

The trace (sum of diagonal elements) of $\underline{\underline{C}}_{ss}$ is equal to the sum of the expected variances at each location $\mathbf{r}_i$ and is also equal to the expected value of the *inner product* of $\underline{s} - \langle \underline{s}\rangle$ with itself:

$$\text{Trace}(\underline{\underline{C}}_{ss}) = \sum_{i=1}^{I} \langle [s(\mathbf{r}_i) - \langle s(\mathbf{r}_i)\rangle]^2\rangle = \langle [\underline{s} - \langle \underline{s}\rangle]^{\mathrm{T}}[\underline{s} - \langle \underline{s}\rangle]\rangle \tag{D15}$$

A well-known theorem of linear algebra (Wilkinson 1965) states that the trace of a matrix is equal to the sum of its eigenvalues. Suppose the eigenvalues of $\underline{C}_{ss}$ are denoted μ_j, $1 \le j \le I$. Then $\sum_{j=1}^{I} \mu_j$ is equal to the sum of the expected variances at each location $\mathbf{r}_i$. Consequently, μ_j, $1 \le j \le I$, can be thought of as the expected variance of the jth eigenvector of $\underline{C}_{ss}$.

$\underline{\rho}_{ss}$ is symmetric, and the diagonal elements of $\underline{\rho}_{ss}$ are all equal to 1. Trace$(\underline{\rho}_{ss}) = I$, and the sum of the eigenvalues of $\underline{\rho}_{ss}$ is equal to I.

For the sake of simplicity, assume that $\langle s(\mathbf{r}_i)\rangle = \langle q(\mathbf{r}_i)\rangle = 0$ for $1 \le i \le I$; thus, $\mathrm{cov}[s(\mathbf{r}_i), q(\mathbf{r}_j)] = \langle s(\mathbf{r}_i)q(\mathbf{r}_j)\rangle$. The statistical structure of s and q is said to be spatially *homogeneous* if $\langle s(\mathbf{r}_i)q(\mathbf{r}_j)\rangle$ depends only on the relative displacement $\tilde{\mathbf{r}} = \mathbf{r}_j - \mathbf{r}_i$, rather than on the absolute locations $\mathbf{r}_i$ and $\mathbf{r}_j$. In the homogeneous case,

$$C_{sq}(\mathbf{r}_i, \mathbf{r}_j) = \langle s(\mathbf{r}_i)q(\mathbf{r}_i + \tilde{\mathbf{r}})\rangle = C_{sq}(\tilde{\mathbf{r}}) \tag{D16}$$

and the covariance in (D16) is a function only of $\tilde{\mathbf{r}}$ and not of $\mathbf{r}_i$ or $\mathbf{r}_j$. In particular, the diagonal elements of $\underline{C}_{sq}$ are all equal in the homogeneous case:

$$C_{sq}(\mathbf{r}_i, \mathbf{r}_i) = \langle s(\mathbf{r}_i)q(\mathbf{r}_i)\rangle = C_{sq}(0) \tag{D17}$$

is independent of position. Then, using (D16–17) gives

$$\begin{aligned} C_{sq}(\tilde{\mathbf{r}}) &= \langle s(\mathbf{r}_i)q(\mathbf{r}_i + \tilde{\mathbf{r}})\rangle = \langle s(\mathbf{r}_i - \tilde{\mathbf{r}})q(\mathbf{r}_i)\rangle \\ &= \langle q(\mathbf{r}_i)s(\mathbf{r}_i - \tilde{\mathbf{r}})\rangle = C_{qs}(-\tilde{\mathbf{r}}) \end{aligned} \tag{D18}$$

Now consider $\underline{C}_{ss}$ under conditions of homogeneity, and continue to assume that $\langle s(\mathbf{r}_i)\rangle = 0$. From (D18), it is evident that

$$C_{ss}(\tilde{\mathbf{r}}) = C_{ss}(-\tilde{\mathbf{r}}) \tag{D19}$$

Moreover, because $C_{ss}(0) = \langle s^2(\mathbf{r}_i)\rangle = \langle s^2\rangle$ is independent of location,

$$C_{ss}(\tilde{\mathbf{r}}) = \langle s^2\rangle \rho_{ss}(\tilde{\mathbf{r}}) = C_{ss}(0)\rho_{ss}(\tilde{\mathbf{r}})$$

and

$$C_{ss}(0) = \langle s^2\rangle \ge \langle s^2\rangle |\rho_{ss}(\tilde{\mathbf{r}})| = |C_{ss}(\tilde{\mathbf{r}})| \tag{D20}$$

The temporal analogue of spatial homogeneity is called stationarity. Define s and q at times t_1 and t_2, respectively, and define $\tau = t_2 - t_1$. Under stationary conditions,

$$C_{sq}(t_1, t_2) = \langle s(t_1)q(t_2)\rangle = \langle s(t_1)q(t_1 + \tau)\rangle = C_{sq}(\tau) \tag{D21}$$

is only a function of the time difference τ and not of the absolute times t_1 and t_2.

Now suppose that $s(\mathbf{r}, t)$ is the true value of s (the signal) and define an estimate $s_e(\mathbf{r}, t)$ that is in error:

$$s_e(\mathbf{r}, t) = s(\mathbf{r}, t) + \varepsilon(\mathbf{r}, t) \tag{D22}$$

where $\varepsilon(\mathbf{r}, t)$ is the error. The estimate $s_e(\mathbf{r}, t)$ of $s(\mathbf{r}, t)$ could be obtained by measurement (observation), by a forecast using a numerical model (background), or by an objective analysis algorithm. The expectation operator (D1) can be applied to the error $\varepsilon(\mathbf{r}, t)$ as well:

$$\langle \varepsilon \rangle = \int_{-\infty}^{\infty} \varepsilon p(\varepsilon)\, d\varepsilon \qquad \text{and} \qquad \langle \varepsilon^2 \rangle = \int_{-\infty}^{\infty} \varepsilon^2 p(\varepsilon)\, d\varepsilon \tag{D23}$$

where $p(\varepsilon)$ is the probability that the error lies between ε and $\varepsilon + d\varepsilon$. A number of simplifying assumptions can be made about the error:

If $\langle \varepsilon(\mathbf{r}, t) \rangle = 0$, there is no systematic error or bias. (D24)

If $\langle \varepsilon(\mathbf{r}_i, t)\varepsilon(\mathbf{r}_j, t) \rangle = 0$ for $\mathbf{r}_i \neq \mathbf{r}_j$, the error is not spatially correlated. (D25)

If $\langle \varepsilon(\mathbf{r}, t_1)\varepsilon(\mathbf{r}, t_2) \rangle = 0$ for $t_1 \neq t_2$, the error is not temporally correlated. (D26)

If $\langle s(\mathbf{r}, t)\varepsilon(\mathbf{r}, t) \rangle = 0$, the error is not correlated with the signal. (D27)

If the error is unbiased (D24), then $\langle s_e(\mathbf{r}, t) \rangle = \langle s(\mathbf{r}, t) \rangle$. (D28)

That is, the expected value of the estimate over many realizations is equal to the expected value of the signal. $s_e(\mathbf{r}, t)$ is then called an unbiased estimate of $s(\mathbf{r}, t)$.

A measure of the importance of the error is the signal-to-noise ratio, which is defined as

$$\frac{\langle [s(\mathbf{r}, t) - \langle s(\mathbf{r}, t) \rangle]^2 \rangle}{\langle \varepsilon^2(\mathbf{r}, t) \rangle} \tag{D29}$$

Appendix E
Classical interpolation

Interpolation is used in the data assimilation cycle primarily to determine values of the background field at observation stations. This is known as the forward problem and is discussed in Sections 1.6, 3.1, 4.2, and 5.6. Usually, we know the background field at the gridpoints of a regular mesh, and we use interpolation formulas of various types to obtain estimates of the background field at the observation stations. The interpolation algorithms are usually two- or three-dimensional formulations, but we examine only the one-dimensional case here. The subject is a classical numerical analysis topic and is discussed in many books on numerical analysis, such as Hildebrand (1956).

Suppose the function $y=f(x)$ is known exactly at K regularly or irregularly spaced values of the independent variable in the domain $x_a \le x \le x_b$. Thus, the $f(x_1), f(x_2), \ldots, f(x_K)$ are assumed known. The process of determining an approximate (or sometimes exact) value of the function at an arbitrary point x is known as interpolation. For example, function tables tabulate functional values at constant increments in the independent variables. To determine values of the function at intermediate values of the independent variable requires interpolation.

Perhaps the best-known interpolation formula is that of Lagrange:

$$\begin{aligned} f_{\mathrm{A}}(x) = {} & \frac{(x-x_2)(x-x_3)\cdots(x-x_K)}{(x_1-x_2)(x_1-x_3)\cdots(x_1-x_K)} f(x_1) \\ & + \cdots \\ & + \frac{(x-x_1)(x-x_2)\cdots(x-x_{K-1})}{(x_K-x_1)(x_K-x_2)\cdots(x_K-x_{K-1})} f(x_K) \end{aligned} \tag{E1}$$

where $f_{\mathrm{A}}(x)$ is an approximation of the true function $f(x)$. This formula requires that $f(x)$ be known exactly at K regularly or irregularly spaced values of x. $f_{\mathrm{A}}(x)=f(x)$ at the points $x_1, x_2, \ldots, x_K$.

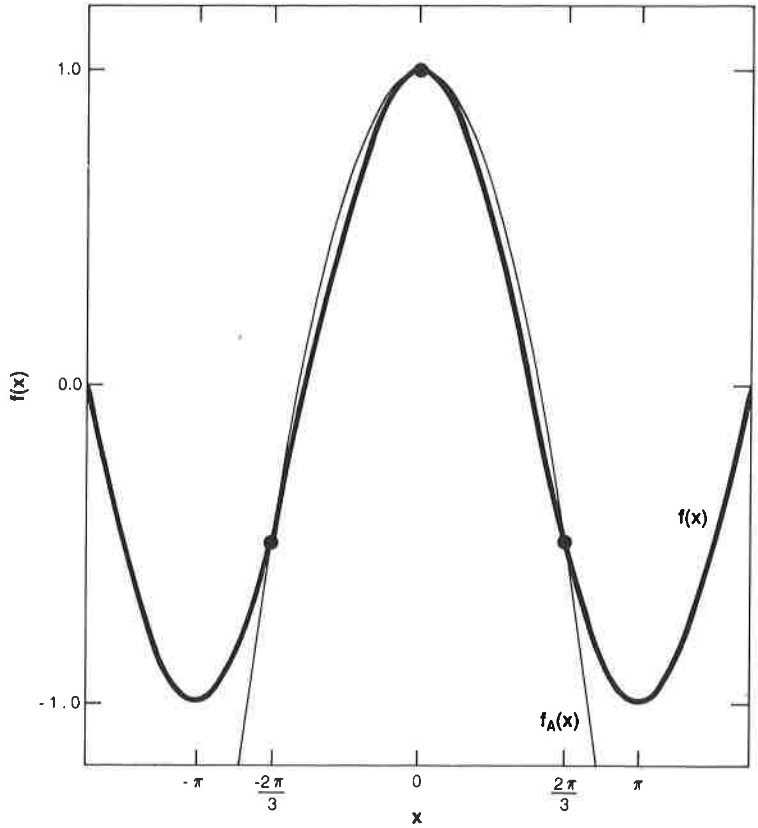

Figure E1 Plot of $f(x) = \cos(x)$ (heavy line) and the Lagrange interpolated approximation $f_A(x)$ (light line) as a function of x. The known values of $f(x)$ at $x = 0$, $\pm 2\pi/3$ are indicated by heavy dots.

If $f(x)$ is the polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_N x^N$$

then Lagrange's interpolation formula is exact for any value of x provided that $N + 1 \leq K$. If $f(x)$ is any other function, Lagrange's interpolation formula is not exact but only approximate. Suppose $f(x) = \cos(x)$ and $f(x)$ is assumed known at the points $x_1 = -2\pi/3$, $x_2 = 0$, and $x_3 = 2\pi/3$. Then the application of Lagrange's interpolation formula yields

$$f_A(x) = -\frac{27x^2}{8\pi^2} + 1 \tag{E2}$$

The functions $f(x)$ and $f_A(x)$ are plotted in Figure E1. It is apparent that for $-2\pi/3 \leq x \leq 2\pi/3$, $f_A(x)$ is a good approximation to $f(x)$; but outside this range, $f_A(x)$ is an increasingly poor approximation. For $x \leq -2\pi/3$ and $x \geq 2\pi/3$, Lagrange's formula is actually doing extrapolation, which is generally much less accurate than interpolation.

Another commonly used interpolation procedure is spline interpolation (Ahlberg, Nilson, and Walsh 1967). As above, assume $f(x_k)$, $1 \le k \le K$, is known. Find the function $f_A(x)$ that is continuous, has continuous first and second derivatives, and passes through the points $f(x_k)$. Let $S_k = f''_A(x_k)$ be the unknown values of the second derivative evaluated at the points x_k. Then, $f''_A(x)$ is linear between x_{k-1} and x_k:

$$f''_A(x) = S_{k-1}\left(\frac{x_k - x}{\Delta_k}\right) + S_k\left(\frac{x - x_{k-1}}{\Delta_k}\right) \tag{E3}$$

where $\Delta_k = x_k - x_{k-1}$.

Integrate (E3) twice and evaluate the constants of integration using the known values $f(x_k)$. Thus,

$$f_A(x) = S_{k-1}\frac{(x_k - x)^3}{6\Delta_k} + S_k\frac{(x - x_{k-1})^3}{6\Delta_k} + \left[f(x_{k-1}) - \frac{S_{k-1}\Delta_k^2}{6}\right]\left[\frac{x_k - x}{\Delta_k}\right] + \left[f(x_k) - \frac{S_k\Delta_k^2}{6}\right]\left[\frac{x - x_{k-1}}{\Delta_k}\right] \tag{E4}$$

$$f'_A(x) = -S_{k-1}\frac{(x_k - x)^2}{2\Delta_k} + \frac{S_k(x - x_{k-1})}{2\Delta_k} + \frac{f(x_k) - f(x_{k-1})}{\Delta_k} - \frac{(S_k - S_{k-1})\Delta_k}{6} \tag{E5}$$

Equation (E5) applies in the interval $x_{k-1} \le x \le x_k$. A similar equation applies in the interval $x_k \le x \le x_{k+1}$:

$$f'_A = -S_k\frac{(x_{k+1} - x)^2}{2\Delta_{k+1}} + S_{k+1}\frac{(x - x_k)^2}{2\Delta_{k+1}} + \frac{f(x_{k+1}) - f(x_k)}{\Delta_{k+1}} - \frac{(S_{k+1} - S_k)\Delta_{k+1}}{6} \tag{E6}$$

Because $f'_A(x)$ must be continuous, the limit of $f'_A(x)$ when $x \to x_k$ should be the same when approached from above or below. Setting $x = x_k$ in (E5) and (E6) and equating the two gives

$$\frac{\Delta_k}{6}S_{k-1} + \frac{(\Delta_k + \Delta_{k+1})}{3}S_k + \frac{\Delta_{k+1}}{6}S_{k+1} = \frac{f(x_{k+1}) - f(x_k)}{\Delta_{k+1}} - \frac{f(x_k) - f(x_{k-1})}{\Delta_k} \tag{E7}$$

Consider the periodic case, $S_{K+1} = S_1$, $f(x_{K+1}) = f(x_1)$, $\Delta_{K+1} = \Delta_1$. Then (E7) can be written in matrix form as

$$\underline{T}\,\underline{S} = \underline{\underline{Q}}^{T}\underline{f} \tag{E8}$$

where $\underline{S}$ is the column vector of length K of unknown $S_k = f''_A(x_k)$ and $\underline{f}$ is the column vector of length K of known functional values of $f(x_k)$. $\underline{T}$ is a symmetric positive definite, (almost) tri-diagonal $K \times K$ matrix with elements $t_{k,k} = (\Delta_k + \Delta_{k+1})/3$, $t_{k,k+1} = \Delta_{k+1}/6$, and $t_{k,k-1} = \Delta_k/6$. $\underline{\underline{Q}}$ is a $K \times K$ tri-diagonal diagonal matrix with elements $q_{k-1,k} = 1/\Delta_k$, $q_{k,k} = -1/\Delta_k - 1/\Delta_{k+1}$, $q_{k+1,k} = 1/\Delta_{k+1}$. In accord with usual matrix notation, the first index indicates the row and the second the column. $\underline{T}$ is a simple sparse matrix and can be inverted simply and efficiently. Substitution of the S_k into (E4) yields the approximation to $f(x)$.

Spline functions have a minimum curvature property. It was shown by Holladay (see Ahlberg et al. 1967) that of all the functions that have continuous second derivatives in the domain and that exactly fit $f(x_k)$, $1 \leq k \leq K$, the spline function (E8) minimizes the integral

$$\int_{x_a}^{x_b} \{f''(x)\}^2 \, dx \tag{E9}$$

There are many types of spline functions; (E8) defines an interpolating cubic spline because (E4) is a cubic polynomial in the interval $x_{k-1} \leq x \leq x_k$.