MULTIVARIATE, MINIMUM-CURVATURE SPLINES FOR RANDOMLY SPACED DATA

JAMES R. CLOUTIER

JULY 1983
FOREWORD

The multivariate splines presented in this report have been designed for the direct analysis, smooth representation, and efficient storage of data which is randomly spaced in multiple dimensions and which, additionally, may be periodic along one or more of these directions. Of special interest to the U.S. Naval Oceanographic Office is the applicability of these splines to randomly sampled geophysical and oceanographic features and/or processes.

The univariate, minimum-curvature spline has been applied as a smoother and "gap filler" in the SEASAT ephemeris correction; this spline also has been used to generate a pseudomonthly Generalized Digital Environmental Model (GDEM) and employed to model the north wall of the Gulf Stream.

Possible future applications of the multivariate, minimum-curvature splines are as a closed-form representation of the gravimetric geoid as an efficient, closed-form upward continuation of gravity anomalies and as a parametric, closed-form representation of GDEM based on latitude, longitude, depth, and time of month.

This work was carried out within the Advanced Technology Staff and has been reviewed by its head, Dr. Thomas M. Davis.

[Signature]

E. H. CRAIGLOW
Captain, USN
Acting Commanding Officer
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ABSTRACT

This paper develops a collection of multivariate splines which are applicable to randomly spaced data. The splines are constructed from a linear combination of spline basis functions having evenly spaced nodes. A pseudoinverse solution of coefficients is obtained via a singular value decomposition (SVD). Spurious oscillations are damped by zeroing out an appropriate number of the singular values. A transformation is performed prior to entering the SVD so that, whenever the solution is nonunique, the "minimum-curvature" solution is obtained. An added feature of these splines is an option through which a periodic fit may be produced in one or more dimensions if it is so desired.
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1. **INTRODUCTION**

Geophysicists and oceanographers are constantly faced with the task of analyzing and interpreting randomly spaced data. Moreover, it is not unusual for such data to have been collected nonuniformly; some portions of the sampled area may be data dense, while other portions may contain no data at all. This nature of geophysical sampling presents a problem to the analyst attempting to represent the data as a parameterized curve or surface. What often happens is that the linear system resulting from the parameterization has an infinite number of solutions, or is highly ill-conditioned, or both.

In this report, we will develop a collection of multivariate splines which are immune to these difficulties. This will be accomplished by first representing the splines as a linear combination of spline basis functions. The linear system resulting from this parameterization will then be transformed into a new reference frame and a singular value decomposition in conjunction with pseudoinversion will be used to solve the new system. The reference frame transformation will be derived so that whenever the solution is nonunique, the "minimum-curvature" solution is obtained.

Another important aspect of geophysical and oceanographic data is that of periodicity. This is the case when one considers geophysical phenomena on a global scale, or the seasonal dependence of many types of oceanographic data, the latter data being at least quasi-periodic as a function of time of year. For this reason, we will also consider the concept of a periodic spline and derive an elegant way of representing multivariate, periodic splines.

The first step in the development is the construction of sets of basis functions for the multivariate splines.
2. **MULTIVARIATE SPLINE BASIS FUNCTIONS**

Let $S$ be the set of all cubic, univariate spline functions having evenly spaced nodes (or knots) $s_1, s_2, \ldots, s_n$ separated by the distance $h$. A function $f$ is a member of $S$ if and only if $f$ is a cubic polynomial on each sub-interval $[s_j, s_{j+1}]$ and is twice continuously differentiable throughout the interval $[s_1, s_n]$.

It is well known that the set $S$ constitutes an $(n+2)$-dimensional linear space of functions. Thus any set of $n+2$ linearly independent members of $S$, e.g. \( \{ \phi_j : j = 1, \ldots, n+2 \} \), forms a basis for $S$. This means that each $f \in S$ can be uniquely represented as

$$f(t) = \sum_{j=1}^{n+2} x_j \phi_j(t).$$  \hspace{1cm} (1)

One of the most commonly used bases [Lawson (1974), Schoenberg (1973), Ahlberg (1967), deBoor (1978)] can be defined using the two cubic polynomials

$$p_1(\theta) = .25\theta^3$$  \hspace{1cm} (2)

and

$$p_2(\theta) = 1 - .75(1+\theta)(1-\theta)^2.$$  \hspace{1cm} (3)

With $\theta_j$ defined as

$$\theta_j = \frac{t-s_j}{h}, \quad j=1, \ldots, n-1$$  \hspace{1cm} (4)

where

$$h = s_{j+1} - s_j, \quad j=1, \ldots, n-1$$  \hspace{1cm} (5)

the following set of functions,

$$\phi_j(t) = \begin{cases} 
0 & \text{for } s_1 \leq t \leq s_{j-3} \text{ and } 5 \leq j \leq n+2 \\
p_1(\theta_{j-3}) & \text{for } s_{j-3} \leq t \leq s_{j-2} \text{ and } 4 \leq j \leq n+2 \\
p_2(\theta_{j-2}) & \text{for } s_{j-2} \leq t \leq s_{j-1} \text{ and } 3 \leq j \leq n+1 \\
p_2(1-\theta_{j-1}) & \text{for } s_{j-1} \leq t \leq s_j \text{ and } 2 \leq j \leq n \\
p_1(1-\theta_j) & \text{for } s_j \leq t \leq s_{j+1} \text{ and } 1 \leq j \leq n-1 \\
0 & \text{for } s_{j+1} \leq t \leq s_n \text{ and } 1 \leq j \leq n-2 
\end{cases}$$  \hspace{1cm} (6)
represents a basis for $S$. This spline basis is illustrated in figure 1 for the case $h=1, n=11$. (Note: Figures are located on pages 39 through 59.)

Multivariate spline bases can be generated from this univariate spline basis through the use of tensor products [de Boor (1978) and Schultz (1973)]. To simplify the multivariate development, it will be required that the nodal spacing in each direction be equal to the distance $h$. This can be done without any loss of generality; different nodal spacings in each of the multidirections can be achieved by appropriate nodal scaling of the independent variables of the data.

The bivariate spline basis is composed of the functions

$$\phi_{ij}(t_1, t_2) = \phi_i(t_1)\phi_j(t_2) \quad i=1, \ldots, n_1+2 \quad j=1, \ldots, n_2+2$$

(7)

Orthogonal subsets of this basis are depicted in figures 2-17 for the case $h=1, n_1=11, n_2=11$. The entire basis is represented by the superposition of these figures.

The trivariate spline basis is made up of the functions

$$\phi_{ijk}(t_1, t_2, t_3) = \phi_i(t_1)\phi_j(t_2)\phi_k(t_3) \quad i=1, \ldots, n_1+2 \quad j=1, \ldots, n_2+2 \quad k=1, \ldots, n_3+2$$

(8)

In general, the $M$-variate spline basis consists of the functions

$$\phi_{j_1\ldots j_M}(t_1, t_2, \ldots, t_M) = \phi_{j_1}(t_1)\phi_{j_2}(t_2)\ldots\phi_{j_M}(t_M) \quad j_1=1, \ldots, n_1+2 \quad j_2=1, \ldots, n_2+2 \quad \vdots \quad j_M=1, \ldots, n_M+2$$

(9)

Hence, any bivariate spline with evenly spaced nodes can be uniquely represented as

$$f(t_1, t_2) = \sum_{i=1}^{n_1+2} \sum_{j=1}^{n_2+2} x_{ij} \phi_i(t_1)\phi_j(t_2),$$

(10)
any trivariate spline with evenly spaced nodes can be uniquely represented as

\[ f(t_1, t_2, t_3) = \sum_{i=1}^{n_1+2} \sum_{j=1}^{n_2+2} \sum_{k=1}^{n_3+2} x_{ijk} \phi_i(t_1) \phi_j(t_2) \phi_k(t_3), \]

and so forth.
THE LINEAR SYSTEM

Using such bases, the problem of finding a multivariate spline that best fits a set of data reduces to solving a linear system

$$Ax = b \quad (12)$$

in some sense (usually a least-squares sense) where $A$ is an $m \times N$ matrix. For example, in the univariate case, given a set of data $\{(t_i, y_i) : t_i \in [s_1, s_n]; i=1, \ldots, m\}$, employment of equation (1) leads to the linear system

$$y_1 = \sum_{j=1}^{n+2} x_j \phi_j(t_1)$$
$$y_2 = \sum_{j=1}^{n+2} x_j \phi_j(t_2)$$
$$\vdots$$
$$y_m = \sum_{j=1}^{n+2} x_j \phi_j(t_m). \quad (13)$$

In this instance, $N = n+2$ and

$$A = \begin{bmatrix}
\phi_1(t_1) & \phi_2(t_1) & \cdots & \phi_{n+2}(t_1) \\
\phi_1(t_2) & \phi_2(t_2) & \cdots & \phi_{n+2}(t_2) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_1(t_m) & \phi_2(t_m) & \cdots & \phi_{n+2}(t_m)
\end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n+2} \end{bmatrix}, \quad b = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}. \quad (14)$$

In the multivariate cases, use of equations (10) and (11) leads to similar linear systems. The matrix $A$ will always contain the basis functions evaluated at the appropriate points in time or space, the vector $\vec{x}$ will contain the spline coefficients to be solved for, and the vector $\vec{b}$ will contain the dependent values of the data.

If the data is relatively uniformly dense and there exist several data points within each nodal division (subinterval, subarea, subvolume, etc.), then
the columns of the matrix A will be linearly independent and the system will have a unique least-squares solution

\[
\vec{x} = A^\# b
\]  

(15)

where

\[
A^\# = (A^T A)^{-1} A^T
\]  

(16)

is the pseudoinverse of A. In practice, \((A^T A)^{-1}\) is rarely computed, but rather \(\vec{x}\) is obtained by performing a Cholesky decomposition on \(A^T A\) or employing a sequential Householder processing procedure [Lawson and Hanson (1974)].

If the data is not uniformly dense, and there exist nodal divisions containing no data, then the columns of the matrix A may be linearly dependent, thus making \(A^T A\) singular. Hence, there will be an infinite number of least-squares solutions. The system may be highly ill-conditioned as well. Under these conditions, the Cholesky and Householder approaches, per se, break down, and an alternative approach must be taken. Such an alternative is the use of a singular value decomposition in conjunction with pseudoinversion [LeSchack (1976), Golub (1965), (1970), Van Loan (1976), Rao (1971), Ben-Israel (1974)].
4. THE SINGULAR VALUE DECOMPOSITION

The singular value decomposition of an \( m \times N \) matrix \( A \) of real elements [LeSchack (1976), Golub (1965), (1970), Van Loan (1976)] is a factorization of the form

\[
A = U S_K V^T
\]  
(17)

where \( U \) is an \( m \times m \) orthogonal matrix, \( V \) is an \( N \times N \) orthogonal matrix, and \( S_K \) is an \( m \times N \) matrix whose only nonzero elements are \( K \) positive diagonal elements \( \lambda_i^2, i = 1, \ldots, K \) called the singular values of \( A \). The singular values are arranged in descending order of magnitude, with \( K \) being the rank of \( A \).

Remarkably efficient algorithms exist to numerically perform the decomposition (17). An SVD algorithm in conjunction with pseudoinversion represents a practical and accurate technique for solving ill-conditioned, least-squares problems which originate in, or are transformed to, the form of equation (12). Using a matrix outer product expansion, equation (17) can be written as

\[
A = \sum_{i=1}^{K} \lambda_i^2 \mathbf{u}_i \mathbf{v}_i^T
\]
(18)

where \( \mathbf{u}_i \) and \( \mathbf{v}_i \) are the \( i^{th} \) column vectors of the matrices \( U \) and \( V \), respectively, and \( \lambda_i^2 \) is the \( i^{th} \) singular value of the matrix \( A \). The pseudoinverse of \( A \) is then given by

\[
A^\dagger = \sum_{i=1}^{K} \lambda_i^{-2} \mathbf{v}_i \mathbf{u}_i^T.
\]
(19)

In the event that \( K=N \), this pseudoinverse is identical to the pseudoinverse (16). For \( K<N \), the matrix \( A \) is rank defective, and the pseudoinverse (19) yields the least-squares solution of minimum length.

Ill-conditioning of the system originates from some singular values being relatively much smaller than other ones. This ill-conditioning can be overcome by setting the smaller singular values to zero, that is, terminating the summation in (19) short of \( K \). Hence, a truncated pseudoinverse can be obtained via

\[
A_t^\dagger = \sum_{i=1}^{L} \lambda_i^{-2} \mathbf{v}_i \mathbf{u}_i^T
\]
(20)
where L < K. Whenever L < K, the full solution (L = K) has been deemed unstable and has been replaced by a stable solution at the expense of a slightly larger least-squares residual error.

A procedure for determining the termination index L was presented by Shim and Cho (1981) for use in image restoration problems. An optimal termination index was derived assuming that both the signal and noise were white (with respect to a Karhunen-Loeve transform) and is given by

\[ L_{opt} = \max_k \left\{ k : \lambda_k \geq \frac{m}{N \cdot (SNR)} \right\} \]  

(21)

where SNR is the signal-to-noise ratio and \( \lambda_k \) is the \( k^{th} \) singular value squared. This simple formula produced good image restorations in Shim and Cho’s computer simulations. In practice, this author has found that the formula works equally well in curve-fitting applications.
5. **REFERENCE FRAME TRANSFORMATION**

The SVD technique just discussed yields the least-squares solution of minimum length. Thus, if the method were applied directly to the linear system (12), the vector \( \hat{x} \) of spline coefficients would be minimized. Since it is known [deBoor (1978)] that these coefficients model the surface they represent (i.e., a plot of the coefficients yields a shape similar to the surface, at least to within a scale factor), minimizing the spline coefficients is roughly equivalent to minimizing the spline surface itself. Unfortunately, there is no physical justification for doing so. It is more desirable, therefore, to produce a solution which optimizes some physically justifiable performance index. This can be achieved by representing the system in a new reference frame prior to application of the SVD.

Let the performance index \( P \) be given by

\[
P = \hat{x}^T Q \hat{x} \tag{22}
\]

where \( Q \) is a positive definite matrix and let

\[
\hat{y} = L^T \hat{x} \tag{23}
\]

where \( L \) is the lower triangular Cholesky factor of \( Q \). This implies that

\[
\hat{x} = (L^{-1})^T \hat{y}. \tag{24}
\]

Substituting (24) into equation (12), we have

\[
B \hat{y} = \hat{b} \tag{25a}
\]

where

\[
B = A(L^{-1})^T. \tag{25b}
\]

If the SVD technique is now applied to the system (25), the vector \( \hat{y} \) will be minimized, forcing the performance index

\[
P = \hat{x}^T Q \hat{x} = \hat{x}^T L L^T \hat{x} = (L^T \hat{x})^T (L^T \hat{x}) = \hat{y}^T \hat{y} \tag{26}
\]

to be a minimum. The appropriate spline coefficients can then be obtained via equation (24).

The problem now is to find a positive definite matrix \( Q \) such that \( P \) will represent a physically important aspect of the solution. Before doing so, however, the concept of a periodic spline is introduced.
6. **PERIODIC SPLINES**

For a univariate spline

\[ f(t) = \sum_{j=1}^{n+2} x_j \phi_j(t) \]  

(27)

to be periodic over the interval \([s_1, s_n]\), the spline along with its first and second derivatives must match at the interval end points, that is,

\[ f(s_1) = f(s_n) \]  

(28a)

\[ f'(s_1) = f'(s_n) \]  

(28b)

\[ f''(s_1) = f''(s_n) \]  

(28c)

This means that

\[ \sum_{j=1}^{n+2} x_j \phi_j(s_1) = \sum_{j=1}^{n+2} x_j \phi_j(s_n) \]  

(29a)

\[ \sum_{j=1}^{n+2} x_j \phi_j'(s_1) = \sum_{j=1}^{n+2} x_j \phi_j'(s_n) \]  

(29b)

\[ \sum_{j=1}^{n+2} x_j \phi_j''(s_1) = \sum_{j=1}^{n+2} x_j \phi_j''(s_n) \]  

(29c)

These equations reduce to

\[ \sum_{j=1}^{3} x_j \phi_j(s_1) = \sum_{j=n}^{n+2} x_j \phi_j(s_n) \]  

(30a)

\[ \sum_{j=1}^{3} x_j \phi_j'(s_1) = \sum_{j=n}^{n+2} x_j \phi_j'(s_n) \]  

(30b)

\[ \sum_{j=1}^{3} x_j \phi_j''(s_1) = \sum_{j=n}^{n+2} x_j \phi_j''(s_n) \]  

(30c)
since these are the only nonzero contributors to the sums.

Evaluating the functions at the interval end points yields

\[
\begin{align*}
\frac{1}{4}x_1 + x_2 + \frac{1}{4}x_3 &= \frac{1}{4}x_n + x_{n+1} + \frac{1}{4}x_{n+2} \\
\frac{-3}{4}x_1 + \frac{3}{4}x_3 &= \frac{-3}{4}x_n + \frac{3}{4}x_{n+2} \\
\frac{3}{2}x_1 - 3x_2 + \frac{3}{2}x_3 &= \frac{3}{2}x_n - 3x_{n+1} + \frac{3}{2}x_{n+2}.
\end{align*}
\]

(31a) (31b) (31c)

If we let

\[
\begin{align*}
a &= x_1 - x_n \\
b &= x_2 - x_{n+1} \\
c &= x_3 - x_{n+2}
\end{align*}
\]

(32a) (32b) (32c)

then system (31) becomes

\[
\begin{align*}
\frac{1}{4}a + b + \frac{1}{4}c &= 0 \\
\frac{-3}{4}a + \frac{3}{4}c &= 0 \\
\frac{3}{2}a - 3b + \frac{3}{2}c &= 0
\end{align*}
\]

(33a) (33b) (33c)

which has the unique solution \(a = 0, \ b = 0, \ c = 0\). Hence, the equations

\[
\begin{align*}
x_1 &= x_n \\
x_2 &= x_{n+2} \\
x_3 &= x_{n+2}
\end{align*}
\]

(34) (35) (36)

represent the necessary and sufficient conditions for \(f(t)\) to be periodic over the interval \([s_1, s_n]\) [deBoor (1978)].

One way to implement these conditions would be to augment system (12) with the three additional equations (34) - (36), strongly weighting these latter equations; that would only slightly increase the size of the system. However, our aim is to develop a collection of multivariate splines, and in the higher dimensions, the number of conditions which must be satisfied for periodicity significantly increases. This is due to the fact that the multivariate spline, along with its first and second partial derivatives, must match everywhere.
along the boundaries of the domain (bivariate area, trivariate volume, etc.) considered. Hence, such an augmenting procedure is rejected.

Instead, we will develop an elegant and efficient way of representing and computing the periodic splines. This will be done by determining a spline basis for the univariate, periodic spline. Multivariate, periodic spline bases can then be generated through the use of tensor products. By taking this approach, the size of the system to be solved will be reduced.

Substituting equations (34) - (36) into equation (27) yields, for \( n > 4 \),

\[
\begin{align*}
  f(t) &= \sum_{j=1}^{n-1} x_j \psi_j(t) \\
  \psi_j(t) &= \phi_j(t) + \phi_{j+n-1}(t) \quad j=1, \ldots, 3 \quad (38a) \\
  \psi_j(t) &= \phi_j(t) \quad j=4, \ldots, n-1 \quad (38b)
\end{align*}
\]

For \( n = 3 \)

\[
\begin{align*}
  x_1 &= x_3 = x_5 \\
  x_2 &= x_4
\end{align*}
\]

so that

\[
f(t) = x_1 \psi_1(t) + x_2 \psi_2(t)
\]

where

\[
\begin{align*}
  \psi_1(t) &= \phi_1(t) + \phi_3(t) + \phi_4(t) \quad (41a) \\
  \psi_2(t) &= \phi_2(t) + \phi_4(t) \quad (41b)
\end{align*}
\]

For \( n = 2 \)

\[
\begin{align*}
  x_1 &= x_2 = x_3 = x_4
\end{align*}
\]
so that
\[ f(t) = x_1 \psi_1(t) \] (43)
where
\[ \psi_1(t) = \phi_1(t) + \phi_2(t) + \phi_3(t) + \phi_4(t). \] (44)

Combining these results, we have that
\[ f(t) = \sum_{j=1}^{n-1} x_j \psi_j(t) \] (45)
where
\[ \psi_j(t) = \sum_{i=j}^{n+2} \phi_i(t) \quad j=1, \ldots, n-1 \] (46)

Hence, the set of functions \( \{\psi_j(t), j=1, \ldots, n-1\} \) represents a basis for the \((n-1)\)-dimensional space of all cubic, univariate, periodic splines with evenly spaced nodes. Figure 18 depicts the first three basis functions \( \psi_1(t), \psi_2(t), \psi_3(t) \) for the case \( h=1, n=11 \). (Note their periodicity.) Figure 19 shows a typical univariate, periodic spline fit.

A basis for a bivariate spline that is periodic in both the \( t_1 \) and \( t_2 \) directions is given by
\[ \rho_{ij}(t_1, t_2) = \psi_i(t_1) \psi_j(t_2) \quad i=1, \ldots, n_1-1 \quad j=1, \ldots, n_2-1 \] (47)

A basis for a trivariate spline that is periodic in all three directions is given by
\[ \rho_{ijk}(t_1, t_2, t_3) = \psi_i(t_1) \psi_j(t_2) \psi_k(t_3) \quad i=1, \ldots, n_1-1 \quad j=1, \ldots, n_2-1 \quad k=1, \ldots, n_3-1 \] (48)

If we are only concerned with periodicity in one direction, e.g., the \( t_2 \) direction, then appropriate bicubic and tricubic spline bases can be generated via
\[ \rho_{ij}(t_1, t_2) = \phi_i(t_1) \psi_j(t_2) \quad \text{for } i=1, \ldots, n_1+2 \quad j=1, \ldots, n_2-1 \]  

(49)

and

\[ \rho_{ijk}(t_1, t_2, t_3) = \phi_i(t_1) \psi_j(t_2) \phi_k(t_3) \quad \text{for } i=1, \ldots, n_1+2 \quad j=1, \ldots, n_2-1 \quad k=1, \ldots, n_3+2 \]  

(50)

Thus, using this technique, multivariate splines which are periodic along one or more arbitrary directions can be produced.

The elegant part of this construction is that the periodic framework now fits neatly within the regular spline framework. Hence, the periodic option will require no additional computer storage. Furthermore, the same computer routine that evaluates the regular spline can be used to evaluate the periodic versions. This is made possible by re-representing the periodic spline in terms of the regular spline basis. For example, in the univariate case, once the \( n-1 \) coefficients have been obtained, we can set

\[ x_n = x_1 \]  

(51a)

\[ x_{n+1} = x_2 \]  

(51b)

\[ x_{n+2} = x_3 \]  

(51c)

then represent the periodic spline via equation (27). In the bivariate case, once the \((n_1-1) \times (n_2-1)\) coefficients have been obtained, we can set

\[ x_{i,n_2} = x_{i,1} \]  

(52a)

\[ x_{i,n_2+1} = x_{i,2} \quad i=1, \ldots, n_1-1 \]  

(52b)

\[ x_{i,n_2+2} = x_{i,3} \]  

(52c)

and

\[ x_{n_1,j} = x_{i,j} \]  

(53a)

\[ x_{n_1+1,j} = x_{i,j} \quad j=1, \ldots, n_2+2 \]  

(53b)

\[ x_{n_1+2,j} = x_{i,j} \]  

(53c)
then represent the periodic spline with equation (10). In the trivariate case, once the \((n_1-1) \times (n_2-1) \times (n_3-1)\) coefficients have been obtained, we can set

\[
x_{i,j,n_3} = x_{i,j,1} \quad (54a)
\]
\[
x_{i,j,n_3+1} = x_{i,j,2} \quad i=1, \ldots, n_1-1 \quad (54b)
\]
\[
x_{i,j,n_3+2} = x_{i,j,3} \quad j=1, \ldots, n_2-1 \quad (54c)
\]

and

\[
x_{i,n_2,k} = x_{i,1,k} \quad i=1, \ldots, n_1-1 \quad (55a)
\]
\[
x_{i,n_2+1,k} = x_{i,2,k} \quad k=1, \ldots, n_3+2 \quad (55b)
\]
\[
x_{i,n_2+2,k} = x_{i,3,k} \quad (55c)
\]

and

\[
x_{n_1,j,k} = x_{1,j,k} \quad j=1, \ldots, n_2+2 \quad (56a)
\]
\[
x_{n_1+1,j,k} = x_{2,j,k} \quad k=1, \ldots, n_3+2 \quad (56b)
\]
\[
x_{n_1+2,j,k} = x_{3,j,k} \quad (56c)
\]

then represent the periodic spline through equation (11). If periodicity had been enforced in only one direction, e.g. the \(t_1\) direction, in the two previous examples, then steps (52) and (53) would be replaced with only step (53) and steps (54)-(56) would be replaced with only step (56).
7. "CURVATURE" MATRICES

One physically important aspect of the solution is that of curvature. Hence, we shall proceed to develop a performance index that is a measure of the "curvature" of the spline surface. We use quotes here because what we will actually do is construct a performance index which measures the Frobenius norm of the second derivative of the spline over the domain of interest. This approximately measures the curvature over that domain for small curvatures.

In general, we will consider quantities of the form

\[ J = \int_{a_1}^{b_1} \int_{a_2}^{b_2} ... \int_{a_M}^{b_M} h^{4-M} ||\nabla^2 f(t_1, t_2, \ldots, t_M)||^2 dt_1 dt_2 ... dt_M \] (57)

where \( \nabla^2 f(t_1, t_2, \ldots, t_M) \) is the second derivative (second gradient) of the spline, \( || \cdot || \) is the Frobenius norm, and \( M \) is the number of variates.

The form (57) reduces to

\[ J = x^T C x \] (58)

where \( x \) is the vector of spline coefficients and \( C \) is a positive semidefinite, "curvature" matrix. The factor \( h^{4-M} \), where \( h \) is the node spacing, is simply a scale factor which has no effect on the minimization of \( J \). However, it does serve an important purpose; its presence results in the curvature matrix \( C \) being a function of the grid size only, and not of the grid spacing as well. Since \( C \) is only positive semidefinite, an epsilon technique will be used to produce the positive definite matrix \( Q \) required for the transformation (23). The matrix \( Q \) will be given by

\[ Q = C + \epsilon I \] (59)

where \( I \) is the identity matrix and \( \epsilon \) is a small number, large enough only for the computer at hand to identify \( Q \) as being positive definite. Thus the performance index \( P \) will be a measure of the weighted sum of the "curvature" and the length of the vector of spline coefficients. Since \( \epsilon \) will be extremely small, essentially only the curvature will be measured.
7.1 UNIVARIATE CURVATURE MATRICES

In the univariate, nonperiodic case,

\[ f(t) = \sum_{j=1}^{n+2} x_j \phi_j(t). \]  

(60)

The second derivative of \( f(t) \) is given by

\[ \frac{d^2f(t)}{dt^2} = \sum_{j=1}^{n+2} x_j \phi_j''(t) \]  

(61)

so that

\[ J = \int_{a=s}^{b=s} h^3 \left[ \frac{d^2f(t)}{dt^2} \right]^2 \, dt \]  

(62a)

\[ = \int_{a}^{b} h^3 \left[ \sum_{j=1}^{n+2} x_j \phi_j''(t) \right]^2 \, dt \]  

(62b)

\[ = \int_{a}^{b} h^3 \left[ \sum_{i=1}^{n+2} x_i \phi_i''(t) \right] \left[ \sum_{j=1}^{n+2} x_j \phi_j''(t) \right] \, dt \]  

(62c)

\[ = \sum_{i=1}^{n+2} \sum_{j=1}^{n+2} x_i \left[ h^3 \int_{a}^{b} \phi_i'(t) \phi_j'(t) \, dt \right] x_j \]  

(62d)

\[ = \frac{\mathbf{x}^T \mathbf{Wx}}{x} \]  

(62e)
where

\[
W(n) = \begin{pmatrix} w_{ij}(n) \end{pmatrix} \quad i=1, \ldots, n+2
\]

\[
w_{ij}(n) = h^3 \int_a^b \phi_i'(t) \phi_j'(t) \, dt.
\]
\[
\int_a^b h^3 \left[ \sum_{i=1}^{n-1} x_i \psi_i''(t) \right] \left[ \sum_{j=1}^{n-1} x_j \psi_j''(t) \right] dt
\]  
(67c)
\[
= \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} \sum_{i=1}^{n-1} \sum_{j=1}^{n-1} x_i \left[ h^3 \int_a^b \psi_i''(t) \psi_j''(t) dt \right] x_j
\]  
(67d)
\[
= x^T W x
\]  
(67e)

where
\[
W^P(n) = \left( w^P_{i,j}(n) \right)_{i=1, \ldots, n-1} \quad k=1, \ldots, n-1
\]  
(68)

with
\[
w^P_{i,j} = h^3 \int_a^b \psi_i''(t) \psi_j''(t) dt.
\]  
(69)

The superscript \( P \) denotes periodicity.

The weighting matrices \( W^P(n), n=2, 3, \ldots \) were computed as in the nonperiodic case, integrating (69) analytically and establishing a pattern for the generation of \( W^P(n) \) for arbitrary \( n \). These weighting matrices are given in appendix B.

In both of the above cases, the curvature matrix \( C \) is identical to the weighting matrix:
\[
C(n) = W(n)
\]  
(70)

for a nonperiodic spline and
\[
C(n) = W^P(n)
\]  
(71)

for a periodic spline.

Figure 20 shows an application of the univariate, minimum-curvature spline which has resulted in an improved NAVOCEANO product. A gross estimate of the north wall of the Gulf Stream is obtained from a gridded, partially-
observed, satellite infrared image. By representing the north wall as a parametric form consisting of two univariate, minimum-curvature splines, a smoothed, gap-filled estimate of the wall can be obtained.

7.2 BIVARIATE CURVATURE MATRICES

In the bivariate, nonperiodic case,

\[
f(t_1, t_2) = \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{j_1 j_2} \phi_{j_1}^*(t_1) \phi_{j_2}^*(t_2).
\]  

(72)

The second partials of \(f(t_1, t_2)\) are given by

\[
\frac{\partial^2 f}{\partial t_1^2} = \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{j_1 j_2} \phi_{j_1}^{**}(t_1) \phi_{j_2}(t_2)
\]  

(73a)

\[
\frac{\partial^2 f}{\partial t_1 \partial t_2} = \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{j_1 j_2} \phi_{j_1}^{**(t_1)} \phi_{j_2}^{*}(t_2)
\]  

(73b)

\[
\frac{\partial^2 f}{\partial t_2^2} = \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{j_1 j_2} \phi_{j_1}^{**}(t_1) \phi_{j_2}^{**}(t_2)
\]  

(73c)

So that

\[
J = \int_{a_2}^{b_2} \int_{a_1}^{b_1} h^2 \left[ \left( \frac{\partial^2 f}{\partial t_1^2} \right)^2 + 2 \left( \frac{\partial^2 f}{\partial t_1 \partial t_2} \right)^2 + \left( \frac{\partial^2 f}{\partial t_2^2} \right)^2 \right] dt_1 dt_2
\]  

(74a)

\[
= \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{j_1 j_2} \left[ h^3 \int_{a_1}^{b_1} \phi_{j_1}^{**}(t_1) \phi_{j_2}^{**}(t_1) dt_1 \int_{a_2}^{b_2} \phi_{j_2}^{*}(t_2) \phi_{j_2}^{*}(t_2) dt_2 \right.
\]

\[
+ h \int_{a_1}^{b_1} \phi_{j_1}^{**}(t_1) \phi_{j_2}^{*}(t_1) dt_1 \int_{a_2}^{b_2} \phi_{j_2}^{*}(t_2) \phi_{j_2}^{**}(t_2) dt_2
\]

\[
+ 2h \int_{a_1}^{b_1} \phi_{j_1}^{*}(t_1) \phi_{j_2}^{*}(t_1) dt_1 \int_{a_2}^{b_2} \phi_{j_2}^{**}(t_2) \phi_{j_2}^{*}(t_2) dt_2
\]  

23
\begin{align*}
+ \frac{1}{h} \int_{a_1}^{b_1} \phi_{i_1}(t_1) \phi_{j_1}(t_1) dt_1 h^3 \int_{a_2}^{b_2} \phi_{i_2}''(t_2) \phi_{j_2}''(t_2) dt_2 \right] x_{j_1 j_2} \tag{74b}
\end{align*}

\begin{align*}
= \sum_{i_1=1}^{n_1+2} \sum_{i_2=1}^{n_2+2} \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2+2} x_{i_1 j_2} \left[ w_{i_1 j_1} (n_1) z_{i_2 j_2} (n_2) + 2 y_{i_1 j_1} (n_1) y_{i_2 j_2} (n_2) \\
+ z_{i_1 j_1} (n_1) w_{i_2 j_2} (n_2) \right] x_{j_1 j_2} \tag{74c}
\end{align*}

where \( w_{i,j}(n) \) is defined as in (64) and

\begin{align*}
y_{i,j}(n) &= h \int_a^b \phi_i'(t) \phi_j'(t) dt \\
&= \int_{a_1}^{b_1} \phi_{i_1}(t) \phi_{j_1}(t) dt \\
&= \int_{a_2}^{b_2} \phi_{i_2}(t) \phi_{j_2}(t) dt \tag{75}
\end{align*}

\begin{align*}
z_{i,j}(n) &= \frac{1}{h} \int_a^b \phi_i(t) \phi_j(t) dt \\
&= \int_{a_1}^{b_1} \phi_{i_1}(t) \phi_{j_1}(t) dt \\
&= \int_{a_2}^{b_2} \phi_{i_2}(t) \phi_{j_2}(t) dt \tag{76}
\end{align*}

The weighting matrices

\begin{align*}
Y(n) &= \left( y_{i,j}(n) \right) \\
&= \left( \begin{array}{cccc}
\vdots & \vdots & \vdots & \vdots \\
i=1 & \ldots & n+2 & \vdots \\
\end{array} \right) \tag{77}
\end{align*}

and

\begin{align*}
Z(n) &= \left( z_{i,j}(n) \right) \\
&= \left( \begin{array}{cccc}
\vdots & \vdots & \vdots & \vdots \\
i=1 & \ldots & n+2 & \vdots \\
\end{array} \right) \tag{78}
\end{align*}

were computed by integrating (75) and (76) analytically and are given in appendices C and D, respectively.

Setting

\begin{align*}
c_{k,1} (n_1, n_2) &= w_{i_1 j_1} (n_1) z_{i_2 j_2} (n_2) + 2 y_{i_1 j_1} (n_1) y_{i_2 j_2} (n_2) \\
&+ z_{i_1 j_1} (n_1) w_{i_2 j_2} (n_2) \tag{79}
\end{align*}

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where

\[ k = i_1 + (i_2 - 1)(n_2 + 2) \quad i_1 = 1, \ldots, n_1 + 2 \]  \hfill (80a)

\[ l = j_1 + (j_2 - 1)(n_2 + 2) \quad j_1 = 1, \ldots, n_1 + 2 \]  \hfill (80b)

and

\[ N = (n_1 + 2)(n_2 + 2) \]  \hfill (81)

we have

\[ J = \sum_{k=1}^{N} \sum_{l=1}^{N} x_k c_{k,l}(n_1, n_2)x_l \]  \hfill (82a)

\[ = \mathbf{x}^T C(n_1, n_2) \mathbf{x}. \]  \hfill (82b)

Here, the curvature matrix \( C(n_1, n_2) \) is defined via (79) and the vector \( \mathbf{x} \) contains the spline coefficients stored columnwise.

Figure 21 displays an application of the bivariate, minimum-curvature spline. This spline was applied to nineteen data points identifying Eddy F in the Gulf of Mexico. The figure depicts the resulting minimum-curvature surface and its contour.

In the bivariate, periodic case,

\[ f(t_1, t_2) = \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} x_j \psi_j(t_1) \psi_j(t_2). \]  \hfill (83)

The second partials of \( f(t_1, t_2) \) are given by

\[ \frac{\partial^2 f}{\partial t_1^2} = \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} x_j \psi_j(t_1) \psi_j(t_2) \]  \hfill (84a)
\[
\frac{\partial^2 f}{\partial t_1 \partial t_2} = \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} x_{j_1 j_2} j_1^j(t_1) j_2^j(t_2)
\]

(84b)

\[
\frac{\partial^2 f}{\partial t_2^2} = -\sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} x_{j_1 j_2} j_1^j(t_1) j_2^j(t_2)
\]

(84c)

so that

\[
J = \int_{a_1}^{b_1} \int_{a_2}^{b_2} h^2 \left[ \left( \frac{\partial^2 f}{\partial t_1^2} \right)^2 + 2 \left( \frac{\partial^2 f}{\partial t_1 \partial t_2} \right)^2 + \left( \frac{\partial^2 f}{\partial t_2^2} \right)^2 \right] dt_1 dt_2
\]

(85a)

\[
- \sum_{i_1=1}^{n_1-1} \sum_{i_2=1}^{n_2-1} \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2-1} x_{i_1 i_2} \left[ h^3 \int_{a_1}^{b_1} \psi_{-1}^i(t_1) \psi_{-1}^i(t_1) dt_1 \int_{a_2}^{b_2} \psi_{-2}^i(t_2) dt_2 \right]
\]

(85b)

\[
+ \frac{1}{h} \int_{a_1}^{b_1} \psi_{-1}^i(t_1) \psi_{-1}^i(t_1) dt_1 h^3 \int_{a_2}^{b_2} \psi_{-2}^i(t_2) \psi_{-2}^i(t_2) dt_2 \right] x_{i_1 i_2}
\]

(85c)

\[
+ 2y_{i_1 i_2} (n_1) y_{i_1 i_2}^p (n_2) + z_{i_1 i_2} (n_1) w_{i_1 i_2}^p (n_2) \right] x_{i_1 i_2}
\]
where \( w_{ij}^P(n) \) is defined as in (69) and

\[
y_{ij}^P(n) = \int_a^b \psi_i(t) \psi_j(t) \, dt \quad i=1, \ldots, n-1
\]

\[
z_{ij}^P(n) = \frac{1}{h} \int_a^b \psi_i(t) \psi_j(t) \, dt \quad j=1, \ldots, n-1
\]

The weighting matrices

\[
y^P(n) = \begin{pmatrix} y_{ij}^P(n) \end{pmatrix} \quad i=1, \ldots, n-1
\]

\[
z^P(n) = \begin{pmatrix} z_{ij}^P(n) \end{pmatrix} \quad j=1, \ldots, n-1
\]

were computed by integrating (86) and (87) analytically and are given in appendices E and F, respectively.

Setting

\[
c_{k,l}^P(n_1, n_2) = w_{i_1 j_1}^P(n_1) z_{i_2 j_2}^P(n_2) + 2y_{i_1 j_1}^P(n_1) y_{i_2 j_2}^P(n_2) + z_{i_1 j_1}^P(n_1) z_{i_2 j_2}^P(n_2)
\]

where

\[
k = i_1 + (i_2-1)(n_1-1)
\]

\[
l = j_1 + (j_2-1)(n_1-1)
\]

\[
i_1, i_2, j_1, j_2 = 1, \ldots, n_1 - 1
\]

\[
i_1, i_2, j_1, j_2 = 1, \ldots, n_2 - 1
\]
and

\[ N = (n_1 - 1)(n_2 - 1) \]  \hspace{1cm} (92)

we have

\[ J = \sum_{k=1}^{N} \sum_{l=1}^{N} x_k c_{k, l} (n_1, n_2) x_l \]  \hspace{1cm} (93a)

\[ = \vec{x}^T C(n_1, n_2) \vec{x} \]  \hspace{1cm} (93b)

with the curvature matrix \( C(n_1, n_2) \) being defined by (90).

If periodicity is desired only in the \( t_1 \) direction, then

\[ f(t_1, t_2) = \sum_{j_1=1}^{n_1-1} \sum_{j_2=1}^{n_2+2} x_{j_1} j_1 \psi_{j_1} (t_1) \phi_{j_2} (t_2) \]  \hspace{1cm} (94)

and the curvature matrix \( C \) is obtained from

\[ c_{k, l} (n_1, n_2) = w_{i_1 j_1}^P (n_1) z_{i_2 j_2}^P (n_2) + 2 v_{i_1 j_1}^P (n_1) y_{i_2 j_2}^P (n_2) \]

\[ + z_{i_1 j_1}^P (n_1) w_{i_2 j_2}^P (n_2) \]  \hspace{1cm} (95)

where

\[ k = i_1 + (i_2 - 1)(n_1 - 1) \hspace{1cm} i_1 = 1, \ldots, n_1 - 1 \]  \hspace{1cm} (96a)

\[ i_2 = 1, \ldots, n_2 + 2 \]

\[ l = j_1 + (j_2 - 1)(n_1 - 1) \hspace{1cm} j_1 = 1, \ldots, n_1 - 1 \]  \hspace{1cm} (96b)

\[ j_2 = 1, \ldots, n_2 + 2 \]
If periodicity is desired only in the $t_2$ direction, then

$$f(t_1, t_2) = \sum_{j_1=1}^{n_1+2} \sum_{j_2=1}^{n_2-1} x_{j_1 j_2} \phi_{j_1}(t_1) \psi_{j_2}(t_2)$$

(97)

and the curvature matrix $C$ is obtained from

$$c_{k, l}^{(n_1, n_2)} = w_{i_1 j_1}^{(n_1)} z_{i_2 j_2}^{(n_2)} + 2y_{i_1 j_1}^{(n_1)} y_{i_2 j_2}^{(n_2)} + z_{i_1 j_1}^{(n_1)} w_{i_2 j_2}^{(n_2)}$$

(98)

where

$$k = i_1 + (i_2 - 1)(n_1 + 2) \quad i_1 = 1, \ldots, n_1 + 2$$

(99a)

$$l = j_1 + (j_2 - 1)(n_1 + 2) \quad j_1 = 1, \ldots, n_1 + 2$$

(99b)

### 7.3 TRIVARIATE CURVATURE MATRICES

In the trivariate case,

$$f(t_1, t_2, t_3) = \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \sum_{j_3=1}^{d_3} x_{j_1 j_2 j_3} \xi_{j_1}(t_1) \xi_{j_2}(t_2) \xi_{j_3}(t_3)$$

(100)

where

$$\xi_{j_1}(t_1) = \phi_{j_1}(t_1) \text{ for nonperiodicity in the } t_1 \text{ direction}$$

(101a)

$$\xi_{j_1}(t_1) = \psi_{j_1}(t_1) \text{ for periodicity in the } t_1 \text{ direction}$$

(101b)

and

$$d_1 = n_1 + 2 \text{ for nonperiodicity in the } t_1 \text{ direction}$$

(102a)

$$d_1 = n_1 - 1 \text{ for periodicity in the } t_1 \text{ direction}.$$
Taking the second partials of \( f(t_1, t_2, t_3) \) and proceeding as in the two previous sections,

\[
J = \int_{a_3}^{b_3} \int_{a_2}^{b_2} \int_{a_1}^{b_1} h \left[ \frac{\partial^2 f}{\partial t_1^2} + \frac{\partial^2 f}{\partial t_2^2} + \frac{\partial^2 f}{\partial t_3^2} \right] dt_1 dt_2 dt_3 \tag{103a}
\]

\[
= \sum_{k=1}^{N} \sum_{l=1}^{N} x_k c_{k,l} (n_1, n_2, n_3) x_l \tag{103b}
\]

\[
= \bar{x}^T C(n_1, n_2, n_3) \bar{x} \tag{103c}
\]

where the curvature matrix \( C(n_1, n_2, n_3) \) is given by

\[
c_{k,l} (n_1, n_2, n_3) = w_{1i1}^K (n_1) z_{12j2}^K (n_1) y_{13j3}^K (n_2) + z_{1i1}^K (n_1) w_{12j2}^K (n_2) y_{13j3}^K (n_3) + \]

\[
+ 2 y_{1i1}^K (n_1) y_{12j2}^K (n_2) y_{13j3}^K (n_3) \tag{104}
\]

with

\[
K^i = "\text{blank}" \text{ for nonperiodicity in the } t_i \text{ direction} \tag{105a}
\]

\[
K^i = "p" \text{ for periodicity in the } t_i \text{ direction} \tag{105b}
\]

\[
i_1 = 1, \ldots, d_1 \]

\[
k = i_1 + (i_2 - 1)d_1 + (i_3 - 1)d_1d_2 \quad i_2 = 1, \ldots, d_2 \quad i_3 = 1, \ldots, d_3 \tag{106a}
\]
\[ l = j_1 + (j_2 - 1)d_1 + (j_3 - 1)d_1d_2 \quad j_1 = 1, \ldots, d_1 \]
and
\[ j_3 = 1, \ldots, d_3 \]
\[ N = d_1d_2d_3. \]

The weighting matrices \( w_{ij}(n), y_{ij}(n), z_{ij}(n) \) are defined as in (64), (77), (78), (69), (86), (87), respectively.

For example, if periodicity is desired only in the \( t_2 \) direction, equation (104) becomes
\[
c_{k,l}(n_1, n_2, n_3) = w_{1j_1}(n_1)z_{2j_2}(n_2)z_{3j_3}(n_3) + z_{1j_1}(n_1)w_{2j_2}(n_2)z_{3j_3}(n_3)
\]
\[+ z_{1j_1}(n_1)w_{2j_2}(n_2)y_{3j_3}(n_3) + 2y_{1j_1}(n_1)y_{2j_2}(n_2)z_{3j_3}(n_3)\]
\[+ 2z_{1j_1}(n_1)y_{2j_2}(n_2)y_{3j_3}(n_3). \]

7.4 QUADRIVARIATE CURVATURE MATRICES

In the quadrivariate case,
\[
f(t_1, t_2, t_3, t_4) = \sum_{j_1=1}^{d_1} \sum_{j_2=1}^{d_2} \sum_{j_3=1}^{d_3} \sum_{j_4=1}^{d_4} \xi_{j_1j_2j_3j_4} \xi_{j_1}(t_1) \xi_{j_2}(t_2) \xi_{j_3}(t_3) \xi_{j_4}(t_4) \]
(109)

with \( \xi_{j_i}(t_i) \) and \( d_i \), \( i=1,2,3,4 \) defined as in (101) and (102). Taking the second partials of \( f(t_1, t_2, t_3, t_4) \) and proceeding as before,
\[
J = \int_{a_4}^{b_4} \int_{a_3}^{b_3} \int_{a_2}^{b_2} \int_{a_1}^{b_1} \left[ \left( \frac{\partial^2 f}{\partial t_1^2} \right)^2 + \left( \frac{\partial^2 f}{\partial t_2^2} \right)^2 + \left( \frac{\partial^2 f}{\partial t_3^2} \right)^2 + \left( \frac{\partial^2 f}{\partial t_4^2} \right)^2 \right]
\]
\[+ 2 \left( \frac{\partial^2 f}{\partial t_1 \partial t_2} \right)^2 + 2 \left( \frac{\partial^2 f}{\partial t_1 \partial t_3} \right)^2 \]
31
+ 2 \left( \frac{\partial^2 f}{\partial t_3 \partial t_4} \right)^2 dt_1 dt_2 dt_3 dt_4
\right)
\right]
= \sum_{k=1}^{N} \sum_{l=1}^{N} x_k c_{k,l} (n_1, n_2, n_3, n_4) x_l
\right)
= \bar{x}^T C(n_1, n_2, n_3, n_4) \bar{x}
\right)
\right)
(110a)
(110b)
(110c)

where the curvature matrix $C(n_1, n_2, n_3, n_4)$ is given by

$$c_{k,l} (n_1, n_2, n_3, n_4) = w_{11}^k (n_1) z_{12}^k (n_2) z_{13}^k (n_3) z_{14}^k (n_4)
\right)
+ w_{12}^k (n_1) z_{13}^k (n_2) z_{14}^k (n_3) z_{14}^k (n_4)
\right)
+ w_{13}^k (n_1) z_{14}^k (n_2) z_{14}^k (n_3) w_{14}^k (n_4)
\right)
+ 2 y_{11}^k (n_1) z_{12}^k (n_2) y_{13}^k (n_3) z_{14}^k (n_4)
\right)
+ 2 y_{12}^k (n_1) z_{13}^k (n_2) y_{14}^k (n_3) z_{14}^k (n_4)
\right)
+ 2 y_{13}^k (n_1) z_{14}^k (n_2) y_{14}^k (n_3) z_{14}^k (n_4)
\right)
+ 2 z_{11}^k (n_1) y_{12}^k (n_2) y_{13}^k (n_3) z_{14}^k (n_4)
\right)
+ 2 z_{12}^k (n_1) y_{13}^k (n_2) y_{13}^k (n_3) y_{14}^k (n_4)
\right)
+ 2 z_{13}^k (n_1) y_{14}^k (n_2) y_{14}^k (n_3) y_{14}^k (n_4)
\right)
(111)
with

\[ K_i^i = \text{"blank" for nonperiodicity in the } t_1 \text{ direction} \]  
\[ K_i^i = \text{"P" for periodicity in the } t_1 \text{ direction} \]

\[ k = i_1 + (i_2-1)d_1 + (i_3-1)d_1d_2 + (i_4-1)d_1d_2d_3 \]  
\[ i_1=1, \ldots, d_1 \]  
\[ i_2=1, \ldots, d_2 \]  
\[ i_3=1, \ldots, d_3 \]  
\[ i_4=1, \ldots, d_4 \]  

\[ l = j_1 + (j_2-1)d_1 + (j_3-1)d_1d_2 + (j_4-1)d_1d_2d_3 \]  
\[ j_1=1, \ldots, d_1 \]  
\[ j_2=1, \ldots, d_2 \]  
\[ j_3=1, \ldots, d_3 \]  
\[ j_4=1, \ldots, d_4 \]  

and

\[ N = d_1d_2d_3d_4. \]  

(114)
8. SUMMARY AND CONCLUDING REMARKS

A collection of multivariate, minimum-curvature splines for randomly spaced data has been developed. The splines are represented as a linear combination of spline basis functions having evenly spaced nodes. This parameterization results in a linear system of the form

$$AX = \hat{b}$$

(115)

where the $m \times N$ matrix $A$ contains the spline basis functions evaluated at the appropriate points in time or space, the vector $\hat{x}$ contains the spline coefficients to be solved for, and the vector $\hat{b}$ contains the dependent values of the data. A reference frame transformation is then performed to yield

$$A(L^{-1})T_{x} = \hat{b}.$$  \hspace{1cm} (116)

The matrix $L$ is the lower triangular Cholesky factor of a positive definite matrix $Q$ which essentially is a measure of the curvature of the spline surface. The matrix $Q$ is given by

$$Q = C + \epsilon I$$

(117)

where $C$ is the so-called "curvature" matrix, $I$ is the identity matrix, and $\epsilon$ is a small number, large enough only for the computer at hand to identify $Q$ as being positive definite. The new system (116) is then solved using a singular value decomposition in conjunction with pseudoinversion. Finally, the spline coefficients are computed via

$$\hat{x} = (L^{-1})T_{y}.$$ \hspace{1cm} (118)

The end result of this procedure is a spline solution having the property of "minimum curvature."

Several pertinent remarks should be made in closing. First, there is no need to have the entire matrix $[A:\hat{b}]$ in computer storage at one time. A sequential Householder procedure [Lawson and Hanson (1974)] can be employed to convert $[A:\hat{b}]$ to an upper triangular form; only $m_{1}$ rows of data need to be operated on at a time, requiring at most $m_{1} + N + 1$ rows of storage. The integers $m_{1}$ can be as small as 1, which permits the greatest economy of storage. The resulting least-squares problem

$$\begin{bmatrix} R \\ 0 \end{bmatrix} \hat{x} = \begin{bmatrix} d \\ e \end{bmatrix}$$  \hspace{1cm} (119)
where $R$ is upper triangular, is equivalent to (115) in that it has the same set of solutions and the same minimal residual norm. Furthermore, the matrix $R$ has the same set of singular values as the matrix $A$. The $N \times N$ reference frame transformation $(L^{-1})^T$ can then be applied to the $R$ matrix to yield

$$R(L^{-1})^T_y = \tilde{d}$$

(120)

and the SVD can be applied to this result. Since the matrix $L^{-1}$ is lower triangular, it can be read into the lower triangular portion of $R$ (plus one additional row of storage) and a packed multiply can be performed.

Second, the curvature matrix $C$ is easily computed using the weighting matrices $W(n)$, $Y(n)$, $Z(n)$ and/or $W^P(n)$, $Y^P(n)$, $Z^P(n)$.

Third, since $L$ is lower triangular, $L^{-1}$ can be computed strictly through back substitutions.

Fourth, the spline fit is controlled through specification of the nodal spacing and the signal-to-noise ratio. A good rule of thumb is to have the nodal spacing in each direction equal to one-fourth of the shortest wavelength present in that direction. This, in part, must be done through appropriate scaling of the independent variables of the data.

Finally, if an $M$-variate, minimum-curvature spline is applied to $M+1$ randomly spaced data points, an $M$-dimensional hyperplane is obtained. While this last observation has little practical application, it does nicely illustrate the minimum-curvature property of these multivariate splines.
REFERENCES


Figure 8: Subset of Bivariate Basis
Figure 10. Subset of Bivariate Basis
Figure 15. Subset of Bivariate Basis
Figure 18. Three Periodic Basis Functions
Figure 21. Gulf of Mexico Eddy F
APPENDIX A

The Weighting Matrices W(n)
The weighting matrices $W(n)$, $n=2, 3, \ldots$ defined via

$$W(n) = \begin{pmatrix} w_{ij}(n) \end{pmatrix} \quad i=1, \ldots, n+2$$
$$j=1, \ldots, n+2$$  \hspace{1cm} (A-1)$$

$$w_{ij}(n) = h^3 \int_a^b \phi_i''(t) \phi_j''(t) dt$$  \hspace{1cm} (A-2)$$

are given below.

$$W(2) = \frac{3}{8} \begin{bmatrix} 2 & -3 & 0 & 1 \\ -3 & 6 & -3 & 0 \\ 0 & -3 & 6 & -3 \\ 1 & 0 & -3 & 2 \end{bmatrix}$$  \hspace{1cm} (A-3)$$

$$W(3) = \frac{3}{8} \begin{bmatrix} 2 & -3 & 0 & 1 & 0 \\ -3 & 8 & -6 & 0 & 1 \\ 0 & -6 & 12 & -6 & 0 \\ 1 & 0 & -6 & 8 & -3 \\ 0 & 1 & 0 & -3 & 2 \end{bmatrix}$$  \hspace{1cm} (A-4)$$

$$W(4) = \frac{3}{8} \begin{bmatrix} 2 & -3 & 0 & 1 & 0 & 0 \\ -3 & 8 & -6 & 0 & 1 & 0 \\ 0 & -6 & 14 & -9 & 0 & 1 \\ 1 & 0 & -9 & 14 & -6 & 0 \\ 0 & 1 & 0 & -6 & 8 & -3 \\ 0 & 0 & 1 & 0 & -3 & 2 \end{bmatrix}$$  \hspace{1cm} (A-5)$$
where there are $n-4$ 16's on the main diagonal.
APPENDIX B

The Weighting Matrices $W^p(n)$
The weighting matrices $W^p_{\cdot}(n)$, $n=2$, 3, \ldots defined via

$$W^p_{\cdot}(n) = \begin{pmatrix} w^p_{ij}(n) \end{pmatrix}_{i=1, \ldots, n-1 \atop j=1, \ldots, n-1} \quad (B-1)$$

$$w^p_{ij}(n) = h^3 \int_a^b \psi_1^{(i)}(t) \psi_j^{(i)}(t) dt \quad (B-2)$$

are given below.

$$W^p_{\cdot}(2) = \frac{3}{8} \begin{bmatrix} 0 \end{bmatrix} \quad (B-3)$$

$$W^p_{\cdot}(3) = \frac{3}{8} \begin{bmatrix} 16 & -16 \\ -16 & 16 \end{bmatrix} \quad (B-4)$$

$$W^p_{\cdot}(4) = \frac{3}{8} \begin{bmatrix} 18 & -9 & -9 \\ -9 & 18 & -9 \\ -9 & -9 & 18 \end{bmatrix} \quad (B-5)$$

$$W^p_{\cdot}(5) = \frac{3}{8} \begin{bmatrix} 16 & -8 & 0 & -8 \\ -8 & 16 & -8 & 0 \\ 0 & -8 & 16 & -8 \\ -8 & 0 & -8 & 16 \end{bmatrix} \quad (B-6)$$

$$W^p_{\cdot}(6) = \frac{3}{8} \begin{bmatrix} 16 & -9 & 1 & 1 & -9 \\ -9 & 16 & -9 & 1 & 1 \\ 1 & -9 & 16 & -9 & 1 \\ 1 & 1 & -9 & 16 & -9 \\ -9 & 1 & 1 & -9 & 16 \end{bmatrix} \quad (B-7)$$
\[
W^P(7) = \frac{3}{8} \begin{bmatrix}
16 & -9 & 0 & 2 & 0 & -9 \\
-9 & 16 & -9 & 0 & 2 & 0 \\
0 & -9 & 16 & -9 & 0 & 2 \\
2 & 0 & -9 & 16 & -9 & 0 \\
0 & 2 & 0 & -9 & 16 & -9 \\
-9 & 0 & 2 & 0 & -9 & 16
\end{bmatrix}
\]

(B-8)

\[
W^P(8) = \frac{3}{8} \begin{bmatrix}
16 & -9 & 0 & 1 & 1 & 0 & -9 \\
-9 & 16 & -9 & 0 & 1 & 1 & 0 \\
0 & -9 & 16 & -9 & 0 & 1 & 1 \\
1 & 0 & -9 & 16 & -9 & 0 & 1 \\
1 & 1 & 0 & -9 & 16 & -9 & 0 \\
0 & 1 & 1 & 0 & -9 & 16 & -9 \\
-9 & 0 & 1 & 1 & 0 & -9 & 16
\end{bmatrix}
\]

(B-9)

\[
W^P(9) = \frac{3}{8} \begin{bmatrix}
16 & -9 & 0 & 1 & 0 & 1 & 0 & -9 \\
-9 & 16 & -9 & 0 & 1 & 0 & 1 & 0 \\
0 & -9 & 16 & -9 & 0 & 1 & 0 & 1 \\
1 & 0 & -9 & 16 & -9 & 0 & 1 & 0 \\
0 & 1 & 0 & -9 & 16 & -9 & 0 & 1 \\
1 & 0 & 1 & 0 & -9 & 16 & -9 & 0 \\
0 & 1 & 0 & 1 & 0 & -9 & 16 & -9 \\
-9 & 0 & 1 & 0 & 1 & 0 & -9 & 16
\end{bmatrix}
\]

(B-10)
\[ w^p(n) = \begin{cases} \frac{3}{8} & \text{if } n \geq 9 \\ \end{cases} \]

\[
\begin{bmatrix}
16 & -9 & 0 & 1 & \ldots & \ldots & 1 & 0 & -9 \\
-9 & 16 & -9 & 0 & 1 & \ldots & \ldots & 1 & 0 \\
0 & -9 & 16 & -9 & 0 & \ldots & \ldots & 1 & 0 \\
1 & 0 & -9 & 16 & \ldots & \ldots & \ldots & \ldots & \ldots \\
\end{bmatrix}
\]

n-8 minor diagonals of zeroes (B-11)
APPENDIX C

The Weighting Matrices $Y(n)$
The weighting matrices $Y(n)$, $n=2, 3, \ldots$ defined via

$$Y(n) = \begin{pmatrix} y_{ij}(n) \end{pmatrix}_{i=1, \ldots, n+2, \ j=1, \ldots, n+2} \quad (C-1)$$

$$y_{ij} = \int_a^b \phi_i^R(t) \phi_j^R(t) dt \quad (C-2)$$

are given below.

$$Y(2) = \frac{3}{160} \begin{bmatrix} 6 & 7 & -12 & -1 \\ 7 & 34 & -29 & -12 \\ -12 & -29 & 34 & 7 \\ -1 & -12 & 7 & 6 \end{bmatrix} \quad (C-3)$$

$$Y(3) = \frac{3}{160} \begin{bmatrix} 6 & 7 & -12 & -1 & 0 \\ 7 & 40 & -22 & -24 & -1 \\ -12 & -22 & 68 & -22 & -12 \\ -1 & -24 & -22 & 40 & 7 \\ 0 & -1 & -12 & 7 & 6 \end{bmatrix} \quad (C-4)$$

$$Y(4) = \frac{3}{160} \begin{bmatrix} 6 & 7 & -12 & -1 & 0 & 0 \\ 7 & 40 & -22 & -24 & -1 & 0 \\ -12 & -22 & 74 & -15 & -24 & -1 \\ -1 & -24 & -15 & 74 & -22 & -12 \\ 0 & -1 & -24 & -22 & 40 & 7 \\ 0 & 0 & -1 & -12 & 7 & 6 \end{bmatrix} \quad (C-5)$$
where there are $n-4$ 80's on the main diagonal.
APPENDIX D

The Weighting Matrices $Z(n)$
The weighting matrices $Z(n)$, $n=2, 3, \ldots$ defined via

$$Z(n) = \begin{pmatrix} z_{ij}(n) \end{pmatrix}_{i=1, \ldots, n+2, \ j=1, \ldots, n+2} \tag{D-1}$$

$$z_{ij} = \frac{1}{h} \int_{a}^{b} \phi_i(t)\phi_j(t)dt \tag{D-2}$$

are given below.

$$Z(2) = \frac{1}{2240} \begin{bmatrix} 20 & 129 & 60 & 1 \\ 129 & 1188 & 933 & 60 \\ 60 & 933 & 1188 & 129 \\ 1 & 60 & 129 & 20 \end{bmatrix} \tag{D-3}$$

$$Z(3) = \frac{1}{2240} \begin{bmatrix} 20 & 129 & 60 & 1 & 0 \\ 129 & 1208 & 1062 & 120 & 1 \\ 60 & 1062 & 2376 & 1062 & 60 \\ 1 & 120 & 1062 & 1208 & 129 \\ 0 & 1 & 60 & 129 & 20 \end{bmatrix} \tag{D-4}$$

$$Z(4) = \frac{1}{2240} \begin{bmatrix} 20 & 129 & 60 & 1 & 0 & 0 \\ 129 & 1208 & 1062 & 120 & 1 & 0 \\ 60 & 1062 & 2396 & 1191 & 120 & 1 \\ 1 & 120 & 1191 & 2396 & 1062 & 60 \\ 0 & 1 & 120 & 1062 & 1208 & 129 \\ 0 & 0 & 1 & 60 & 129 & 20 \end{bmatrix} \tag{D-5}$$
\[ Z(n) = \frac{1}{2240} \]

for \( n \geq 5 \)

where there are \( n-4 \) 2416's on the main diagonal.
APPENDIX E

The Weighting Matrices $Y^P(n)$
The weighting matrices $Y^p(n)$, $n=2,3, \ldots$ defined via

$$Y^p(n) = \begin{pmatrix} y^p_{ij}(n) \end{pmatrix}_{i=1, \ldots, n-1 \atop j=1, \ldots, n-1} \quad (E-1)$$

$$y^p_{ij}(n) = \frac{h}{b-a} \int_a^b \psi_i^-(t) \psi_j^+(t) \, dt \quad (E-2)$$

are given below.

$$Y^p(2) = \frac{1}{160} \begin{bmatrix} 0 \end{bmatrix} \quad (E-3)$$

$$Y^p(3) = \frac{3}{160} \begin{bmatrix} -32 & -32 \\ -32 & -32 \end{bmatrix} \quad (E-4)$$

$$Y^p(4) = \frac{3}{160} \begin{bmatrix} 78 & -39 & -39 \\ -39 & 78 & -39 \\ -39 & -39 & 78 \end{bmatrix} \quad (E-5)$$

$$Y^p(5) = \frac{3}{160} \begin{bmatrix} 80 & -16 & -48 & -16 \\ -16 & 80 & -16 & -48 \\ -48 & -16 & 80 & -16 \\ -16 & -48 & -16 & 80 \end{bmatrix} \quad (E-6)$$

\[
Y^p(7) = \frac{3}{160} \begin{bmatrix}
\end{bmatrix}
\] (E-8)

\[
Y^p(8) = \frac{3}{160} \begin{bmatrix}
-1 & -24 & -15 & 80 & -15 & -24 & -1 \\
-24 & -1 & -1 & -24 & -15 & 80 & -15 \\
\end{bmatrix}
\] (E-9)

\[
Y^p(9) = \frac{3}{160} \begin{bmatrix}
80 & -15 & -24 & -1 & 0 & -1 & -24 & -15 \\
-15 & 80 & -15 & -24 & -1 & 0 & -1 & -24 \\
-24 & -15 & 80 & -15 & -24 & -1 & 0 & -1 \\
-1 & -24 & -15 & 80 & -15 & -24 & -1 & 0 \\
0 & -1 & -24 & -15 & 80 & -15 & -24 & -1 \\
-1 & 0 & -1 & -24 & -15 & 80 & -15 & -24 \\
-24 & -1 & 0 & -1 & -24 & -15 & 80 & -15 \\
\end{bmatrix}
\] (E-10)
\[ Y^p(n) = \frac{3}{160} \quad \text{if } n > 9 \]

\[
\begin{bmatrix}
80 & -15 & -24 & -1 \\
-15 & 80 & -15 & -24 & -1 \\
-24 & -15 & 80 & -15 & -24 \\
-1 & -24 & -15 & 80 & -24 \\
-24 & -1 & -24 & -15 & 80 \\
-15 & -24 & -1 & -24 & -15 \\
\end{bmatrix}
\]

n-8 minor diagonals of zeroes

(E-11)
APPENDIX F

The Weighting Matrices $Z^P(n)$
The weighting matrices $Z^P(n)$, $n=2, 3, \ldots$ defined via

$$Z^P(n) = \begin{pmatrix} z^P_{ij}(n) \end{pmatrix}_{i=1, \ldots, n-1, \quad j=1, \ldots, n-1} \quad (F-1)$$

$$z^P_{ij}(n) = \frac{1}{h} \int_a^b \psi_i(t) \psi_j(t) dt \quad (F-2)$$

are given below.

$$Z^P(2) = \frac{1}{2240} \begin{bmatrix} 5040 \end{bmatrix} \quad (F-3)$$

$$Z^P(3) = \frac{1}{2240} \begin{bmatrix} 2656 & 2384 \\ 2384 & 2656 \end{bmatrix} \quad (F-4)$$

$$Z^P(4) = \frac{1}{2240} \begin{bmatrix} 2418 & 1311 & 1311 \\ 1311 & 2418 & 1311 \\ 1311 & 1311 & 2418 \end{bmatrix} \quad (F-5)$$

$$Z^P(5) = \frac{1}{2240} \begin{bmatrix} 2416 & 1192 & 240 & 1192 \\ 1192 & 2416 & 1192 & 240 \\ 240 & 1192 & 2416 & 1192 \\ 1192 & 240 & 1192 & 2416 \end{bmatrix} \quad (F-6)$$

$$Z^P(6) = \frac{1}{2240} \begin{bmatrix} 2416 & 1191 & 121 & 121 & 1191 \\ 1191 & 2416 & 1191 & 121 & 121 \\ 121 & 1191 & 2416 & 1191 & 121 \\ 121 & 121 & 1191 & 2416 & 1191 \\ 1191 & 121 & 121 & 1191 & 2416 \end{bmatrix} \quad (F-7)$$
\[ z^p(7) = \frac{1}{2240} \begin{bmatrix} 2416 & 1191 & 120 & 2 & 120 & 1191 \\ 1191 & 2416 & 1191 & 120 & 2 & 120 \\ 120 & 1191 & 2416 & 1191 & 120 & 2 \\ 2 & 120 & 1191 & 2416 & 1191 & 120 \\ 120 & 2 & 120 & 1191 & 2416 & 1191 \\ 1191 & 120 & 2 & 120 & 1191 & 2416 \end{bmatrix} \] (F-8)

\[ z^p(8) = \frac{1}{2240} \begin{bmatrix} 2416 & 1191 & 120 & 1 & 1 & 120 & 1191 \\ 1191 & 2416 & 1191 & 120 & 1 & 1 & 120 \\ 120 & 1191 & 2416 & 1191 & 120 & 1 & 1 \\ 1 & 1 & 120 & 1191 & 2416 & 1191 & 120 \\ 120 & 1 & 1 & 120 & 1191 & 2416 & 1191 \\ 1191 & 120 & 1 & 1 & 120 & 1191 & 2416 \end{bmatrix} \] (F-9)

\[ z^p(9) = \frac{1}{2240} \begin{bmatrix} 2416 & 1191 & 120 & 1 & 0 & 1 & 120 & 1191 \\ 1191 & 2416 & 1191 & 120 & 1 & 0 & 1 & 120 \\ 120 & 1191 & 2416 & 1191 & 120 & 1 & 0 & 1 \\ 1 & 120 & 1191 & 2416 & 1191 & 120 & 1 & 0 \\ 0 & 1 & 120 & 1191 & 2416 & 1191 & 120 & 1 \\ 1 & 0 & 1 & 120 & 1191 & 2416 & 1191 & 120 \\ 120 & 1 & 0 & 1 & 120 & 1191 & 2416 & 1191 \\ 1191 & 120 & 1 & 0 & 1 & 120 & 1191 & 2416 \end{bmatrix} \] (F-10)
\[
Z^P(n) = \frac{h}{2240}
\]

for \( n \geq 9 \)

The diagram depicts a matrix with zeroes and non-zero elements, illustrating the concept of minor diagonals (F-11) of zeroes.

- **Minor Diagonals of Zeroes**
  - The matrix shows two sets of minor diagonals:
    - One set is highlighted to indicate the minor diagonals (F-11).
    - The other set is shaded to indicate the minor diagonals of zeroes.

The matrix is structured with elements 1, 2416, 1191, and 120, forming the diagonals and off-diagonals, with zeroes filling in the remaining spaces.
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