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On the Matrix $[|x_i - x_j|^3]$ and the Cubic Spline Continuity Equations

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1. INTRODUCTION

Let $x_1 < x_2 < \cdots < x_N$ be $N > 1$ given points of $\mathbb{R}$. Then each of the functions, $s_k(x) = |x - x_k|^3$ $1 \leqslant k \leqslant N$, is a twice continuously differentiable piecewise cubic, i.e., a cubic spline. They must, therefore, satisfy the standard spline continuity equations. The application of this simple observation to each of the s_k yields a remarkable factorization. Let F and T be the $N \times N$ matrices given by $F_{ij} = |x_i - x_j|$ and $T_{ij} = |x_i - x_j|^3$; then

$$T = FCF.$$

Here C is a near tridiagonal $N \times N$ matrix essentially expressing the C^2 continuity of a cubic spline.

An easy consequence of this factorization is that T is positive definite on a certain $N-2$ dimensional subspace of $\mathbb{R}^N$. See also [2] for more general and related results. This latter fact will be used to show that T is nonsingular, thus showing that the set of translates, $\{|x - x_k|^3\}$, is "unisolvent".

2. THE CUBIC SPLINE CONTINUITY EQUATIONS

Although these equations are well known we present a derivation which we believe to be novel and somewhat more economical than the standard. This approach can also be extended to derive possible factorizations of matrices of higher odd powers of point distances.

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Let s be a cubic spline and y_1, y_2, y_3 any three consecutive knots of s. Then s'' is continuous and piecewise linear on $[y_1, y_3]$ with a possible knot at $x = y_2$. Now by the Hermite Gennochi formula, the second divided difference of s at y_1, y_2, y_3 is given by

$$s[y_1, y_2, y_3] = \int_0^1 \int_0^{1-t} s''(t(y_3 - y_1) + u(y_2 - y_1) + y_1)\, du\, dt.$$

But $s''(t(y_3 - y_1) + u(y_2 - y_1) + y_1)$ is piecewise linear in (t, u) with knot line given by

$$t(y_3 - y_1) + u(y_2 - y_1) + y_1 = y_2,$$

that is

$$t(y_3 - y_1) + u(y_2 - y_1) = y_2 - y_1,$$

a straight line passing through the points (0, 1) and $(t^*, 0)$ where $t^* = (y_2 - y_1)/(y_3 - y_1)$. (See Fig. 1)

Now for any linear $p(t, u)$ and Δ a triangle with vertices v_1, v_2 and v_3,

$$\iint_\Delta p(t, u)\, du\, dt = \frac{area(\Delta)}{3}\,(p(v_1) + p(v_2) + p(v_3)).$$

Thus, referring to Fig. 1,

$$\begin{aligned} s[y_1, y_2, y_3] &= \int_0^1 \int_0^{1-t} s''(t(y_3 - y_1) + u(y_2 - y_1) + y_1)\, du\, dt \\ &= \left(\iint_{\Delta_1} + \iint_{\Delta_2}\right) s''(t(y_3 - y_1) + u(y_2 - y_1) + y_1)\, du\, dt \\ &= \frac{1}{6}\frac{y_2 - y_1}{y_3 - y_1}\{s''(y_1) + 2s''(y_2)\} \\ &\quad + \frac{1}{6}\left(1 - \frac{y_2 - y_1}{y_3 - y_1}\right)\{s''(y_3) + 2s''(y_2)\}. \end{aligned}$$

If we define $h_i = y_{i+1} - y_i$ $1 \leq i \leq 2$, this expression simplifies to

$$\frac{1}{6(h_1 + h_2)}\{h_1 s''(y_1) + 2(h_1 + h_2)\, s''(y_2) + h_2 s''(y_3)\}.$$

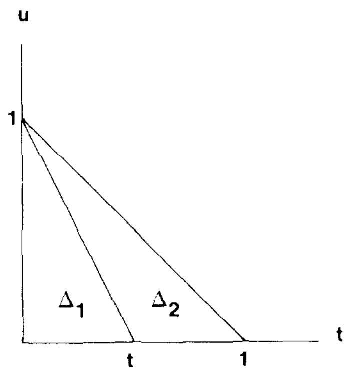

FIGURE 1

Now substitute the explicit expression for $s[y_1, y_2, y_3]$ and simplify to obtain

$$\frac{h_1}{2}\frac{s''(y_1)}{6} + (h_1 + h_2)\frac{s''(y_2)}{6} + \frac{h_2}{2}\frac{s''(y_3)}{6}$$
$$= \frac{1}{2h_1} s(y_1) - \frac{h_1 + h_2}{2h_1 h_2} s(y_2) + \frac{1}{2h_2} s(y_3). \tag{2.2}$$

We emphasize that for any spline, s, these are just the conditions which express the continuity of $s''(x)$ at the interior knots [1, p. 11].

3. THE FACTORIZATION OF T

For simplicity we make use of the differences $h_i \triangleq x_{i+1} - x_i$, $1 \leqslant i \leqslant N-1$. We apply the continuity equations (2.2) to each of the $s_k(x)$ at the interior knots, x_i $2 \leqslant i \leqslant N-1$, and obtain the $(N-2) \times N$ matrix equations

$$\begin{bmatrix} \frac{h_1}{2} & h_1 + h_2 & \frac{h_2}{2} & & & & \bigcirc \\ & \frac{h_2}{2} & h_2 + h_3 & \frac{h_3}{2} & & & \\ & & \frac{h_3}{2} & h_3 + h_4 & \frac{h_4}{2} & & \\ & \bigcirc & & & \ddots & & \\ & & & & \frac{h_{N-2}}{2} & h_{N-2} + h_{N-1} & \frac{h_{N-1}}{2} \end{bmatrix} \begin{bmatrix} s_k''(x_1)/6 \\ s_k''(x_2)/6 \\ \\ \vdots \\ s_k''(x_N)/6 \end{bmatrix}$$

$$
= \begin{bmatrix}
\frac{1}{2h_1} & -\frac{h_1+h_2}{2h_1h_2} & \frac{1}{2h_2} & & & \bigcirc \\
 & \frac{1}{2h_2} & -\frac{h_2+h_3}{2h_2h_3} & \frac{1}{2h_3} & & \\
 & & \frac{1}{2h_3} & & & \\
 & & & \ddots & & \\
 & \bigcirc & & \frac{1}{2h_{N-2}} & -\frac{h_{N-2}+h_{N-1}}{2h_{N-1}h_{N-2}} & \frac{1}{2h_{N-1}}
\end{bmatrix}
\begin{bmatrix}
s_k(x_1) \\ s_k(x_2) \\ \\ \vdots \\ s_k(x_N)
\end{bmatrix},
$$

$$1 \leqslant k \leqslant N, \qquad (3.1)$$

We "square up" these equations with the following two identities.

LEMMA 3.2. *For* $x_1 < x_2 < \cdots < x_N$ *and* $s(x) = |x - x_k|^3$ *the following hold*:

$$
(x_2 - x_N)\frac{s''(x_1)}{6} + \frac{x_2 - x_1}{2}\frac{s''(x_2)}{6} + \frac{x_N - x_1}{2}\frac{s''(x_N)}{6}
$$

$$
= \frac{x_2 - x_N}{2(x_N - x_1)(x_2 - x_1)}s(x_1) + \frac{1}{2(x_2 - x_1)}s(x_2) + \frac{1}{2(x_N - x_1)}s(x_N) \qquad (3.2)
$$

and

$$
\frac{x_N - x_1}{2}\frac{s''(x_1)}{6} + \frac{x_N - x_{N-1}}{2}\frac{s''(x_N - 1)}{6} + (x_1 - x_{N-1})\frac{s''(x_N)}{6}
$$

$$
= \frac{1}{2(x_N - x_1)}s(x_1) + \frac{1}{2(x_N - x_{N-1})}s(x_{N-1}) \qquad (3.3)
$$

$$
+ \frac{x_1 - x_{N-1}}{2(x_N - x_1)(x_N - x_{N-1})}s(x_N).
$$

Proof. It suffices to demonstrate (3.2); (3.3) will then follow by symmetry.

If $k = 1$ it is readily seen that both sides reduce to $0.5\{(x_2 - x_1)^2 + (x_N - x_1)^2\}$ whereas for $k \geqslant 2$ both sides equal $0.5(x_N - x_2)(x_1 + x_2 + x_N - 3x_k)$. ∎

We now add identity (3.2) as the first row of (3.1) and (3.3) as the last and write $S = h_1 + h_2 + \cdots + h_{N-1}$, obtaining

$$\begin{bmatrix} h_1 - S & \frac{h_1}{2} & 0 & \cdots & 0 & \frac{S}{2} \\ \frac{h_1}{2} & h_1 + h_2 & \frac{h_2}{2} & 0 & \cdots & 0 \\ 0 & \frac{h_2}{2} & h_2 + h_3 & \frac{h_3}{2} & 0 \cdots & 0 \\ \vdots & & \ddots & & & \\ 0 & & & \frac{h_{N-2}}{2} & h_{N-2} + h_{N-1} & \frac{h_{N-1}}{2} \\ \frac{S}{2} & 0 & \cdots & 0 & \frac{h_{N-1}}{2} & h_{N-1} - S \end{bmatrix} \begin{bmatrix} |x_k - x_1| \\ |x_k - x_2| \\ \vdots \\ |x_k - x_N| \end{bmatrix}$$

$$= \begin{bmatrix} \frac{h_1 - S}{2h_1 S} & \frac{1}{2h_1} & 0 & \cdots & 0 & \frac{1}{2S} \\ \frac{1}{2h_1} & -\frac{h_1 + h_2}{2h_1 h_2} & \frac{1}{2h_2} & 0 & \cdots & 0 \\ 0 & \frac{1}{2h_2} & -\frac{h_2 + h_3}{2h_2 h_3} & \frac{1}{2h_3} & & \vdots \\ \vdots & & & \ddots & & 0 \\ 0 & & & \frac{1}{2h_{N-2}} & -\frac{h_{N-2} + h_{N-1}}{2h_{N-1} h_{N-2}} & \frac{1}{2h_{N-1}} \\ \frac{1}{2S} & 0 & \cdots & 0 & \frac{1}{2h_{N-1}} & \frac{h_{N-1} - S}{2h_{N-1} S} \end{bmatrix} \begin{bmatrix} |x_k - x_1|^3 \\ |x_k - x_2|^3 \\ \vdots \\ |x_k - x_N|^3 \end{bmatrix},$$

$$1 \leqslant k \leqslant N. \qquad (3.4)$$

Denote the first matrix in (3.4) by C. The following lemma identifies the second.

LEMMA 3.6. *The second matrix in* (3.4) *is the inverse of* F.

Proof. This fact is verified by a straightforward calculation. We suppress the details. ▌

If we now collect the N matrix times vector equations of (3.4) we obtain the matrix equation

$$CF = F^{-1}T, \qquad (3.5)$$

and have proven:

THEOREM 3.7. $T = FCF$. ▌

4. The Conditional Positive Definiteness of T

Since the diagonal is strictly dominant for the $N-2$ interior rows of the matrix C, C is strictly positive definite on the subspace

$$V' = \{\mathbf{a} \in \mathbb{R}^N : a_1 = a_N = 0\}.$$

Clearly then T is strictly positive definite on the subspace $V = F^{-1}V'$.

Lemma 4.1. $V = F^{-1}V' = \{\mathbf{a} \in \mathbb{R}^N : \sum_{i=1}^N a_i = \sum_{i=1}^N a_i x_i = 0\}$.

Proof. Consider $\mathbf{u} \in V'$ and let $\mathbf{a} = F^{-1}\mathbf{u}$. Then

$$\sum_{i=1}^N a_i = \mathbf{u}^T F^{-1} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix},$$

and

$$\sum_{i=1}^N a_i x_i = \mathbf{u}^T F^{-1} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}.$$

But from the formula for F^{-1} given in Lemma 3.6, it follows easily that the $N-2$ *interior* components of both

$$F^{-1} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} \quad \text{and} \quad F^{-1} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}$$

are zero. Since the *first* and *last* components of $\mathbf{u}$ are both zero the result follows. ∎

We have therefore:

Theorem 4.2 (cf. [2]). *The matrix T is strictly positive definite on the $N-2$ dimensional subspace $V = \{\mathbf{a} \in \mathbb{R}^N : \sum_{i=1}^N a_i = \sum_{i=1}^N a_i x_i = 0\}$.*

5. The Invertibility of T

THEOREM 5.1. *The matrix T is non-singular.*

Proof. The $N=2$ case is easily disposed of. By Theorem 4.2, T is strictly positive definite on an $N-2$ dimensional subspace. As T is symmetric, it is readily seen that, counting multiplicities, T must have at least $N-2$ strictly positive eigenvalues. We claim that for $N>2$, T has exactly $N-2$ strictly positive and two strictly negative eigenvalues. To see this consider T_3, the upper 3×3 block of T. If we write

$$T_3 = \begin{bmatrix} 0 & a & b \\ a & 0 & c \\ b & c & 0 \end{bmatrix},$$

we may compute $\operatorname{trace}(T_3)=0$ and $\det(T_3)=2abc>0$. Thus T_3 must have two strictly negative eigenvalues and one strictly positive. Let $E\subset\mathbb{R}^3$ be the two dimensional eigenspace corresponding to the two negative eigenvalues. Then for $\mathbf{0}\neq\mathbf{x}\in E$, $\mathbf{x}^T T_3\mathbf{x}<0$ and if we extend $\mathbf{x}$ to $\mathbf{y}\in\mathbb{R}^N$ by zeroes we have

$$\mathbf{y}^T T\mathbf{y} = \mathbf{x}^T T_3 \mathbf{x} < 0.$$

Thus T is strictly negative definite on a 2-dimensional subspace and must have two strictly negative eigenvalues. The result follows. ∎

6. Remarks

We point out that the analogue of T in 2 dimensions need not be non-singular. In fact, for the four points in the plane, $(-1, 0)$, $(0, 0)$, $(1, 0)$, and $(0, 1)$, the matrix of distances cubed is

$$\begin{bmatrix} 0 & 1 & 8 & 2\sqrt{2} \\ 1 & 0 & 1 & 1 \\ 8 & 1 & 0 & 2\sqrt{2} \\ 2\sqrt{2} & 1 & 2\sqrt{2} & 0 \end{bmatrix}$$

with determinant $64(1-\sqrt{2})<0$. But the matrix for the points, $(-1, 0)$, $(0, 0)$, $(1, 0)$, and $(2, 0)$, is

$$\begin{bmatrix} 0 & 1 & 8 & 27 \\ 1 & 0 & 1 & 8 \\ 8 & 1 & 0 & 1 \\ 27 & 8 & 1 & 0 \end{bmatrix}$$

with determinant $1188>0$. There must, therefore, be points (u, v) when the matrix for $(-1, 0)$, $(0, 0)$, $(1, 0)$, and (u, v) is singular.

REFERENCES

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