SOME INTERPOLATION FORMULAS FOR APPROXIMATING THE SOLUTION OF THE HEAT EQUATION

by

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Some Interpolation Formulas for Approximating the Solution of the Heat Equation

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Summary Interpolation formulas of the form

$$u(x_{*1}, \ldots, x_{*n}, t_*) \simeq \sum_{i=1}^{N} A_i \, u(v_{i1}, \ldots, v_{in}, t_i)$$

are presented. These formulas are based on the heat polynomials of Appell. The point $(x_{*1}, \ldots, x_{*n})$ is in the interior of an (n+1) dimensional region, R_{n+1}, and the points $(v_{i1}, \ldots, v_{in}, t_i)$ are on the boundary of R_{n+1}. These formulas can be used to approximate the solution of the heat conduction problem in R_{n+1}. The relationship between formulas of the above type of degree 2 in R_{n+1} and the second degree harmonic interpolation formulas of Stroud, Chen, Wang, and Mao [1] in R_n is presented. Some higher degree formulas for special regions in R_2 are also developed.

1. INTRODUCTION

In this paper we discuss interpolation formulas of the type

$$u(x_{*1}, \ldots, x_{*n}, t_*) \simeq \sum_{i=1}^{N} A_i \, u(v_{i1}, \ldots, v_{in}, t_i) \qquad (1)$$

which are based on the heat polynomials of Appell [2]. The point $p_* \equiv (x_{*1}, \ldots, x_{*n}, t_*)$ is in the interior of a region, Int R_{n+1}, in (n+1)-dimensional space. The points $p_i \equiv (v_{i1}, \ldots, v_{in}, t_i)$, $i=1, \ldots, N$, lie on the boundary of this region, Bd R_{n+1}, and the weights (also called coefficients), A_i, $i=1, \ldots, N$ are positive constants. We will sometimes deal with the cylinder

$$R_{n+1} \equiv R_n \times [0, T) = \{(x,t) \mid x \in \bar{R}_n, \ 0 \le t < T\}. \qquad (2)$$

It will be assumed that Bd R_{n+1} is sufficiently smooth so that the initial boundary value problem of heat conduction,

$$\begin{aligned} L_n \, [u(x,t)] &= 0 \text{ in Int } R_{n+1} \\ u(x,0) &= f(x) \text{ on } R_n \\ u(x,t) &= g(x) \text{ on Bd } R_{n+1} \end{aligned} \qquad (3)$$

where $$L_n \, [u] \equiv \sum_{i=1}^{N} \frac{\partial^2 u}{\partial x_i^2} - \frac{\partial u}{\partial t} \qquad (4)$$

has a solution. Then formula (1) can serve to approximate the solution of (3) at $p_* \in$ Int R_{n+1}.

In section 2 we introduce the heat polynomials in 2 variables and state some of their properties. We then extend the heat polynomials of degree ≤ 2 to higher dimensional spaces. In section 3 we demonstrate the existence of (n+1)-point formulas of degree 2 in cylindrical regions (2). We also show that for both cylindrical and non-cylindrical regions there is a formula of degree 2 for which the n+1 points in the formula (1) lie on a hyperplane t = constant. The theorems of this section state some of the geometrical properties of these formulas and their relationship to the harmonic interpolation formulas of Stroud, Chen, Wang, and Mao [1]. In Section 4 we investigate n-point formulas of degree 2n-1 in 2 variables. In section 5 we briefly discuss open questions related to investigating formulas (1).

2. THE HEAT POLYNOMIALS

2.1 Heat Polynomials in 2 Variables

Appell introduced in [2] the fundamental heat polynomials, $\upsilon_n(x, t)$, which he defined as the coefficients of $z^n/n!$ in the power series expansion of $\exp(zx+z^2t)$, i.e.,

$$e^{zx+z^2 t} = \sum_{n=o}^{\infty} \upsilon_n(x, t) \frac{z^n}{n!} \quad .$$

He showed that each of these linearly independent polynomials is a solution of

$$L_1 [u] \equiv \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} = 0. \tag{5}$$

Rosenbloom and Widder [3], Widder [4], and Haimo [5] have investigated expansions of solutions $u(x, t)$ to (5) in terms of the heat polynomials. These polynomials are directly related to the Hermite polynomials and are given by the following recursion formulas (see, for example, Shohat [6]),

$$\begin{aligned} \upsilon_0(x, t) &= 1, \\ \upsilon_1(x, t) &= x, \\ \upsilon_n(x, t) &= x\, \upsilon_{n-1}(x, t) + 2(n-1)t\, \upsilon_{n-2}(x, t) \quad n=2, \ldots \quad . \end{aligned} \tag{6}$$

Examples of (6) are

$$\begin{aligned} \upsilon_2(x, t) &= x^2 + 2t, \\ \upsilon_3(x, t) &= x^3 + 6xt, \\ \upsilon_4(x, t) &= x^4 + 12x^2 t + 12t^2, \\ \upsilon_5(x, t) &= x^5 + 20x^3 t + 60xt^2, \\ \upsilon_6(x, t) &= x^6 + 30x^4 t + 180x^2 t^2 + 120t^3. \end{aligned}$$

It can be shown that $\upsilon_n(x, t)$ can be written as

$$\upsilon_n(x, t) = n! \sum_{k=0}^{[n/2]} \frac{n^{n-2k}\, t^k}{(n-2k)!\, k!} \tag{7}$$

where $[n/2]$ means the integer part of $n/2$. Note, $v_n(x,t)$ is of degree n in x and of degree $[n/2]$ in t. We will call any linear combination of the fundamental heat polynomials (6) a "heat polynomial". It is obvious such a linear combination also satisfies equation (5).

Lemma 1. A heat polynomial $p(x,t)$ is transformed into another heat polynomial $q(r,s)$ under any affine transformation

$$x = r+h, \quad t = s+k$$

which is a simple translation of the origin. □

Because of this lemma, we can assume that R_2 is situated so that any given interior point (x_*, t_*) coincides with the origin.

2.2 Heat Polynomials of Degree ≤2 in (n+1) Variables.

We now extend the heat polynomials of degree ≤2 to higher dimensional spaces.

Definition 1. We will call the following independent polynomials the fundamental heat polynomials of degree ≤2 in the n+1 variables x_i, i=1, . . . , n, and t

$$\begin{aligned} &1, \\ &x_i \qquad\qquad i, j = 1,\dots,n, \; i \neq j \\ &x_i x_j \\ &x_i^2 + 2t. \end{aligned} \tag{8}$$

We note that there are $(n+1)(n+2)/2$ such polynomials. This definition is motivated by the fact we wish to construct polynomials similar in form to those of (6). Linear combinations of (8) satisfy (4) and will be called "heat polynomials".

Lemma 2. A heat polynomial $p(x_1,\dots,x_n, t)$ is transformed into another heat polynomial $q(r_1,\dots,r_n, s)$ under the simple affine trnasformation consisting of a translation of the origin combined with a rotation about the t-axis. □

This lemma allows us to assume that R_{n+1} is situated so that any given interior point $(x_{*1},\dots,x_{*n}, t_*)$ corresponds to the origin and that any particular point on the Bd R_{n+1}, say p_1, is such that

$$p_1 = (v_{11}, \ldots, v_{1n}, t_1) = (v_{11}, 0, \ldots, 0, t_1), \quad v_{11} > 0.$$

3. FORMULAS OF DEGREE 2 IN R_{n+1}, $n+1 > 2$

For a given region R_{n+1} and $p_* \in \text{Int } R_{n+1}$ we wish to determine the points and weights p_i, A_i, $i=1, \ldots, n$ so that formula (1) is exact for the heat polynomials (8). We therefore introduce the following definition.

Definition 2. We say that the interpolation formula (1) has degree d if it is exact for all fundamental heat polynomials $\upsilon(x_1, \ldots, x_n, t)$ of degree $\leq$ d in the x_i's and there is at least one heat polynomial of degree d+1 for which it is not exact.

In this section we discuss interpolation formulas of type (1) of degree 2 in R_{n+1}, $n+1 > 2$. These formulas are directly related to the second degree harmonic interpolation formu las discussed by Stroud, Chen, Wang, and Mao [1] which are used in approximating the solution of the Dirichlet problem and some of the proofs are in a similar vein. In fact, the proofs for theorems 1-3 are quite similar to those in [1] and are not given here but can be found in Shriver [7].

If the points and weights p_i, A_i, $i=1, \ldots, n+1$ are to specify a formula of degree 2 for $p_* = (0, \ldots, 0)$, then they must satisfy the following $(n+1)(n+2)/2$ equations based on Definition 2,

$$\begin{aligned}
&A_1 &&+ A_2 &&+ \ldots + A_{n+1} &&= 1 \\
&A_1 v_{1i} &&+ A_2 v_{2i} &&+ \ldots + A_{n+1} v_{n+1,i} &&= 0 \\
&A_1 v_{1i} v_{1j} &&+ A_2 v_{2i} v_{2j} &&+ \ldots + A_{n+1} v_{n+1,i} v_{n+1,j} &&= 0 \\
&A_1 (v_{1i}^2 + 2t_1) &&+ A_2 (v_2^2 + 2t_2) &&+ \ldots + A_{n+1} (v_{n+1,i}^2 + 2t_{n+1}) &&= 0
\end{aligned} \qquad (9)$$
$$i, j = 1, \ldots, n, \quad i \neq j.$$

In the following, we assume R_{n+1} is convex.

Theorem 1. If the p_i, A_i, $i=1, \ldots, n+1$ are the points and weights of a formula of degree 2 where all of the $p_i \in$ Bd R_{n+1}, then all of the A_i are positive and the point $p_* = (0,\ldots,0,0)$ is an interior point of the n-simplex, T_n, which has vertices given by

$$p_i' = (v_{i1},\ldots, v_{in}, t_i), \quad i=1,\ldots,n+1,$$

where $t_1 = t_2 = \ldots = t_{n+1} = 0$. □

Theorem 2. An interpolation formula (1) of degree 2 cannot be obtained with fewer than $N = n+1$ points. □

If we are given a set of points p_i, $i=1,\ldots,n+1$, which can be used as points in a formula of degree 2 for $p_* = (0,\ldots,0)$ then the A_i, $i=1,\ldots,n+1$, are uniquely determined as a solution to the first n+1 (linear) equations of (9),

$$\begin{aligned} A_1 + \ldots + A_{n+1} &= 1 \\ A_1 V_{1i} + \ldots + A_{n+1} V_{n+1,i} &= 0, \quad i=1,\ldots,n. \end{aligned} \tag{10}$$

We now state a theorem which can be used to determine the n+1 points, p_i.

Theorem 3. In order that the p_i, $i=1,\ldots,n+1$, will be the points in a formula of degree 2 for R_{n+1} and $p_* = (0,\ldots,0)$, it is necessary and sufficient that the following conditions be satisfied:

(i) p_* is an interior point of the n-simplex which has vertices $p_i' = (v_{i1},\ldots, v_{in}, 0)$, $i=1,\ldots,n+1$,

(ii) for each i, the vector p_i' is perpendicular to the plane containing the other p_j', $j \neq 1$, i, $j = 1,\ldots,n+1$,

(iii) assuming R_{n+1} is rotated so that $p_1 = (v_{11}, 0,\ldots,0, t_1)$, $v_{11} > 0$, the t_i must satisfy

$$A_1 t_1 + \ldots + A_{n+1} t_{n+1} = v_{11} v_{21}/2. \quad □$$

When n=2, for example, this theorem means that the point $p_* = (0,0,0)$ is the orthocenter + of the trinagle with vertices $p_1' = (v_{11}, 0, 0)$, $p_2' = (v_{21}, v_{22}, 0)$, and $p_3' = (v_{21}, v_{32}, 0)$ where p_1, p_2, p_3 are the interpolation points of a formula of degree 2 for $p_* = (0, 0, 0)$.

We will now need the following theorem from Stroud, Chen, Wang, and Mao [1].

Theorem 4. Given any $v_1 \equiv (v_{11}, \ldots, v_{1n}) \in \mathrm{Bd}\, R_n$, R_n a bounded simply connected convex n-dimensional region, there exist $v_2, \ldots, v_{n+1}$, and positive $A_1, \ldots, A_{n+1}$ so that the v_i, $i=1, \ldots n+1$ satisfy conditions (i) and (ii) of theorem 3 and the A_i, v_i, $i=1, \ldots, n+1$ satisfy system (10). Furthermore these are the points and weights of a harmonic interpolation formula of degree 2 for R_n.

As a direct result of this we can show

Theorem 5. Given R_{n+1} is the cylinder (2) and given a point, $p_* \in R_{n+1}$, there exist points $p_i \in \mathrm{Bd}\, R_{n+1}$, $i=1, \ldots, n+1$, and positive weights A_i, $i=1, \ldots, n+1$, so that the p_i, A_i, $i=1, \ldots, n+1$, are the points and weights of a formula of degree 2 for R_{n+1} and p_*.

Proof. Assume that R_{n+1} has been translated so the p_* corresponds to the origin and rotated so that $p_1' = (v_{11}, 0, \ldots, 0) \in \mathrm{Bd}\, R_n \in \mathrm{Bd}\, R_{n+1}$. From Theorem 4 we can find $p_i' = (v_{i1}, \ldots, v_{in}, 0) \in \mathrm{Bd}\, R_n$, $i=2, \ldots, n+1$, so that conditions (i) and (ii) of theorem 3 are satisfied, and $A_i > 0$, $i=1, \ldots, n+1$ so that system (10) is satisfied. Now choose the t_i, $-T \leq -t_* \leq t_i < 0$, $i=1, \ldots, n+1$ so that

$$A_1 t_1 + \ldots + A_{n+1} t_{n+1} = v_{11} v_{21}/2.$$

We have n free parameters to do this. Thus we have satisfied the conditions of theorem 3 and system (10) and the p_i, A_i, $i=1, \ldots, n+1$ are a formula of degree 2. □

\+ The orthocenter of a triangle is the point of intersection of three altitudes.

We now ask the following question: Are there interpolation formulas (1) for which all of the points, p_i, in the formula lie on the hyperplane t=constant, i.e., $t_i = t$, $i=1,\ldots,n+1$. These formulas bear a resemblance to explicit finite difference methods when viewed as interpolation formulas. We can state,

Theorem 6. Given R_{n+1} is the cylinder (2) and given a point $p_* \in \text{Int}\, R_{n+1}$, there exists points $p_i = (v_{i1}, \ldots, v_{in}, t) \in \text{Bd}\, R_{n+1}$, $0 < t \leq t_* \leq T$, and weights $A_i > 0$, $i=1,\ldots,n+1$ so that the p_i, A_i, $i=1,\ldots,n+1$ are an interpolation formula if degree 2 for R_{n+1} and p_*.

Proof. Assume that R_{n+1} has been translated so that p_* corresponds to the origin and rotated so that point $p_1' = (v_{11}, 0, \ldots, 0) \in \text{Bd}\, R_n \in \text{Bd}\, R_{n+1}$. From theorem 4, we can find points $p_i' = (v_{i1}, \ldots, v_{in}, 0) \in \text{Bd}\, R_{n+1}$ and weights, $A_i > 0$, $i=1,\ldots,n+1$ so that conditions (i) and (ii) of Theorem 3 and system (10) are satisfied. If all of the points are to be on the hyperplane, t=constant, then, since $\Sigma A_i = 1$, condition (iii) of theorem 3 becomes

$$t = v_{11} v_{21}/2. \tag{11}$$

If the t calculated from the above points, p_i, with formula (11) lies in the interval $-t_* \leq t < 0$, then the required formula has been found. However, the calculated t may be such that $t < -t_*$. We will show the required formula lies on the portion of the boundary of the translated R_{n+1} given by

$$B_{t_*} \equiv R_n \cap \{t = -t_*\}.$$

Consider $B'_{t_*} = R'_n \cap \{t = -t_*\} \in B_{t_*}$, where $R'_n \subset R_n$ and $\text{Bd}\, R'_n$ is formed by contracting the $\text{Bd}\, R_n$, i.e., reducing the distance between the origin and every point on the $\text{Bd}\, R_n$ in some fashion. Choose $p_1' = (v'_{11}, 0, \ldots, 0, -t_*) \in \text{Bd}\, R'_n$, $v'_{11} > 0$, and note that $v'_{11} < v_{11}$ and compute $t' = -v'_{11} v_{21}/2$. We note that when $B'_{t_*} = B_{t_*}$, then $v'_{11} = v_{11}$ and $t' = t$. Since we can shrink the $\text{Bd}\, R_n$ in any continuous fashion, we can make v'_{11} as small as we please. Therefore, t' will take on all values in the interval $t \leq t' < 0$. Thus we can find a $t' = -t_*$ and the conjectured formula exists. □

Theorem 6 can be extended to hold for more general regions than the cylindrical regions heretofore discussed. We denote by D a bounded (n+1)-dimensional domain in E^{n+1}. Let $(x, t) = (x_1, \ldots, x_n, t)$ be a variable point in E^{n+1}. D is bounded by a region B lying on the hyperplane t=0, a region B_T lying on the hyperplane t=T, $0 < T < \infty$, and a hypersurface (manifold) S is lying in the strip $0 < t < T$. We assume that the Bd D is sufficiently smooth so that the following initial boundary value problem has a solution (see, for example, Friedman [8]),

$$\begin{aligned} L_n[u(x,t)] &= 0 \text{ on } D + B_T \\ u(x,0) &= f(x) \text{ on } \overline{B} \\ u(x,t) &= g(x,t) \text{ on } S \end{aligned} \qquad (12)$$

Formula (1) can serve to approximate the solution of (12).

<u>Theorem 7.</u> Given a region D as described above and a point $p_* \in \text{Int } D$, there exist points $p_i = (v_{i1}, \ldots, v_{in}, t) \in \text{Bd } D$, $0 < t \le t_* \le T$ and weights $A_i > 0$, $i=1, \ldots, n+1$, so that the p_i, A_i, $i=1, \ldots, n+1$ are an interpolation formula of degree 2 for D and p_*.

Proof. Assume that D has been translated so that p_* corresponds to the origin and rotated so that p_1 lies on the positive x_1-axis, i.e., $p_1 = (v_{11}, 0, \ldots, 0, t) \in D$, $v_{11} > 0$.

Consider the 2-dimensional curve, C, which is the intersection of the sets $x_2 = 0$, $x_3 = 0, \ldots, x_n = 0$, $x_1 \ge 0$, $-t_* \le t \le 0$, and the Bd D. C is such that either (a) as t varies from t to $-t_*$ in a continuous fashion the point p_1 moves along C with v_{11} taking on all values in the interval $-F < v_{11} < M$, M, F constants, $M > 0$, $F \ge 0$, or (b) as t varies from 0 to $-t_*$ in a continuous fashion the point p_1 moves along C with v_{11} taking on all values im the interval $0 < N \le v_{11} \le M$, N a constant, i.e., C contains a straight line segment parallel to the x_1-axis at $t = -t_*$ which intersects the t-axis.

Let us choose a t', $-t_* \le t' < 0$, and a point $p_1' = (v_{11}', 0, \ldots, 0, t')$ $\in \text{Bd } D$, $v_{11}' > 0$. From theorem 4 we can find $p_i' = (v_{i1}, \ldots, v_{in}, t')$ $\in \text{Bd } D$, $i=2, \ldots, n+1$, and $A_i > 0$, $i=1, \ldots, n+1$ so that conditions (i) and (ii) of theorem 3 and system(10) are satisfied. If all of the points

p_i, are to lie on the hyperplane, t = constant, then condition (iii) of Theorem 3 again becomes equation (11). All we need to show is that for some choice of t' equation (11) holds. In case (a) above, vary t' in a continuous decreasing fashion from 0 to $-t_*$. But then v_{11} assumes, in a continuous increasing fashion, values from M to $-F$, and the right hand side of (11) varies continuously between $MV_{21} < 0$ and $-FV_{21} > 0$. Thus there is a t' for which the required formula exists. In case (b), it may be possible that we do not yet have a t' such that (11) holds when $t = -t_*$, t having varied from 0 to $-t_*$. We can however employ the contraction argument of Theorem 6 and show that the formula exists on the portion of the translated Bd D defined by B_{t_*}. □

Theorems 5, 6, and 7 show that given a second degree harmonic interpolation formula of the Stroud, Chen, Wang, and Mao type, we can construct a second degree formula of the type described in this paper. We will now give some examples:

Let S_n be the n-sphere of unit radius with center at the origin,

$$S_n : \{(x_1, \ldots, x_n) \mid x_1^2 + \ldots + x_n^2 \leq 1\}.$$

We give some examples of formulas of degree 2 of Theorems 5 and 6 in the cylindrical region $S_n \times [-T, 0]$. The point p_* is assumed to lie on on the x_1-axis,

$$p_* = (x_{*1}, \ldots, 0, 0), \quad x_{*1} \in (-1, 1), \quad t_* = 0.$$

One can verify directly that the points and weights

$$p_i - p_*, \quad A_i, \quad i=1, \ldots, n+1,$$

given in Table 1, satisfy equations (9). The points p_j, $j=2, \ldots, n+1$, ($t_j = 0$, $j=2, \ldots, n+2$), are the vertices of a simplex, T_{n-1}, lying in the plane $x_1 = v_{21}$. The points p_j, $j=2, \ldots, n+1$ may be rotated about the x_1-axis in any manner we desire and we still obtain a formula of degree 2.

Table 1

A Formula of Degree 2 for $S_n \times [-T, 0]$

$$p_1 = (v_{11}, 0, 0, 0, \ldots, 0, 0, t_1)$$

$$p_2 = (v_{21}, v_{22}, 0, 0, \ldots, 0, 0, t_2)$$

$$p_3 = (v_{21}, v_{32}, v_{33}, 0, \ldots, 0, 0, t_3)$$

$$p_4 = (v_{21}, v_{32}, v_{43}, v_{44}, \ldots, 0, 0, t_4)$$

$$\ldots$$

$$p_n = (v_{21}, v_{32}, v_{43}, v_{54}, \ldots, v_{n,n-1}, v_{n,n}, t_n)$$

$$p_{n+1} = (v_{21}, v_{32}, v_{43}, v_{54}, \ldots, v_{n,n-1}, v_{n+1,n}\ t_{n+1})$$

where,

$$r = r_0(1-\epsilon), \tag{13}$$

$$x'_{*1} = x_{*1} + \epsilon, \tag{14}$$

$$\bar{x}_{*1} = x'_{*1}/r, \tag{15}$$

$$\beta = (n+1) - (n-1)x_{*1}, \tag{16}$$

$$v_{11} = r - \epsilon, \tag{17}$$

$$v_{21} = \frac{(n-1)\bar{x}_{*1} - 1}{n}\ r - \epsilon, \tag{18}$$

$$v_{i,i} = \left[\frac{(n-i+1)(1+\bar{x}_{*1})\beta}{n(n-i+2)}\right]^{\frac{1}{2}} r, \quad i=2,\ldots,n. \tag{19}$$

$$v_{i+1,i} = -\left[\frac{(1+\bar{x}_{*1})\beta}{n(n-i+2)(n-i+1)}\right]^{\frac{1}{2}} r, \quad i=2,\ldots,n. \tag{20}$$

$$A_1 = \frac{1+\bar{x}_{*1}}{\beta}, \quad A_2 = \ldots = A_{n+1} = \frac{1-\bar{x}_{*1}}{\beta} \tag{21}$$

$$A_1 t_1 + \ldots + A_{n+1} t_{n+1} = \frac{r^2 - (x'_{*1})^2}{2n}\ . \tag{22}$$

Example 1. Formulas of Theorem 5.

In equations (13) through (22) of Table 1 let $r_0 = 1$ and $\epsilon = 0$. The points p_i lie on the surface of S_n. By choosing the $t_i \in [-T, 0]$, $i=1,\ldots,n+1$, so that (22) holds, we have a desired formula.

Example 2. Formulas of Theorem 6.

Here we are interested in formulas with all points lying on the hyperplane t'=constant. Let $r_0=1$ and $\epsilon=0$ in equations (13) through (21). If $t_1 = \ldots = t_{n+1} = t'$, equation (22) becomes

$$t' = -\frac{r^2 - (x^!_{*1})^2}{2n} \quad .$$

If $-T \leq t' < 0$, then we have a desired formula and the points p_i, $i=1,\ldots,n+1$ lie on the surface of S_n. If $t' < -T$, perform the boundary contractions below with $t_i = -T$, $i=1,\ldots,n+1$:

case i) $x_{*1} = 0$

choose r_0 such that $r_0{}^2 = -2nT$ and with $\epsilon = 0$ recompute (13-21). The points p_i, $i=1,\ldots,n+1$ lie on the surface of S_{n, r_0} which is the n-sphere of radius r_0 with center at the origin.

case ii) $x_{*1} < 0$.

If $$-\frac{1-x^2_{*1}}{2n} \leq T \leq -\frac{(1-|x_{*1}|)^2}{2n}$$

then choose ϵ so that

$$\epsilon = \frac{2nT - (x^2_{*1} - 1)}{2(1+x_{*1})}$$

and with $r_0=1$ recompute (13-21). The points p_i, $i=1,,\ldots,n+1$, lie on the surface of $S_{n,r,-\epsilon}$ which is the n-sphere of radius $r=1-\epsilon$ and center at $p_{-\epsilon} = (-\epsilon, 0, \ldots, 0)$;

If $$\frac{(1-|x_{*1}|)^2}{2n} \leq T < 0$$

then choose r_0 so that

$$r_0^2 = - \frac{2nT}{(1-|x_{*1}|)^2}$$

and with $\epsilon = |x_{*1}|$ recomputer(13-21). The points p_i, with $t_i=0$, $i=1,\ldots,n+1$, lie on the surface of $S_{n,r,-\epsilon}$ which is the n-sphere of radius $r=r_0(1-|x_{*1}|)$ and center of $p_{-\epsilon} = (x_{*1},0,\ldots,0)$.

case iii) $x_{*1} > 0$.

In this case, make the following changes to the equations of Table 1:

(14) becomes $x'_{*1} = -x_{*1} + \epsilon$,

(17) becomes $v_{11} = -(r-\epsilon)$,

(18) becomes $v_{21} = - \left[\frac{(n-1)\bar{x}_{*1} - 1}{n} \quad r-\epsilon \right]$,

and perform the previous analysis of case (ii). The points p_i, with $t_i=0$, $i=1,\ldots,n+1$ lie on the surface of $S_{n,r,-\epsilon}$ which is the n-n-sphere of radius $r=r_0(1-\epsilon)$ with center at $p_\epsilon = (\epsilon,0,\ldots,0)$.

<u>Example 3. Formulas of Theorem 7.</u>

Here we give an example of a formula of Theorem 7 for the non-cylindrical region defined by the paraboloid of revolution, P_3,

$$x_1^2 + x_2^2 \leq r_T^2 \,(|T|+t), \; T \leq t \leq 0,$$

where r_T and T are given constants which describe the paraboloid. The point p_* is assumed to lie on the x_1-axis,

$$p_* = (x_{*1},0,0), \; x_{*1} \in (-r_T\,(|T|)^{1/2}, \; r_T(|T|)^{1/2}).$$

One can verify directly that the points and coefficients

$$p_i - p_*, \; A_i, \; i=1,2,3$$

satisfy equations (9) with n=2. The p_i, A_i, i=1,2,3 are given in Table 2. Since the cross sections of the paraboloid are circles, the relationship between the formulas of Table 1 and Table 2 for n=2 is clear. If we define a general (n+1)-dimensional paraboloid, P_{n+1}, as

$$x_1^2 + \ldots + x_n^2 \leq r^2 = r_\tau^2\ (|T| + t),\ T \leq t \leq 0,$$

so that any cross section is $S_{n,r}$, the n-sphere of radius r with center at the origin, the extensions of formulas of Table 2 based on those of Table 1 is direct.

Table 2

A Formula of Degree 2 for P_3

$$p_1 = (v_{11},\ 0\ ,t')$$
$$p_2 = (v_{21}, v_{22}, t')$$
$$p_3 = (v_{21}, v_{32}, t')$$

where,

$$t' = \frac{x_{*1}^2 - r_\tau^2 |T|}{4 + r_\tau^2},$$

$$r = r_\tau^2(|T| + t'),$$

$$\bar{x}_{*1} = x_{*1}/r,$$

$$\beta = 3 - \bar{x}_{*1}$$

$$v_{11} = r,$$

$$v_{21} = \frac{\bar{x}_{*1} - 1}{2}\ r,$$

$$v_{22} = -v_{32} = \left[\frac{(\bar{x}_{*1} + 1)\beta}{4}\right]^{\frac{1}{2}} r,$$

$$A_1 = \frac{\bar{x}_{*1} + 1}{\beta},\ A_2 = A_3 = \frac{1 - \bar{x}_{*1}}{\beta}.$$

4. n-POINT FORMULAS OF DEGREE 2n-1 IN 2 VARIABLES

In this section we shall consider n-point interpolation formulas

$$u(x_*, t_*) \approx \sum_{i=1}^{n} A_i \; u(x_i, t_i) \tag{23}$$

of degree 2n-1 for the half plane $t \geq 0$, $-\infty < x < \infty$, and for the rectangular region, G, shown in Figure 1.

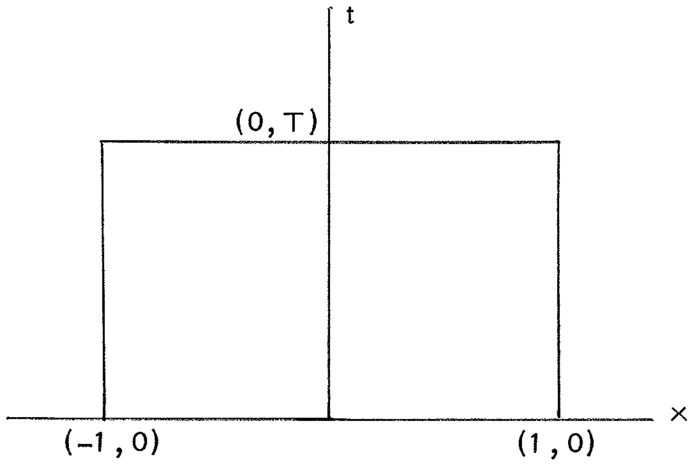


Figure 1

Rectangular Region G: $\{(x,t) \mid -1 < x < 1,\ 0 < t \leq T\}$

We shall consider various configurations of interpolation points on the boundary of the rectangular region.

4.1 The Half Plane, $t > 0$, $-\infty < x < \infty$

Consider the following Cauchy (initial value) problem of heat conduction

$$\begin{aligned} L_1[u(x,t)] &= 0 \text{ for } -\infty < x < \infty,\ t > 0 \\ u(x,0) &= f(x) \end{aligned} \tag{24}$$

If we wish to approximate the value of $u(x,t)$ by a linear combination of its boundary values, we must have all of the interpolation points, p_i, lying on the x-axis, i.e., $p_i = (x_i, 0)$, $i=1,\ldots,n$. Because of Lemma 1 we can choose, without loss of generality, $p_* = (x_*, t_*) = (0, t_*)$.

If formula (23) is to be of degree 2n-1, then the p_i, A_i, $i=1, \ldots, n$ must satisfy (from Definition 2) the following non-linear system of 2n equations in 2n unknowns,

$$\begin{array}{lllll} A_1 & + A_2 & + \ldots + A_n & = c_0 \\ A_1 x_1 & + A_2 x_2 & + \ldots + A_n x_n & = c_1 \\ \vdots & \vdots & \vdots & \\ A_1 x_1^{2n-2} & + A_2 x_2^{2n-2} & + \ldots + A_n x_n^{2n-2} & = c_{2n-2} \\ A_1 x_1^{2n-1} & + A_2 x_2^{2n-1} & + \ldots + A_n x_n^{2n-1} & = c_{2n-1} \end{array} \qquad (25)$$

where the $c_i = \upsilon_i\ (0, t_*)$ are given by

$$c_i = \begin{cases} 0 & i=1, 3, \ldots, 2n-1 \\ \dfrac{i!}{(i/2)!}\ (t_*)^{\frac{1}{2}} & i=0, 2, \ldots, 2n-2 \end{cases} \qquad (26)$$

This representation for the c_i is obtained from (7) with $x=0$ and $t=t_*$. System (25) closely resembles the nonlinear system of equations which arises in the determination of the points and weights of Gaussian Quadrature formulas. Let us review, for a moment, a few elementary concepts and results from this theory which is concerned with obtaining approximations of the following type,

$$\int_a^b w(y)\ f(y)\ dy \simeq \sum_{i=1}^{n} B_i\ (f(y_i)) \qquad (27)$$

We will say the y_i, B_i, $i=1, \ldots, n$, are a quadrature formula. A quadrature formula is said to have degree d if it is exact whenever f(y) is a polynomial of degree $\leq d$ (or equivalently, whenever $f(y) =$ $f(y) = 1, y, \ldots, y^d$) and it is not exact for $f(y) = y^{d+1}$. Thus, if we are to have a formula of degree $d = 2n-1$, the y_i, B_i, $\epsilon=1, \ldots, n$ must satisfy the following system of 2n equations in 2n unknowns,

$$\begin{array}{lllll} B_1 & + B_2 & + \ldots + B_n & = c_0 \\ B_1 y_1 & + B_2 y_2 & + \ldots + B_n y_n & = c_1 \\ \vdots & \vdots & \vdots & \vdots \\ B_1 y_1^{2n-2} & + B_2 y_2^{2n-2} & + \ldots + B_n y_n^{2n-2} & = c_{2n-2} \\ B_1 y_1^{2n-1} & + B_2 y_2^{2n-2} & + \ldots + B_n y_n^{2n-1} & = c_{2n-1} \end{array} \qquad (28)$$

where the c_k are given by

$$c_k = \int_a^b w(y)\, y^k\, dy, \quad k=0,1,\ldots,2n-1.$$

The following result is known (see, for example, Krylov [9]),

Theorem 8. If the weight function, $w(y)$, is nonnegative in $[a,b]$, ($[a,b]$ finite or infinite), the points y_i and weights B_i, $i=1,\ldots,n$ can be found so that (27) has degree $d=2n-1$, i.e., such that (28) has a solution. Moreover, the y_i, $i=1,\ldots,n$ are roots of the unique n'th degree polynomial which is orthogonal with respect to $w(y)$ on the interval $[a,b]$, and the weights B_i, $i=1,\ldots,n$ are positive. □

Thus, to show that p_i, A_i, $i=1,\ldots,n$ can be found such that (25) has a solution, it is sufficient to show that the $\overline{c}_i$ defined by (26) are the moments of a nonnegative weight function on the interval $-\infty$ to ∞. That this is not unreasonable is suggested

a) by the fact that the heat polynomials are related to the Hermite polynomials, $H_j(y)$, as mentioned in Section 2,

$$v_j(x,-t) = t^{j/2}\, H_j\left(x/(4t)^{1/2}\right) \tag{29}$$

and,

b) because the fundamental solution

$$k(x,t) \equiv \frac{e^{-x^2/4t}}{(4\pi t)^{1/2}}$$

is the "heat kernel" + of the Cauchy Problem (24), i.e., if $u(x,t)$ is bounded, then we have

$$u(x,t) = \int_{-\infty}^{\infty} k(x-y,t)\, f(y)\, dy.$$

Rosenbloom and Widder [3] have shown

+ see, for example, Weinberger [10].

Theorem 9. The heat polynomials $v_n(x,t)$ have the following representation

$$v_n(x,t) = \int_{-\infty}^{\infty} k(x-\xi, t)\xi^n d\ . \quad \square$$

Thus, we have

Theorem 10. (i) The $\bar{c}_i$ of (26) are the monomial integrals of the positive weight function $k(-\xi, t_*)$, (ii) p_i, A_i, $i=1,\ldots,n$ can be found so that (25) has a solution, i.e., so that formula (23) has degree $2n-1$, (iii) moreover, the x_i, $i=1,\ldots,n$ are the roots of the n'th degree Hermite polynomial $H_n(x/(4t_*)^{\frac{1}{2}})$, and the A_i, $i=1,\ldots,n$ are positive.

Proof. Since $\bar{c}_i = v_i(0, t_*)$, the first statement is a direct application of Theorem 9 and the second statement then follows from Theorem 8, Also, we note the Hermite polynomials, $H_n(x/(4t_*)^{\frac{1}{2}})$, form an orthogonal system on the interval $-\infty$ to ∞ with respect to the weight function $e^{-x/4t_*}$. Thus (iii) is a direct application of (i), equation (29), and Theorem 8 to system (25). $\square$

Due to the relationship between systems (25) and (28), the weights A_i can be formulated in terms of the orthogonal polynomials related to system (25) just as the weights B_i are formulated in terms of the orthogonal polynomials associated with system (28); (see, Stroud and Secrest [11]); for example, we can write

$$A_i = [k_0^2 v_0(x_i, -t_*) + \ldots + k_{n-1}^2 v_{n-1}(x_i, -t_*)]^{-1}, \quad i=1,\ldots,n$$

or,

$$A_i = [k_n^2 v_n'(x_i, -t_*) v_{n+1}(x_i, -t_*)]^{-1}, \quad i=1,\ldots,n$$

where

$$k_n = \int_{-\infty}^{\infty} k(x, t_*)\,[v_n(x, -t_*)]^2\,dx = n!\,(2t_*)^n$$

and

$$x_i = y_i(4t_*)^{\frac{1}{2}}, \quad i=1,\ldots,n \tag{30}$$

The y_i, $i=1,\ldots,n$ are the roots of the n'th degree Hermite polynomial, $H_n(y)$. These roots are symmetrically distributed about $y=0$. We can also write the A_i as

$$A_i = \frac{(n-1)!\,2^n}{H_{n-1}(y_i)\,H_{n+1}(y_i)} \quad , \ i=1,\ldots,n \tag{31}$$

Tbale 3 gives the y_i and A_i, $i=1,\ldots,n$ where $n=2(1)10$. The A_i were calculated from (31) with the y_i given in Stroud and Secrest [11].

4.2 The Rectangular Region G

A. All points on the x-axis.

The results of Theorem 10 for the half plane can be immediately extended to the rectangular region G of Figure 1 for interpolation formulas with all of the interpolation points on the portion of the boundary given by $S_2 : \{(x,y) \mid -1\le x\le 1,\ t=0\}$. For this case, we are solving system (25) subject to the constraint that

$$|x_i| \le 1, \quad i=1,\ldots,n$$

Let $y_{n,max}$ be the largest root of the n'th degree Hermite polynomial. We see immediately from (30) that for any point $p_* = (x_*, t_*) \in \text{Int } G$ such that

$$t_* \le \frac{(1-|x_*|)^2}{4y^2_{n,max}}$$

the x_i given by (30) satisfy the constraint $|x_i| \le 1$. The region for which formulas (23) exist with all points on S_2 is shown in Figure 2.

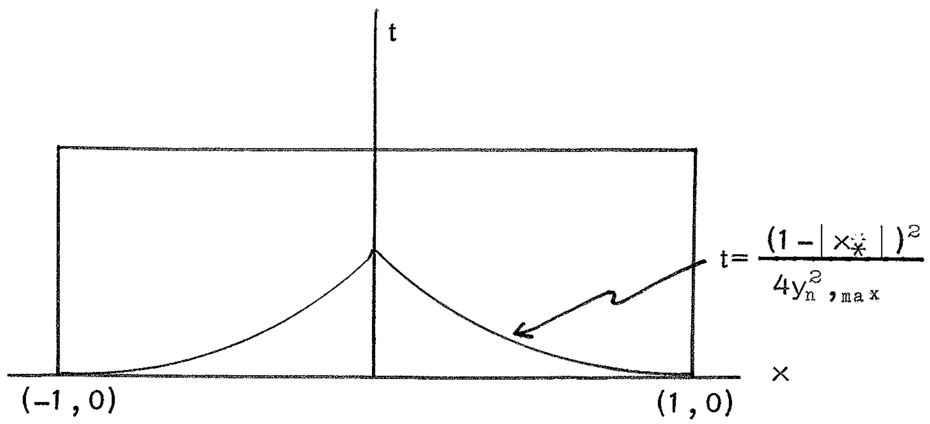


Figure 2

Region for formulas (23) in region G with all points on x-axis

Table 3

Formulas of Degree 2n-1 for the Half Plane

n	y_i	A_i
2	.7071 0678 12	.5000 0000 00
3	.1224 7448 71	.1666 6666 67
	.0000 0000 00	.6666 6666 67
4	.1650 6801 24 (1)	.4587 5854 77 (-1)
	.5246 4762 33	.4541 2414 52
5	.2020 1828 70 (1)	.1125 7411 33 (-1)
	.9585 7246 46	.2220 7592 20
	.0000 0000 00	.5333 3333 33
6	.2350 6049 74 (1)	.2555 7844 02 (-2)
	.1335 8490 74 (1)	.8861 5746 04 (-1)
	.4360 7741 19	.4088 2846 96
7	.2651 9613 57 (1)	.5482 6885 60 (-3)
	.1673 5516 29	.3075 7123 97 (-1)
	.8162 8788 29	.2401 2317 86
	.0000 0000 00	.4571 4285 71
8	.2930 6374 20 (1)	.1126 1453 84 (-3)
	.1981 6567 57 (1)	.9635 2201 21 (-2)
	.1157 1937 12 (1)	.1172 3990 77
	.3811 8699 02	.3730 1225 77
9	.3190 9932 02 (1)	.2234 5844 01 (-4)
	.2266 5805 85 (1)	.2789 1413 21 (-2)
	.1468 5532 89 (1)	.4991 6406 77 (-1)
	.7235 5101 88	.2440 9750 29
	.0000 0000 00	.4063 4920 63
10	.3436 1591 19	.4310 6526 31 (-5)
	.2532 7316 74 (1)	.7580 7093 43 (-3)
	.1756 6836 49 (1)	.1911 1580 50 (-1)
	.1036 6108 30 (1)	.1354 8370 30
	.3429 0132 72	.3446 4233 49

It should be noted here that for n=2 and n=3 these formulas become

$$u(x_*, t_*) \simeq \tfrac{1}{2} u(x_* - \sqrt{2t_*}, 0) + \tfrac{1}{2} u(x_* + \sqrt{2t_*}, 0), \quad t_* \le \frac{(1-|x_*|)^2}{2}$$

and

$$u(x_*, t_*) \simeq \tfrac{1}{6} u(x_* - \sqrt{6t_*}, 0) + \tfrac{2}{3} u(x_*, 0) + \tfrac{1}{6} u(x_* + \sqrt{6t_*}, 0), \quad t_* \le \frac{(1-|x_*|)^2}{6} .$$

These formulas are directly related to the classical explicit finite difference approximation to $L_1[u] = 0$ given by $(\overset{*}{* * *})$, i.e.,

$$u_{i,j+1} = u_{i,j} + \tau(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}),$$

where $u_{i,j} = u(x_i, t_j)$ and $\tau = \ell/h$, ℓ and h the mesh parameters.

Remark When $\tau = 1/2$ we have the formula for n=2. This is the maximum choice of τ allowable so that the finite difference scheme is stable. When $\tau = 1/6$ we have the formula for n=3. Saul'yev [12, p. 98], notes that for this choice of τ, the finite scheme has the hightest accuracy ($O(h^4)$) which can be obtained with the classical explicit method.

B. General Configuration of Interpolation Points for G.

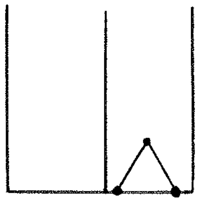
Let S_1 and S_3 be the sets: $S_1 : \{(x,t) \mid x=-1,\ 0 \le t \le T\}$ and $S_3 : \{(x,t) \mid x=1,\ 0 \le t \le T\}$ respectively. We now ask the more general question: Given a point $p_* \in \text{Int } G$, does there exist an interpolation formula (23) of degree 2n-1 with n_{S_1} points on side S_1, n_{S_2} points on side S_2, and n_{S_3} points on side S_3, $n_{S_1} + n_{S_2} + n_{S_3} = n$? Or, assuming the existence of such a formula, the question becomes: What is the distribution of interpolation points on $D = S_1 \cup S_2 \cup S_3$ for a given $p_* \in \text{Int } G$. The points and weights p_i, A_i, i=1,...,n must satisfy the following nonlinear system of 2n equations in 2n unknowns,

$$\sum_{i=1}^{n_{S_1}} A_i v_j(-1, t_i) + \sum_{i=n_{S_1}+1}^{n_{S_1}+n_{S_2}} A_i v_j(x_i, 0) + \sum_{i=n_{S_1}+n_{S_2}+1}^{n} A_i v_j(1, t_i) = v_j(x_*, t_*) \quad (32)$$

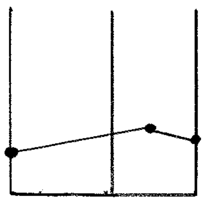
where j=0,...,2n-1. The solution of this system for n=2 for various combinations of n_{S_1}, n_{S_2}, and n_{S_3} is straightforward. After some algebraic manipulation, one arrives at the formulas summarized in Table 4. For n > 2 the situation is much different and closed form solutions to this system are difficult to obtain except in a few special cases for

Table 4

Summary of 2 Point Formulas of Degree 3



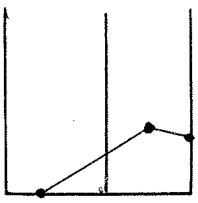
$x_1 = x_* - \sqrt{2t_*}$, $x_2 = x_* + \sqrt{2t_*}$,
$t_1 = t_2 = 0$, $t_* \le \dfrac{(1-x_*)^2}{2}$, $A_1 = A_2 = 1/2$.



$x_1 = -1$, $x_2 = 1$, $t_1 = t_* - \dfrac{(1+x_*)(3-x_*)}{6}$,

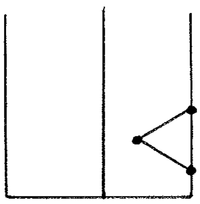
$t_2 = t_* - \dfrac{(3+x_*)(1-x_*)}{6}$, $A_1 = (1-x_*)/2$,

$A_2 = (1+x_*)/2$, $t_* \ge \dfrac{(1+x_*)(3-x_*)}{6}$.



Let $b = \sqrt{(x_*-1)^2 + 6t_*}$, $x_1 = 1-b$, $x_2 = 1$,

$t_1 = 0$, $t_2 = \dfrac{b[(x_*-1)(x_*-1+b) + 2t_*]}{2(b + (x_*-1))}$,
$A_1 = (1-x_*)/b$, $A_2 = 1-(1-x_*)/b$,
$(x_*-1)/2 \le t_* \le (1+x_*)(3-x_*)/6$.



Formulas do not exist.

small n. Here, for example, is a 3 point formula of degree 5 for $p_* = (0, t_*)$, $t_* \geq 1/6$,

$$u(0, t_*) = A_1 u(-1, t_1) + A_2 u(0,0) + A_3 u(1, t_3)$$

where

$$A_1 = A_3 = \frac{t_* \sqrt{9t_*^2 + 6} - 3t_*^2}{2}, \quad A_2 = 1 - 2A_1,$$

$$t_1 = t_3 = \frac{\sqrt{3(3t_*^2+2)} - 3(1-t_*)}{6}$$

To obtain numerical solutions to system (32) the author has employed the Newton- Raphson method of approximating the solution of nonlinear systems. System (32) was rewritten as

$$f_j(\bar{y}) = 0, \quad j=0, \ldots, 2n-1$$

where $\bar{y}$ is a vector having components in the unknowns A_i, x_i, and t_i. The iterative process then becomes

$$\bar{y}_{k+1} = \bar{y}_k + [J]_k^{-1} f_k$$

where k is the iteration step. J is the Jacobian matrix of the system,

$$J_{ij} = \frac{\partial f_i}{\partial y_j}$$

and the notation $\bar{y}_k$, $[J]_k^{-1}$, and f_k means that the components of each of these matrices are evaluated with the values of the components y_i at iteration k. Let the first n components of y be the A_i, the next n_s, be the t_i on side S_1, the next n_{S_2} be the x_i on side S_2, and the last n_{S_3} be the t_i on side S_3. Then, using the following relationships,

$$\frac{\partial f_0}{\partial A_j} = 1, \quad \frac{\partial f_i}{\partial A_j} = \upsilon_i(x_j, t_j), \quad i=1, \ldots, 2n-1, \quad j=1, \ldots, n,$$

$$\frac{\partial f_0}{\partial x_j} = 0, \quad \frac{\partial f_i}{\partial x_j} = iA_j \upsilon_{i-1}(x_j, t_j), \quad i=1, \ldots, 2n-1, \quad j=n_{S_1}+1, \ldots, n_{S_1}+n_{S_2},$$

$$\frac{\partial f_0}{\partial t_j} = \frac{\partial f_1}{\partial t_j} = 0, \quad \frac{\partial f_i}{\partial t_j} = i(i-1)A_j \upsilon_{i-2}(x_j, t_j) \quad i=2, \ldots, 2n-1,$$

$$j=1, \ldots, n_{S_1}, \; j=n_{S_1}+n_{S_2}+1, \ldots, n,$$

$$\begin{bmatrix} \overbrace{\begin{matrix} 1 \\ \upsilon_1(x_i, t_i) \\ \upsilon_2(x_i, t_i) \\ \upsilon_3(x_i, t_i) \\ \vdots \\ \upsilon_{2n-1}(x_i, t_i) \end{matrix}}^{n \text{ columns}} & \overbrace{\begin{matrix} 0 \\ 0 \\ 2A_j \\ 6A_j \upsilon_1(x_j, t_j) \\ \vdots \\ (2n-1)(2n-2)A_j \upsilon_{2n-3}(x_j, t_j) \end{matrix}}^{n_{s_1} \text{ columns}} & \overbrace{\begin{matrix} 0 \\ A_k \\ 2A_k \upsilon_1(x_k, t_k) \\ 3A_k \upsilon_2(x_k, t_k) \\ \vdots \\ (2n-1)A_k \upsilon_{2n-2}(x_k, t) \end{matrix}}^{n_{s_2} \text{ columns}} & \overbrace{\begin{matrix} 0 \\ 0 \\ 2A_\ell \\ 6A_\ell \upsilon_1(x_\ell, t_\ell) \\ \vdots \\ (2n-1)(2n-1)A_\ell \upsilon_{2n-3}(x_\ell, t_\ell) \end{matrix}}^{n_{s_3} \text{ columns}} \end{bmatrix}$$

$$\begin{aligned} \text{where } i &= 1, \ldots, n, \\ j &= 1, \ldots, n_{s_1}, \\ k &= n_{s_1} + 1, \ldots, n_{s_1} + n_{s_2} \\ \ell &= n_{s_1} + n_{s_2} + 1, \ldots, n. \end{aligned}$$

Figure 3

Equation (5.33): The Jacobian Matrix

the Jacobian matrix can be written as shown in Figure 3.

A computer program was written for the solution of this nonlinear system. (Formulas are tabulated for a variety of 3, 4, 5, 6, and 7 point interpolation formulas in Shriver [7].) The solution of this system is not without computational difficulties. For example, given a point $p_* = (x_*, t_*)$, with x_* fixed, as t_* increases the x_i on S_2 become larger and there are values of t_* for which the configuration of points on the boundary and, hence, the structure of the Jacobian matrix change. An example of such a configuration change is shown in Figure 4.

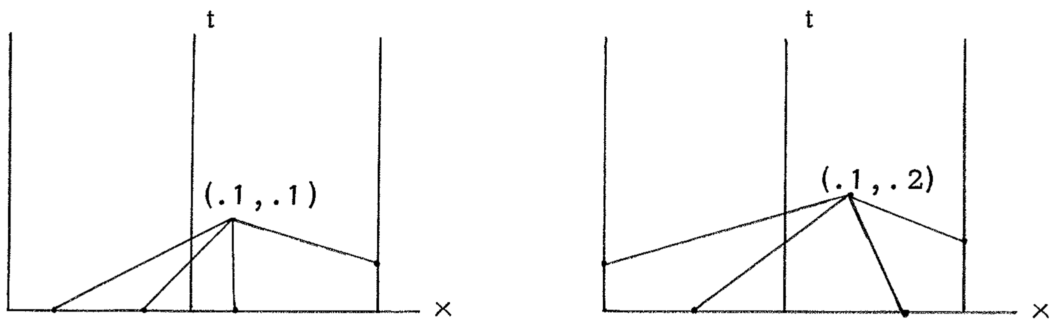


Figure 4

A Change in the Configuration of Interpolation Points

5. CONCLUDING REMARKS

This paper and reference [7] are only the beginning efforts to investigate the existence, construction, and properties of interpolation formulas (1). There are many questions still open. For given integers N and d and a point $p_* \in \text{Int } R_{n+1}$, do there exist points $p_i = (v_{i1}, \ldots, v_{in}, t_i) \in \text{Bd } R_{n+1}$, $i=1,\ldots,N$, and weights A_i, $i=1,\ldots,N$, so that formula (1) has degree d. The existence or nonexistence of such formulas for arbitrary regions and degree is not yet known in general. Moreover, we are interested in those formulas which for a given number of points, N, have the highest degree, d, possible. The questions of appropriate error estimates to be used with such formulas and the identification of the class of solution functions for which they are valid must also be investigated.

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