OPTIMAL QUADRATURE FORMULAE FOR CERTAIN CLASSES OF HILBERT SPACES

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ABSTRACT

Recently there has been growing interest in quadratures with the so called "least estimate of the remainder" or "optimal" quadratures. Sometimes these formulae are preferable to the classical formulae because they provide error bounds in which the dependences of the formula and those of the function are separated.

In this thesis we consider certain Hilbert spaces of functions with known smoothness and develop optimal formulae for these spaces using the techniques of Functional Analysis. It is shown that these results extend similar results obtained elsewhere for the optimal formulae over the spaces $L_q^{(r)}$. The convergence properties of the formulae are derived and certain numerical considerations concerning their use are discussed.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any University and to the best of the author's knowledge and belief the thesis contains no material previously published or written by another person except where due reference is made in the text of the thesis.

Signed...

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1.1 Introduction

In the problem of quadrature we are concerned with the approximation of the integral

$$I(f) = \int_{t_1}^{t_2} f(x)\,dx, \qquad (1.1)$$

by the sum

$$Q_n(f) = \sum_{j=1}^{n} \sum_{i=1}^{N} A_{ij} f^{(i-1)}(x_j). \qquad (1.2)$$

In all that follows we shall consider the interval (t_1, t_2) to be finite and A_{ij}, x_j real, $x_j \in [t_1, t_2]$.

The accuracy of the quadrature depends on n, A_{ij} and the x_j. For simplicity let us for a moment consider that only function values will be used in the sum (1.2) and so $N=1$. Then there are $2n$ parameters to choose in order that the quadrature be completely defined: n parameters A_{ij} called weights, and n parameters x_j called mesh points or nodes. ~~Clearly~~ Within very broad limits, the larger is n the more accurate can our quadrature be made, for then we have more parameters to choose. So we shall consider n to be arbitrarily chosen but fixed throughout this discussion.

The accuracy of a quadrature is measured in terms of the error $E(f) = I(f) - Q_n(f)$ and the choice of the parameters A_{ij}, and x_j is directed to reduce this error. Sometimes some of the parameters may be specified by the particular problem; for example if the values of the integrand are given at prescribed points then the x_j are no longer free parameters and we have only to choose the A_{ij}. Alternatively since the roundoff error committed in computing quadrature sums is reduced the more nearly are the weights equal, we may want to constrain the weights to all be equal. Once again we are restricted, this time to choosing only the x_j. So that in practice, once we have determined the type of quadrature that we seek (i.e. equal weights or, equal mesh or perhaps some other type), we can turn our attention to choosing the remaining parameters so that the error $E(f)$ is reduced.

For example, (1) in the earliest type of quadrature formulae the mesh distribution was the so called "equally-spaced" mesh:

$$x_j - x_{j-1} = \text{constant} = \frac{t_2 - t_1}{n-1}, \quad j=2,\dots,n-1.$$

$$x_1 = t_1, \quad x_n = t_2.$$

The remaining n parameters $A_{11},\dots,A_{1n}$ were then chosen to satisfy certain conditions imposed on $E(f)$. In another case (2) the set $\mathfrak{Q}$ of all quadrature formulae considered consisted of those formulae with all weights equal to some constant, say A. The remaining n+1 parameters $x_1,\dots,x_n$ and the constant A were then chosen to satisfy conditions imposed on $E(f)$. In a third case (3) there were no restrictions on the $A_{11},\dots,A_{1n}$ or on the $x_1,\dots,x_n$ and the 2n conditions on E were used to completely define Q_n.

The important question in all of these cases was however "what are the conditions to be imposed on E(f)?" The following theorem, due to Weierstrass, is often used as a ~~gave the~~ basis. ~~for these conditions~~.

<u>Theorem:</u> Let f(x) be any function which is continuous on the interval $[t_1,t_2]$. Then for every $\varepsilon>0$ there exists a polynomial p(x) such that

$$|f(x) - p(x)| < \varepsilon \quad \text{for all} \quad x \in [t_1,t_2].$$

(For proof see, e.g. [1] chapter 15, p 481.)

Thus any function continuous on a closed finite interval could be approximated to an arbitrary order of precision by a polynomial of some degree. Although the theorem does not apply for all prior choices of x_j ~~gave~~ and gives no indication of the degree required for a particular order of approximation ~~but~~ it nevertheless was a powerful tool ~~none-the-less~~.

Accordingly quadratures were constructed which were exact for polynomials of as high degree as possible. For case (1) the resulting formulae are called Newton-Cotes formulae and are exact for polynomials of degree less than or equal to n-1, and of degree n when n is odd. They are therefore said to have <u>order of</u>

<u>precision</u> n-1. They include such well known rules as the Trapezoidal rule and Simpson's rules. They are amongst the most widely used quadrature formulae - in former years because of their simplicity (when used with desk calculators, for example) and more recently, with the advent of computing machinery, for their generality.

For case (2) the formulae developed were called the Chebyshev Quadrature Formulae and the n+1 "free" parameters were chosen to give the formulae a degree of precision of n. In 1937 Bernstein [4] showed that these formulae exist only for the values of n = 1,2,3,4,5,6,7,9. In spite of this restriction the formulae ~~have been useful~~ could be used because most quadratures used in practice are of low degree.

For case (3) the conditions that the formulae be exact for polynomials of degree less than or equal to 2n-1 led to what are now called the Gauss-Legendre Quadrature Formulae. And once again these formulae are widely used.

A quadrature formula is said to be <u>interpolatory</u> if it can be derived by the integration of an interpolation formula. All the quadratures mentioned so far are interpolatory in nature and each has the same degree of precision as the interpolation formula from which it derives. The generality of these interpolatory quadrature formulae, which one could say derives from the generality of the theorem on which they are based, severely limits the precision of any analysis of their errors. Krylov [7] shows, for example, (for n even) that if the derivative $f^{(n)}(x)$ is continuous on the interval (t_1, t_2) then for any Newton-Cotes ~~interpolatory~~ quadrature formula there exists $\xi \in (t_1, t_2)$ such that the error of the formula satisfies

$$E(f) = \frac{f^{(n)}(\xi)}{n!} \int_{t_1}^{t_2} \omega(x)\,dx, \tag{1.3}$$

$$\omega(x) = (x-x_1)(x-x_2)\dots(x-x_n),$$

and there is a similar formula involving $f^{(n+1)}(x)$ for n odd. ~~this will therefore apply to the Newton-Cotes formulae.~~
For the Gauss-Legendre formulae there is a better form if $f^{(2n)}(x)$ is continuous on $[t_1, t_2]$ for then there exists $\eta \in (t_1, t_2)$ such that remainder satisfies

$$E(f) = \frac{f^{(2n)}(\eta)}{(2n)!} \int_{t_1}^{t_2} \omega^2(x)\,dx.$$

But it is often difficult to use these estimates because, in the first place, the order of derivative on which the error depends varies as n or 2n and, in the second place, we do not, in general, know where ξ and η lie in the interval $[t_1, t_2]$. If, however, we know that $f^{(n)}$ is bounded in absolute value on $[t_1, t_2]$ by some number M_n:

$$|f^{(n)}(x)| \leqslant M_n \quad x \in [t_1, t_2] \qquad (1.3.1)$$

then we can obtain the estimate

$$|E(f)| \leqslant \frac{M_n}{n!} \int_{t_1}^{t_2} |\omega(x)| dx \qquad (1.3.2)$$

for the Newton-cotes formulae, and if $\omega(x)$ does not change sign on $[t_1, t_2]$, this estimate cannot be improved; that is to say there will always exist functions satisfying (1.3.1) which will attain the bound (1.3.2). In fact, for an arbitrary set of nodes we can obtain the precise estimate for $E(f)$ (for any function satisfying (1.3.1))

$$|E(f)| \leqslant M_n \int_{t_1}^{t_2} |K(t)| dt$$

where $K(t)$, the kernel function, is

$$K(t) = \int_{t_1}^{t_2} [J(x-t)-J(t_1-t)] \frac{(x-t)^{r-1}}{(r-1)!} dx$$

$$- \sum_{k=1}^{n} A_{1k} [J(x_k-t)-J(t_1-t)] \frac{(x_k-t)^{r-1}}{(r-1)!},$$

and $J(x)$ is the familiar jump function

$$J(x) = \begin{cases} 1 & x > 0, \\ \frac{1}{2} & x = 0, \\ 0 & x < 0. \end{cases}$$

Clearly then these quadratures ~~are~~ may be poor when the bound M_n on the derivative of f is large. In fact these rules of highest degree of precision sometimes give worse results than the simpler rules such as the Mid-point rule, the Trapezoidal or Simpson's rule. This occurs usually when they are applied to functions of low order of differentiability or functions with singularities near the interval of integration.

Thus whenever we try to improve the accuracy of a quadrature formula of this type by increasing the number of points and so the degree of precision of the formula, we may introduce a coarser estimate of the error because then the error depends on a higher derivative of the integrand. To avoid this situation composite or compound integration rules were devised. These formulae are applied in the following way: the interval (t_1, t_2) is divided up into say m subsegments and on each of these subsegments a formula of low degree of precision is applied. Consequently more points have been used, the formula is more accurate and the error depends on a derivative of the integrand which is of a low order.

These composite formulae, while they offer a simple solution to the problem of increasing the accuracy of a formula without increasing the order of the formula, use in-formation of a local nature and not a <u>global</u> one. That is to say the information used on any subsegment of the interval of integration comes from that subsegment only. For example the compound rules take no account of any smoothness properties that the integrand may possess at the end-points of the subsegment. Therefore more accurate rules can be devised which do take account of all the information that is available about the integrand. Such formulae are the "quadratures with least estimate of error" but before discussing them we need certain notions from the functional analysis.

1.2 Normed Linear Spaces

The set $F = \{f\}$ of elements f is called <u>linear</u> if the operations of addition $f+g$ between elements of F and multiplication αf by a real or complex scalar $\alpha \in S$, a scalar field, define a new element of F. These operations must satisfy:

(a) $f+g = g+f$ (commutivity of addition)

(b) $(f+g)+h = f+(g+h)$ (associativity of addition)

(c) There exists a zero element $\emptyset$ such that

$$f + \emptyset = f$$

(d) There exists an inverse $-f$ to each $f \in F$ such that

$$f + (-f) = \emptyset$$

(e) $\alpha(\beta f) = (\alpha\beta)f$ (associativity of multiplication)

(f) $(\alpha+\beta)f = \alpha f + \beta f$ and $\alpha(f+g) = \alpha f + \alpha g$ (distribution)

(g) $1.f = f$

(h) $0.f = \emptyset$

(i) if $\alpha f = \emptyset$ and $f \neq \emptyset$ then $\alpha = 0$.

We say that the linear space F is <u>normed</u> if for each $f \in F$ there exists a norm, denoted $\|f\|$, that is a real non-negative number satisfying

(a) $\|f\| \geq 0$ with equality iff $f = \emptyset$

(b) $\|f+g\| \leq \|f\| + \|g\|$

(c) $\|\alpha f\| = |\alpha| . \|f\|$

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Associated with a Normed Linear Space are the notions of convergence and completeness.

A sequence $\{f_n\}_{n=1}^{\infty}$, $f_n \in F$ is said to be a "<u>Cauchy Sequence</u>" if

$$\lim_{n,m\to\infty} \|f_n - f_m\| = 0$$

A sequence $\{f_n\}_{n=1}^{\infty}$, is said to be <u>convergent</u> if there exists $f \in F$ such that

$$\lim_{n\to\infty} \|f_n - f\| = 0.$$

A Normed Linear Space is said to be <u>complete</u> if every Cauchy Sequence of its elements is convergent. A complete Normed Linear Space is called a <u>Banach</u> space.

An Inner Product Space is a Linear Space F in which to every pair of elements f and g there exists a bilinear function (f,g) defining a scalar value and satisfying

(a) $(\alpha f, g) = \alpha(f,g)$, α scalar

(b) $(f,f) \geq 0$ with equality iff $f = \emptyset$

(c) $(f+g,h) = (f,h) + (g,h)$

(d) $(f,g) = \overline{(g,f)}$, $(= (g,f)$ if ~~f,g are real~~ the field of scalars is the real numbers ~~valued functions~~).

A complete Inner Product Space with the norm $\|f\|$ defined by $(f,f)^{\frac{1}{2}}$ is called <u>a Hilbert Space</u>.

The properties of orthogonality and distance associated with Hilbert Spaces give rise to the following important result known as the <u>Decomposition</u> Theorem.

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<u>Theorem</u>: Let M be any closed subspace of a Hilbert space H. Then every element $f \in H$ can be <u>uniquely</u> expressed in the form $f = g+h$ where $g \in M$ and $(h,k) = 0$ for any $k \in M$.
In this case g is called the projection of f in M and

$$\|h\| = \|f-g\| \leqslant \|f-k\| \quad \text{for each } k \in M.$$

(for proof see e.g. [13], Chapter III §1)

Functionals over Linear Spaces

An operator ℓ which maps F into the scalar field S is called a <u>linear functional</u> if it is linear and additive i.e.

$$\ell(\alpha f + \beta g) = \alpha\ell(f) + \beta\ell(g)$$

The following theorem will be used later.
A linear functional is continuous if it is bounded.
(proof: Refer to [13], Chapter I §6)
We denote F^* the set of all continuous linear functionals defined on F and we define the norm $\|\ell\|$ of $\ell \in F^*$ by

$$\|\ell\|_{F^*} = \sup_{\|f\|_F = 1} |\ell(f)|$$

F^* is called the <u>dual</u> of F.
One of the most important results relating to Hilbert spaces which we will use is the so called Riesz Representation Theorem which states:
For every linear functional $\ell \in H^*$ defined on a Hilbert space H there exists a unique element $g_\ell \in H$ such that

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$$\ell(f) = \sout{(g_\ell, f)}\ (f, g_\ell)$$

and

$$\|\ell\|_{H^*} = \|g_\ell\|_{H}.$$

1.3 Quadratures with Least Estimate of the Remainder

Suppose we are given a closed and bounded set B_1 of functions f and that we characterize the accuracy of a quadrature formula $Q \in \mathcal{Q} = \{$all quadrature formulae of the type (1.2)$\}$ by the real number

$$\zeta = \sup_{f \in B_1} |I(f) - Q_*(f)|,$$

$$= \sup_{f \in B_1} |E(f)|. \qquad (1.4)$$

We can then reasonably call "optimal for the class B_1" the quadrature formula which has least estimate of the remainder i.e. the one which has the A_{ij} and the x_j chosen so that ζ is smallest for the class B_1.

Now if B_1 is the unit ball of a normed linear space B and $Q \in \mathcal{Q}$ is such that $E(f)$ forms a linear and continuous functional over B then $\zeta = \|E\|_{B*}$ and we immediately have the bound

$$|E(f)| \leqslant \|E\|\|f\|.$$

The dependence of E on the x_j and the A_{ij} occurs only in the multiplier $\|E\|$ and so we can aim to select these to minimize $\|E\|$. In 1949 Sard [9] presented the first discussion on the theory of, and the philosophy behind the use of, "best" quadrature formulae and best approximation formulae. In the same paper he indicated the method by which these could be determined and he tabled, for certain cases, the optimal quadrature formulae themselves.

It should be noted here that quadratures with least estimate of the remainder have been closely linked, in their short history, with spline functions.

A polynomial spline of order $2n-1$, with knots $t_1 = x_0 < x_1 < x_2 < \ldots < x_n < x_{n+1} = t_2$ and interpolating the values of $f(x_j)$, is the function ϕ such that

(i) ϕ is a polynomial of degree $2n-1$ in each interval (x_{i-1}, x_i), $i = 2, \ldots, n$,

(ii) ϕ is a polynomial of degree $n-1$ in each interval $[t_1, x_1]$ and $[x_n, t_2]$,

(iii) $\phi^{(2n-2)}$ is continuous at $x_1, x_2, \ldots, x_n$,

(iv) $\phi(x_j) = f(x_j)$ each $j = 1, 2, \ldots, n$.

These were introduced in 1946 by Schoenberg [11] and since then a substantial body of theory has evolved about them [2]. In 1965 Schoenberg [12] established the relation between best quadrature and polynomial spline functions. He also showed that certain classical formulae, namely the Hermite Formulae and the Euler-Maclaurin Summation Formulae, are best in the least squares sense. Subsequently generalized splines, that is functions which are linear combinations of some basis functions (rather than the powers of x) and which satisfy certain continuity conditions similar to those for polynomial splines, were investigated [3] and as

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a result Karlin and Ziegler [5] established the relation between generalized splines and best quadrature formulae. The relation of generalized splines to present work is discussed in Chapter 3 part (3).

In [7] Krylov considers the set of all quadratures of the type (1.2) (with N=1) for the class $L_q^{(r)}(0,1), q\geq 1$, of functions with derivative $f^{(r-1)}$ that is absolutely continuous on (0,1) and derivative $f^{(r)}$ that is qth power summable on (0,1). From the Taylor series expansion with integral form of the remainder for $f \in L_q^{(r)}(0,1)$ he derives the expression

$$E(f) = \int_0^1 f(x)dx - \sum_{k=1}^{n} A_{1k}\, f(x_k) = \int_0^1 f^{(r)}(t)K(t)dt \tag{1.5}$$

where

$$K(t) = \frac{(1-t)^r}{r!} - \sum_{k=1}^{n} A_{1k}\, J(x_k-t)\, \frac{(x_k-t)^{r-1}}{(r-1)!}$$

and then using the Hölder inequality he derives the bound

$$|E(f)| \leq \left\{\int_0^1 |f^{(r)}|^q dt\right\}^{\frac{1}{q}} \left\{\int_0^1 |K(t)|^p dt\right\}^{\frac{1}{p}}, \quad \frac{1}{p} + \frac{1}{q} = 1,$$

$$(\text{i.e.} \quad |E(f)| \leq \|f\|\|E\|).$$

For the two cases r=1 and r=2 he finds the A_{1k} and x_k which minimize $\int_0^1 |K(t)|^p dt$. Clearly these will also minimize $\|E\|$.

For the case $r=1$ the optimal formula he derives is the well known midpoint rule (see chapter 7) and for $r=2$ he shows that the optimal formula has, denoting $h_j = \frac{1}{2}(x_{j+1}-x_j)$ and $h = \frac{1}{2}[n-1+\sqrt{1-\ell^2}]^{-1}$,

$$\left.\begin{array}{lll} (1) & h_{j-1} = h_j = h & j = 2,3,\dots,n-1, \\ (2) & 1 - x_n = h\sqrt{1-\ell^2}, & \\ (3) & x_1 = h\sqrt{1-\ell^2}, & \end{array}\right\} \quad (1.6)$$

where ℓ is defined by

$$\int_0^{\ell} (\ell^2-x^2)^{p-1}dx = \int_{\ell}^{1} (x^2-\ell^2)^{p-1}dx \qquad (1.7)$$

and has weights

$$\left.\begin{array}{l} A_{1j} = 2h \quad j = 2,\dots,n-1, \\ A_{1j} = A_{1n} = h\,(1+\sqrt{1-\ell^2}). \end{array}\right\} \quad (1.8)$$

He then derives the value of $\|E\|$ at its minimum point:

$$\|E\| = \left\{\int_0^1 |K(t)|^p dt\right\}^{\frac{1}{p}}$$

$$= \tfrac{1}{2}h^2(1-\ell^2)\left(\frac{1}{2p+1}\right)^{\frac{1}{p}}. \qquad (1.9)$$

Kautsky [6] generalizes the results of Krylov by considering the set of quadratures of the type (1.2) with

$N=r$ on the class $L_q^{(r)}(t_1,t_2)$ (i.e. the formula may use values of the derivatives up to order $r-1$ at the mesh points). He shows that the optimal formula for $L_q^{(r)}(t_1,t_2)$ has

$$\left.\begin{array}{ll} (1) & h_{j-1} = h_j = \tfrac{1}{2}h(\text{constant}) \quad j=2,\ldots,n-1, \\ (2) & h = (t_2-t_1)/(n+\rho-1) \\ (3) & x_j-t_1 = (j+\tfrac{1}{2}\rho-1)h, \quad j=1,\ldots,n \end{array}\right\} \quad (1.10)$$

$$\left.\begin{array}{l} \text{where, denoting } M(r,q) = \left\{\int_{t_1}^{t_2} |p(x)|^q dx\right\}^{\frac{1}{q}}, \\ \rho = M^{\frac{1}{r}}(r,q) \left(\frac{rq+1}{2}\right)^{\frac{1}{rq}} \end{array}\right\} \quad (1.11)$$

and $p(x)$ is the polynomial with minimum $L_q^{(r)}$ norm. The corresponding minimum value of $||E||$ is

$$\left(\frac{t_2-t_1}{2}\right)^{r+\frac{1}{q}} \frac{M(r,q)}{(\rho+n-1)^r} \quad . \qquad (1.12)$$

For $q = 2,\infty,1$ the minimum polynomials can be written explicitly and they are the Legendre, Chebyshev first and Chebyshev second kind polynomials respectively. Further he shows for general r, as Krylov does for $r=1$ and 2, that the optimal formula does not use the $r-1$st derivative if r is even.

The spaces $L_q^{(r)}$ considered by Kautsky and Krylov are Banach spaces and except for the case $q=2$, when they are Hilbert spaces, they lack certain properties of symmetry between the dual space and the primal space.

"In a Hilbert space minimizations are related to perpendicularity. Bases may be constructed and projections calculated. Linear continuous functionals are inner products. Linear continuous operators may be studied closely. It is, therefore, advantageous to use Hilbert spaces in the formulation of problems wherever the preproblem allows such use". (Sard [10]).

We consider the Hilbert spaces H_N in which the norm $\|f\|$ involves the function f, the derivative $f^{(N)}$ and may involve the derivatives $f^{(1)}$ up to $f^{(N-1)}$. Using the techniques of functional analysis we find some properties of the quadrature which minimizes ζ and explicitly derive the formulae for the cases $N = 1,2$.

In Chapter 2 we introduce the set G_M^N of generalized splines and show that each spline g with continuous N-1st derivative is uniquely determined by the jumps in g and its derivatives at the mesh points x_j, $j=1,\dots,n$.

In Chapter 3 the properties relating the Hilbert space to its dual are recalled and the method by which these properties are used is discussed. Certain lemmas are established which essentially simplify the optimization procedure. By these lemmas we show that it is possible to find the optimal formula in two stages. In the first stage we find the formula that is best for a prescribed mesh distribution and in the second stage we find the best mesh distribution. Two simple expressions (which are later used to find the optimal mesh and to investigate the convergence properties of the formula) are derived for the norm of the error, $\|E\|$, of the optimal formula on an arbitrary mesh.

In Chapter 4 we solve the case N=1 and in Chapter 5, the case N=2. We then show that the optimal formula does not use the derivative values when used on the optimal mesh. This is the extension to the spaces H_1 and H_2 of the properties derived by Krylov and Kautsky for the spaces $L_q^{(2)}$.

Next we discuss the convergence of the optimal formulae and show that the rate of convergence is as the Nth power of the largest-mesh length.

The Generalized Midpoint Rule (G.M.R.) is introduced in Chapter 7 and there we show that as the largest mesh length tends to zero, the optimal formula tends to the G.M.R. As a consequence of this we find the optimal formulae for the case $\alpha_0 = 0$ (N = 1,2).

In Chapter 8 we determine the optimal closed formula and in Chapter 9 we discuss certain numerical considerations in the use of the optimal formula. We then show, for the case N=1 that if the integrand possesses the quantitative properties of smoothness,

$$\int_{t_1}^{t_2} f^2(x)dx \leqslant M_0 ,$$

$$\int_{t_1}^{t_2} f'^2(x)dx \leqslant M_1 ,$$

M_0 and M_1 some constants, then we can minimize the whole error bound $\|E\|\|f\|$ (instead of just $\|E\|$) by choosing the appropriate metric. The optimal formulae are then applied to a wide range of functions and their errors are compared between themselves and with those of standard formulae.

The material presented in chapters 2-5 and 8 has been published† in slightly different form.

†S. ELHAY, Optimal Quadrature, Bull.Austral.Math.Soc., 1 (1969) 81-108.

2. Definitions and Notation

(1) Let P be the set of all partitions $p = (x_1, x_2, \ldots, x_n)$ which divide the finite interval (t_1, t_2) into $n + 1$ subintervals $I_j = (x_j, x_{j+1})$ for $j = 0, \ldots, n$ and where

$$t_1 = x_0 \leqslant x_1 < x_2 < \ldots < x_n \leqslant x_{n+1} = t_2 \qquad (2.1)$$

(2) Let N be a positive integer and let $\alpha_0, \alpha_1, \alpha_2, \ldots, \alpha_N$ all $\geqslant 0$ be a real sequence such that $\alpha_0 \neq 0$, $\alpha_N \neq 0$. We shall then deal with the following Hilbert spaces:-

(i) For each fixed partition, $p \in P$, let M_N be the space of real functions $f(x)$ such that the Nth derivative $f^{(N)}(x)$ has bounded norm in $L_2(t_1, t_2)$, $f^{(N-1)}(x)$ is absolutely continuous on each subinterval I_j of (t_1, t_2), and the inner product is

$$(f, g)_N = \sum_{j=0}^{N} \alpha_j{}^2 \int_{t_1}^{t_2} f^{(j)}(x) g^{(j)}(x) dx.$$

(ii) Let H_N be the subspace of M_N, independent of p, defined by

$$H_N = \{f; f \in M_N, \text{ and } f^{(N-1)}(x) \text{ is absolutely continuous on the whole interval } (t_1, t_2)\}.$$

(3) We shall call $\tilde{Q}(n,N)$ the set of all n-point quadrature formulae Q_n of the type (1.2) with the A_{ij} real and the x_j given by $p \in P$.

(4) For $p \in P$ we define S_p^N as the collection of all error functionals of the type

$$E(f) = I(f) - Q_n(f),$$

where $Q_n \in \tilde{Q}(n,N)$ and has its mesh points x_j given by p.

(5) Let $\tilde{Q}'$ be a subset of $\tilde{Q}(n,N)$. The quadrature formula $Q_n^* \in \tilde{Q}'$ will be said to be optimal in $\tilde{Q}'$ over H_N when $\|I - Q_n^*\| \leq \|I - Q_n\|$ for all $Q_n \in \tilde{Q}'$, $f \in H_N$.

(6) We will call the function g defined on (t_1, t_2) an exponential spline or e-spline of degree N with n knots if for some partition $p \in P$, g satisfies

$$\sum_{j=0}^{N}(-)^j \alpha_j^2 g^{(2j)}(x) = 1 \quad \text{for} \quad x \in I_i,\ i=0,\ldots,n, \tag{2.2}$$

and

(i) $\sum_{j=m}^{N}(-)^{j-m}\alpha_j^2 g^{(2j-m)}(x_\ell) = 0$, for $m=1,\ldots,N$;
for $\ell=0$ if $x_1 \neq t_1$
and for $\ell = n+1$ if $x_n \neq t_2$

or

(ii) $\sum_{j=m}^{N}(-)^{j-m}\alpha_j^2 g^{(2j-m)}(x_\ell) = \delta_{m,\ell}$, for $m=1,\ldots,N$;
$\ell=1$ and n if $x_1=t_1$ and $x_n=t_2$ for some given constants $\delta_{m,\ell}$. (2.3)

It is convenient to denote

$$g^{(k)}(x_j-) - g^{(k)}(x_j+) = R_{jk}, j=1,\dots,n, \quad k=0,\dots,2N-1. \tag{2.4}$$

We will say the e-spline, g, has order of continuity m when $R_{jk} = 0$ for $j=1,\dots,n$, and all $k=0,1,\dots,m$. Let G^N be the set of all e-splines of degree N defined on the partition $p\in P$. We define

$$G^N_M = \{g;\ g\in G^N \text{ and } g \text{ has order } M\}.$$

Suppose for a moment that $t_1 \neq x_1$ and $t_2 \neq x_n$. In general the solution of (2.2) can be written

$$g(x) = 1/\alpha_0^2 + \sum_{i=1}^{2N} a_{ij} e^{r_i x}, \qquad x\in I_j,\ j=0,\dots,n.$$

(where the r_i are the $2N$ solutions of the auxiliary equation to (2.2) and are assumed to be distinct). Thus $g(x)$ depends on $2N(n+1)$ unknowns called spline coefficients. These spline coefficients are uniquely determined by the $2N(n+1)$ conditions (2.3) (i) which become

$$\sum_{j=m}^{N} (-)^{j-m} \alpha_j^2 \sum_{i=1}^{2N} r_i^{(2j-m)} a_{ij} e^{r_i x} = 0, \quad m=1,\dots,N$$

at $x = t_1$ and $x = t_2$ and (2.4) which become

$$\sum_{i=1}^{2N} r_i^k (a_{i,j-1} e^{r_i(x_j-)} - a_{ij} e^{r_i(x_j+)}) = R_{jk}$$

$$j=1,\dots,n \text{ and } k=0,\dots,2N-1$$

for given R_{jk}. These conditions are linear equations with the spline coefficients as unknowns. To show that the spline is uniquely determined by this system we must show that the system of equations is non-singular. Setting $R_{jk} = 0$ for $j = 1,\ldots,n$ and $k = 0,\ldots,2N-1$ yields the corresponding system of homogeneous equations. Then it is sufficient to show that the trivial solution $g(x) = 1/\alpha_0^2$, is the unique solution to this system. Let g^* be any solution of (2.2). Then

$$(f,g^*)_N = \sum_{j=0}^{N} \alpha_j^2 \int_{t_1}^{t_2} f^{(j)}(x)\, g^{*(j)}(x)\,dx, \qquad f\in H_N \tag{2.5}$$

$$= \sum_{j=0}^{N} \alpha_j^2 \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} f^{(j)}(x)\, g^{*(j)}(x)\,dx$$

$$= \sum_{i=0}^{n} \sum_{j=0}^{N} \alpha_j^2 \int_{x_i}^{x_{i+1}} f^{(j)}(x)\, g^{*(j)}(x)\,dx$$

and integrating N times by parts

$$= \sum_{i=0}^{n} \sum_{j=0}^{N} \alpha_j^2 \left\{ \left[\sum_{k=1}^{j} (-)^{k+1} f^{(j-k)}(x)\, g^{*(j+k-1)}(x) \right]_{x_i}^{x_{i+1}} + (-)^j \int_{x_i}^{x_{i+1}} f(x)\, g^{*(2j)}(x)\,dx \right\}. \tag{2.5.1}$$

Now

$$\sum_{i=0}^{n} \sum_{j=0}^{N} \alpha_j^2 (-)^j \int_{x_i}^{x_{i+1}} f(x)\, g^{*(2j)}(x)\,dx$$

$$= \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} \left[\sum_{j=0}^{N} \alpha_j^2 (-)^j g^{*(2j)}(x) \right] f(x)\,dx$$

and imposing condition (2.2)

$$= \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$= I(f).$$

Considering the other term in (2.5.1)

$$\sum_{i=0}^{n} \sum_{j=0}^{N} \alpha_j{}^2 \left[\sum_{k=1}^{j} (-)^{k+1} f^{(j-k)}(x) g^{*(j+k-1)}(x) \right]_{x_i}^{x_{i+1}}$$

$$= \sum_{i=0}^{n} \left[\sum_{k=1}^{N} \sum_{\ell=0}^{N-k} \alpha^2_{\ell+k} (-)^{k+1} f^{(\ell)}(x) g^{*(\ell+2k-1)}(x) \right]_{x_i}^{x_{i+1}},$$

$$= \sum_{\ell=0}^{N-1} \sum_{i=0}^{n} \left[f^{(\ell)}(x_{i+1}) \sum_{k=\ell+1}^{N} (-)^{k-\ell-1} \alpha_k{}^2 g^{*(2k-\ell-1)}(x_{i+1}-) \right.$$

$$\left. - f^{(\ell)}(x_i) \sum_{k=\ell+1}^{N} (-)^{k-\ell-1} \alpha_k{}^2 g^{*(2k-\ell-1)}(x_i+) \right],$$

$$= \sum_{\ell=0}^{N-1} \left\{ f^{(\ell)}(x_{n+1}) \sum_{k=\ell+1}^{N} (-)^{k-\ell-1} \alpha_k{}^2 (g^{*(2k-\ell-1)}(x_{n+1}-)) \right.$$

$$+ \sum_{i=1}^{n} f^{(\ell)}(x_i) \sum_{k=\ell+1}^{N} (-)^{k-\ell-1} \alpha_k{}^2 (g^{*(2k-\ell-1)}(x_i-) - g^{*(2k-\ell-1)}(x_i+))$$

$$\left. - f^{(\ell)}(x_0) \sum_{k=\ell+1}^{N} (-)^{k-\ell-1} \alpha_k{}^2 g^{*(2k-\ell-1)}(x_0+) \right\},$$

$$= \sum_{m=1}^{N} \left\{ f^{(m-1)}(x_{n+1}) \sum_{k=m}^{N} (-)^{k-m} \alpha_k{}^2 g^{*(2k-m)}(x_{n+1}-) \right.$$

$$+ \sum_{i=1}^{n} f^{(m-1)}(x_i) \sum_{k=m}^{N} (-)^{k-m} \alpha_k{}^2 (g^{*(2k-m)}(x_i-) - g^{*(2k-m)}(x_i+))$$

$$\left. - f^{(m-1)}(x_0) \sum_{k=m}^{N} (-)^{k-m} \alpha_k{}^2 g^{*(2k-m)}(x_0+ \right\}.$$

By setting the required conditions of the homogeneous system on g^*, we have

$$(f, g^*)_N = I(f).$$

Directly expanding the inner product $(f,g)_N$ with $g = 1/\alpha_0^2$ gives

$$(f, 1/\alpha_0^2)_N = I(f). \tag{2.6}$$

Now by the Hölder Inequality

$$|(f, 1/\alpha_0^2)| \leq \|1/\alpha_0^2\| . \|f\|,$$

or

$$|I(f)| \leq M\|f\|,$$

where $M = \|1/\alpha_0^2\|$. Thus the functional $I(f)$ is bounded with respect to $\|f\|$ in H_N and so by Riesz' theorem the function which realizes $I(f)$ is unique; but $R_{jk} = 0$ implies that $g^* \in H_{2N-1} \subset H_N$, so that

$$g^*(x) = 1/\alpha_0^2.$$

Then the system is non-singular whenever $t_1 \neq x_1$ and $t_2 \neq x_n$. If $t_1 = x_1$ and $t_2 = x_n$ then the solution of (2.2) depends on $2N(n-1)$ spline coefficients and these are uniquely determined by the $2N(n-1)$ conditions (2.3) (ii) and (2.4) for given $\delta_{m\ell}$ and R_{jk} respectively. The corresponding system of homogeneous equations is obtained by setting the R_{jk} and $\delta_{m\ell}$ to zero and by the same procedure as before it can be shown that the trivial solution $g = 1/\alpha_0^2$ is the unique solution to this system. Thus any spline of degree N is uniquely determined by the jumps R_{jk} $j=1,\ldots,n,$ and $k=0,\ldots,2N-1.$

The transformation to the new variable h given by

$$h = \begin{cases} x - \dfrac{x_j+x_{j+1}}{2}, & \text{for } x\in I_j,\ j=1,\ldots,n-1, \\ \frac{1}{2}(x-t_1) = \frac{1}{2}(x-x_0), & \text{for } x\in I_0 \text{ if } x_0 \neq t_1, \\ \frac{1}{2}(x-t_2) = \frac{1}{2}(x-x_{n+1}), & \text{for } x\in I_n \text{ if } x_n \neq t_2, \end{cases}$$

is useful as it transforms the subintervals, I_j, as follows

$$I_0 = (x_0,x_1) \to (0, \frac{h_0}{2}),$$

$$I_j = (x_j,x_{j+1}) \to (-\frac{h_j}{2}, \frac{h_j}{2}), \quad 1 \leqslant j \leqslant n-1,$$

$$I_n = (x_n,x_{n+1}) \to (-\frac{h_n}{2}, 0),$$

where $h_j = x_{j+1} - x_j.$

We will consider e-splines to be functions of x or h as is necessary, so implying the appropriate interval and transformation for x.

For convenience we shall denote

$$Q_n(f) = \sum_{j=1}^{n} C_j f(x_j), \quad \text{for the case } N=1,$$

and

$$Q_n(f) = \sum_{j=1}^{n} C_j f(x_j) + D_j f'(x_j), \quad \text{for } N=2.$$

3. Discussion and Method

(1) From the absolute continuity of the functions in H_N and their derivatives of order N-1 it can be seen that $I(f) - Q_n(f)$ forms a linear and bounded functional over H_N. Then if we choose the set, B, as the subset of H_N which contains functions with norm $\|f\| = 1$, the definition (1.4) becomes

$$\zeta = \sup_{f\in H_N, \|f\|=1} |I(f) - Q_n(f)|,$$

$$= \sup_{f\in H_N, \|f\|=1} |E(f)|,$$

and this supremum exists and is just $\|E\|_{H_N^*}$. Then

$$|E(f)| \leq \|E\| . \|f\|,$$

and so, by minimizing ζ we are reducing the size of the bound on $|E(f)|$ in the sense of the norm for functionals defined on H_N.

(2) In practical cases the choice of the metric for our set of functions and so in a sense the definition of H_N will be left open. This choice should seek to give the best measure of the particular properties of interest of the functions in the space. For our case we have chosen an inner product which measures the smoothness of f and its derivatives by integrating them in the square and summing their integrals. The integrals in the sum are weighted by the sequence of α_j's so that for a particular

problem this sequence can be chosen to minimize the product $\|E\| \cdot \|f\|$. The choice of these α_j's is independent of the topology of H_N and only affects our estimates of error. A more detailed discussion of this question will be found in section §1 of chapter 10.

Here we will consider only those sequences of α's such that the polynomial,

$$\sum_{j=0}^{N} (-)^j \alpha_j{}^2 m^{2j} = 0$$

in m, which is the auxiliary equation to (2.2), has $2N$ real and distinct roots

$$\pm m_1, \pm m_2, \pm m_3, \ldots, \pm m_N.$$

(3) For every bounded functional, F, defined on a Hilbert space, H, there exists a unique element, g, in that space which realizes F by the relation

$$(f,g) = F(f) \quad \text{for any} \quad f \in H, \tag{3.1}$$

and

$$\|g\| = \|F\|. \tag{3.2}$$

Consequently for every error functional, E, on H_N there is a function, g, which lies in H_N and which satisfies (3.1) and (3.2). This relation between a Hilbert space and its dual enables us to find a particular element of the dual without dealing directly with the functionals. By finding the set of functions in H_N which realize the

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errors, E, defined on some partition $p \in P$ and isolating that one, (g^*), which has smallest norm we can construct the error which defines the optimal formula on that partition. This set is in fact G^N_{N-1} and the following lemma summarises the relation between G^N_{N-1} and the set, S^N_p, of error functionals on a given partition.

<u>LEMMA</u> 1. Suppose p is a partition from P. There exists a one-to-one correspondence between the elements E of S^N_p and g of G^N_{N-1} such that

$$(f,g)_N = E(f) \quad \text{for any } f \in H_N. \tag{3.3}$$

<u>PROOF</u>: (i) We note first that $G^N_{N-1} \subset H_N$. Let g be from G^N_{N-1} and f from H_N.

$$(f,g)_N = \sum_{i=0}^{N} \alpha_i^2 \int_{t_1}^{t_2} f^{(i)}(x) g^{(i)}(x)\,dx,$$

$$= \sum_{j=0}^{n} \sum_{i=0}^{N} \alpha_i^2 \int_{I_j} f^{(i)}(x) g^{(i)}(x)\,dx.$$

Integrating by parts N times and using the conditions (2.2), (2.3), and

$$R_{jk} = 0, \qquad j=1,\dots,n \text{ and } k=0,\dots,N-1, \tag{3.4}$$

gives

$$\left\{ \begin{array}{l} (f,g)_N = I(f) - \\ \sum_{j=1}^{n} \sum_{i=0}^{N-1} f^{(i)}(x_j) \sum_{k=i+1}^{N} (-1)^{k-i} \alpha_k^2 R_{j,2k-i-1} \end{array} \right. \text{ as before.} \tag{3.5}$$

Therefore if we choose

$$A_{ij} = \sum_{k=i+1}^{N} (-)^{k-1}\alpha_k{}^2 R_{j,2k-i-1}, \qquad (3.6)$$

for all $i = 0,\ldots,N-1$, and $j = 1,\ldots,n$, then we have

$$(f,g)_N = I(f) - Q_n(f),$$
$$= E(f) \text{ as required.}$$

(ii) Suppose now that E is from S_p^N. With the A_{ij}'s given by E and nN of the R_{jk} given by (3.4), the relations (3.6) considered as a system of equations in the remaining R_{jk}'s is in fact a triangular system. Then the $2nN$ real numbers R_{jk} defined by (3.4) and (3.6) uniquely define a spline g. By (3.4) g belongs to G_{N-1}^N.

The elements of S_p^N are bounded linear functionals and so by Riesz' theorem, g is the unique element in H_N which realizes E. This completes the proof of the lemma.

Consider the set G^N defined on the partition $p\in P$. All the elements of G^N realize quadrature formulae and of the subcollection in G^N which realize one quadrature formula, the single spline with smallest norm has a continuous derivative of order $N-1$. This subcollection is

$J_{Q_n}^N = \{g;\ g\in G^N$ such that for $Q_n\in\tilde{Q}(n,N)$ defined on $p\in P$, the R_{jk} satisfy (3.6) where the A_{ij} are given as the weights of $Q_n\}$

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and the continuity property of the spline, in $J_{Q_n}^N$, with smallest norm derives from the following lemma.

<u>LEMMA</u> 2. Let $g_0 \in J_{Q_n}^N$ be such that

$$\|g_0\|_{M^N} \leq \|g\|_{M^N} \quad \text{for any} \quad g \in J_{Q_n}^N.$$

Then $g_0 \in H_N$.

<u>PROOF</u>: Since $J_{Q_n}^N$ is the set of all splines in G^N which realize the single quadrature formula $Q_n(f)$, the set $J_{Q_n}^N \cap H_N$ contains only one element. This is because any function in this intersection will satisfy (3.6) from the definition of $J_{Q_n}^N$ and further it will have order of continuity $N-1$ because it belongs to H_N. Thus it will satisfy $R_{jk} = 0$ for $j=1,\dots,n$ and $k=0,\dots,N-1$. As in the proof of <u>LEMMA</u> 1. this uniquely defines a set of $2nN$ jumps R_{jk} which in turn define a single spline. Let us call this spline g_0. Then if g is any element of $J_{Q_n}^N$ we may write

$$g = g_0 + Z.$$

But because g and g_0 are both from $J_{Q_n}^N$ they both realize the same quadrature formula, and thus the inner product $(g - g_0, f)$ vanishes for any $f \in H_N$. Then $(f, Z) = 0$ for any $f \in H_N$ and g_0 is the projection of g in H_N. By applying Pythagoras' theorem

$$\|g\|^2 = \|g_0\|^2 + \|Z\|^2, \qquad (3.6)$$

we see that

$$\|g_0\| \leq \|g\|$$

for all $g \in J_{Q_n}^N$. Now let $g_1 \in J_{Q_n}^N$ be such that $\|g_1\| \leq \|g\|$ for any $g \in J_{Q_n}^N$. Then $\|g_1\| = \|g_0\|$. Further if we write g_1 as the sum

$$g_1 = g_0 + Z,$$

we see by relation (3.6) that $\|Z\| = 0$. Whence $\|g_0 - g_1\| = 0$ and so $g_0 = g_1$ and the lemma is proved.

<u>COROLLARY</u>: Let $g^* \in G^N$ be such that $\|g^*\|_{M^N} \leq \|g\|_{M^N}$ for any $g \in G^N$. Then $g^* \in H_N$.

The proof follows immediately from the fact that

$$G^N = \bigcup_{Q_n \in \tilde{Q}(n,N)} J_{Q_n}^N.$$

This result leads to an essential saving in the minimization process. It means that we can minimize $\|g\|$ over G^N with respect to the spline coefficients <u>independently</u> on each subinterval and the resulting function will indeed have the properties of continuity which ensure that it lies in G_{N-1}^N. Using this technique we will find this spline g^* and use it to construct the optimal quadrature formula for the mesh p.

It is interesting that for both of the cases $N = 1$ and $N = 2$ the spline with minimal norm has the property

$$g^{*(k)}(x_j) = 0, \quad j=1,\ldots,n \quad \text{and} \quad k=0,\ldots,N-1,$$

independently of the partition p. This leads to the simple form

$$\|E^*\| = \{\int_{t_1}^{t_2} g^*(x)\ dx\}^{\frac{1}{2}},$$

for the error bound of the approximation. The result comes from the following lemma:-

LEMMA 3. Suppose $g_0 \in G^N_{N-1}$ has the property $g_0^{(k)}(x_j) = 0 \quad j=1,\ldots,n, \quad \text{and} \quad k=0,\ldots,N-1,$ then $\|g_0\|^2 = I(g_0)$.

PROOF: For all $f \in H_N$, $g \in G^N_{N-1}$, we have by (3.5)

$$(f,g)_N = I(f) + \sum_{j=1}^{n} \sum_{i=0}^{N-1} f^{(i)}(x_j) \sum_{k=i+1}^{N} (-)^{k-i} \alpha_k{}^2 R_{j,2k-i-1}.$$

Putting $f = g = g_0$ yields

$$(g_0, g_0) = \|g_0\|^2 = I(g_0) + \sum_{j=1}^{n} \sum_{i=0}^{N-1} g_0{}^{(i)}(x_j) \sum_{k=i+1}^{N} (-)^{k-i} R_{j,2k-i-1},$$

$$= I(g_0),$$

since $g_0{}^{(i)}(x_j) = 0$ for each i and j.

This error bound will apply to any mesh distribution and, in particular, it will apply to the optimal mesh. Now $\|g^*\|$ is a function only of the mesh intervals $h_0, h_1, \ldots, h_n$. In order to find the optimal values of these intervals we must minimize $\|g^*\|$ with respect to

$h_0, h_1, \ldots, h_n$. For the case $N=1$ this is done in one step but when $N=2$ we first consider h_0 and h_n to be fixed and minimize $\|g^*\|$ with respect to $h_1, h_2, \ldots, h_{n-1}$, thereby getting as an intermediate result the optimal formula for the case that h_0 and h_n are prescribed. The best values of h_0 and h_n can then be found. The following lemma will be useful later.

LEMMA 4: Let g_0 be as in Lemma 3 and let $E^0(f)=(f,g_0)$ be the error of the formula

$$Q_n^0(f) = \sum_{i=1}^{N} \sum_{j=1}^{n} A_{ij}^0 f^{(i-1)}(x_j^0)$$

Then

$$\|E^0\|^2 = \frac{1}{\alpha_0^2}[(t_2-t_1) - \sum_{j=1}^{n} A_{1j}^0].$$

PROOF: $\|E^0\|^2 = \|g_0\|^2 = I(g_0) = \left(\frac{1}{\alpha_0^2}, g_0\right)$ by relation (2.6).

But $(f,g_0) = E^0(f)$ and so

$$\|E^0\|^2 = E^0\left(\frac{1}{\alpha_0^2}\right) = I\left(\frac{1}{\alpha_0^2}\right) - Q_n^0\left(\frac{1}{\alpha_0^2}\right)$$

$$= \frac{1}{\alpha_0^2}(t_2-t_1) - \sum_{j=1}^{n} A_{1j}^0\left(\frac{1}{\alpha_0^2}\right)$$

$$= \frac{1}{\alpha_0^2}\left[(t_2-t_1) - \sum_{j=1}^{n} A_{1j}^0\right]$$

and the lemma is proved.

4. The Case N=1

The elements of G^1 and G^1_0 defined on the partition $p \in P$ have the form

$$g(x) = 1/\alpha_0{}^2 - (a_j \cosh rx + b_j \sinh rx),$$

for all $x \in I_j$, $(j=0,1,\dots,n)$ where $r = \alpha_0/\alpha_1$ is the solution of the quadratic

$$\alpha_0{}^2 - \alpha_1{}^2 m^2 = 0,$$

and a_j and b_j are the spline coefficients. The results for the optimal formula on a fixed mesh and the description of the optimal mesh can be summarized as follows.

<u>THEOREM</u> I

(1) Let $\mathfrak{Q}_{p_1}$ be the subset of $\mathfrak{Q}(n,1)$ containing all the quadrature formulae defined on the partition $p_1 \in P$. The optimal quadrature formula $Q^*_n(f)$ in $\mathfrak{Q}_{p_1}$ over H_1 has its weights given by

$$C_j = -\alpha_1{}^2 R^*_{j1}, \qquad j=1,\dots,n,$$

where the e-spline g^* is defined by

$$a^*_j = \frac{1}{\alpha_0{}^2 \cosh \frac{rh_1}{2}}, \quad b^*_j = 0, \qquad j=0,\dots,n,$$

and satisfies

$$g^*(x_j) = 0, \qquad j=1,\dots,n.$$

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(2) The optimal formula in $\mathfrak{Q}(n,1)$ has the weights C_j as in (1) and has its mesh defined by

$$h_j = \frac{t_2 - t_1}{n}, \qquad j=0,\ldots,n.$$

PROOF: (1) We shall minimize

$$\|g\|^2 = \sum_{j=0}^{n} \int_{I_j} \alpha_0{}^2 g^2(x) + \alpha_1{}^2 g'^2(x)\, dx$$

with respect to the spline coefficients a_j and b_j.

Denote $M_j = \int_{I_j} \alpha_0{}^2 g^2(x) + \alpha_1{}^2 g'^2(x)\, dx$

In $1 \leqslant j \leqslant n-1$,

$$M_j = \frac{h_j}{\alpha_0{}^2} + \frac{\alpha_0{}^2}{r}(a_j{}^2 + b_j{}^2) \sinh rh_j - \frac{4a_j}{r} \sinh \frac{rh_j}{2},$$

is a quadratic function of a_j, b_j which has a total differential of second order

$$\Phi(da_j, db_j) = \frac{2\alpha_0{}^2 \sinh \frac{rh_j}{2}}{r}((da_j)^2 + (db_j)^2)$$

that is strictly positive whenever h_j is positive.

The normal equations

$$a_j^* \frac{\alpha_0{}^2}{r} \sinh rh_j = \frac{2}{r} \sinh \frac{rh_j}{2},$$

and

$$b_j^* \frac{\alpha_0{}^2}{r} \sinh \frac{rh_j}{2} = 0,$$

therefore define a minimum at the point

$$a_j^* = \frac{1}{\alpha_o^2 \cosh \frac{rh_j}{2}} , \; b_j^* = 0.$$

Now in the interval I_o we have only one free spline coefficient because the end point condition (2.3) with N=1 has the form $[g'(h)]_{h=o} = 0$ implying $b_o^* = 0$. Then

$$M_o = \frac{h_o}{2\alpha_o^2} + \frac{\alpha_o^2}{2r} a_o^2 \sinh rh_o - \frac{2a_o}{r} \sinh \frac{rh_o}{2} ,$$

and the normal equation

$$a_o^* \frac{\alpha_o^2}{r} \sinh rh_o = \frac{\sinh \frac{rh_o}{2}}{r} ,$$

defines

$$a_o^* = \frac{1}{\alpha_o^2 \cosh \frac{rh_o}{2}} .$$

From the symmetry of the situation we can see that $a_n^* = a_o^*$, $b_n^* = -b_o^*$, and so

$$g^*(h) = 1/\alpha_o^2 - \frac{\cosh rh}{\alpha_o^2 \cosh \frac{rh_1}{2}} .$$

From this we have immediately

$$g^*(x_j) = 0, \quad j=1,\ldots,n \tag{4.0}$$

(2) To find the optimal mesh distribution we use the method of the Lagrange multipliers. Let us construct a function

$$\omega = \omega(h_o, h_1, \ldots, h_n),$$

$$= \|g^*\|^2 - \theta\left(\frac{h_o}{2} + \frac{h_n}{2} + \sum_{j=1}^{n-1} h_j - (t_2 - t_1)\right),$$

$$= \|g^*\|^2 - \theta\left(\sum_{j=0}^{n}{}'' h_j - (t_2 - t_1)\right), \quad \theta \text{ real}$$

where Σ'' denotes that the first and last terms in the sum are halved. Recall that $\|g^*\|^2$ is a function of the mesh intervals $h_0, h_1, \ldots, h_n$. If the quadratic form

$\Psi(dh_0, dh_1, \ldots, dh_n) =$

$$\sum_{j=0}^{n} \sum_{m=0}^{n} \left[\frac{\partial^2 \|g^*\|^2}{\partial h_j \partial h_m} + \theta \frac{\partial^2}{\partial h_j \partial h_m} \left(\sum_{j=0}^{n}{}'' h_j - (t_2 - t_1)\right)\right] dh_j\, dh_m$$

is strictly positive whenever $h_0, h_1, \ldots, h_n$ are positive then the normal equations

$$\frac{d\omega}{dh_j} = 0 \qquad j=0,1,\ldots,n$$

define a minimum turning point for the function ω under the constraints

$$\sum_{j=0}^{n}{}'' h_j = t_2 - t_1, \quad h_j \geqslant 0 \quad \text{each} \quad j=1,2,\ldots n-1. \tag{4.1}$$

From the result (4.0) we may apply Lemma 3 to g^* and we arrive at

$$\omega = \sum_{j=0}^{n} \int_{I_j} g^*(h_j;x)\,dx - \theta\left(\sum_{j=0}^{n}{}'' h_j - (t_2 - t_1)\right), \tag{4.2}$$

where we have written $g^*(h_j;x)$ to denote the dependence of g^* on h_j when $x \in I_j$. Since g^* is an even function of h_j in I_j we may write

$$\int_{I_j} g^*(h_j;x)\,dx = 2\int_0^{h_j/2} g^*(h_j;x)\,dx.$$

Now

$$\frac{\partial}{\partial h_j}\left[2\int_0^{h_j/2} g^*(h_j;x)\,dx\right] = g^*(h_j;h_j/2)+2\int_0^{h_j/2}\frac{\partial}{\partial h_j}g^*(h_j;x)\,dx$$

and since $g^*(h_j;h_j/2) = 0$ each j

$$\frac{\partial^2}{\partial h_j^2}\left[2\int_0^{h_j/2} g^*(h_j;x)\,dx\right] = \frac{\partial}{\partial h_j}g^*(h_j;x)\Big|_{x=h_j/2}$$

$$+\int_0^{h_j/2}\frac{\partial^2}{\partial h_j^2}g^*(h_j;x)\,dx$$

Thus by substituting for the spline coefficients in this expression we have

$$\Psi(dh_0,\ldots,dh_n) = \sum_{j=0}^{n}\left[\frac{r\sinh\frac{rh_j}{2}}{2\alpha_0^2\cosh\frac{rh_j}{2}}\right.$$

$$\left.-\frac{r\sinh\frac{rh_j}{2}}{2\alpha_0^2\cosh\frac{rh_j}{2}}\left(\frac{\cosh^2\frac{rh_j}{2}-2\sinh\frac{rh_j}{2}}{\cosh^2\frac{rh_j}{2}}\right)\right](dh_j)^2$$

$$= \sum_{j=0}^{n}\left[\frac{r\tanh^2\frac{rh_j}{2}}{\alpha_0^2\cosh\frac{rh_j}{2}}\right](dh_j)^2,$$

and this expression is positive for all positive r and h_j. By substituting for a_j^* and b_j^* in (4.2) and integrating, we see that

$$\omega = \frac{t_2-t_1}{\alpha_0^2} - \frac{2}{r\alpha_0^2}\left(\sum_{j=0}^{n}{}'' \tanh\frac{rh_j}{2}\right) - \theta\left(\sum_{j=0}^{n}{}'' h_j - (t_2-t_1)\right)$$

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Then $\frac{d\omega}{dh_j} = 0$ implies

$$\cosh^2 \frac{rh_j}{2} = \frac{-1}{\alpha_0{}^2\theta} \quad \text{for each} \quad j=0,\ldots,n.$$

But for each interval the equation for h_j is independent of j and, since all the equations have the same form, we may say that all the h_j are equal and, by relation (4.1),

$$h_j = \frac{t_2 - t_1}{n}, \quad 0 \leqslant j \leqslant n. \qquad (4.3)$$

This completes the proof of THEOREM I.

5. The Case N=2

The elements of G^2 and G_1^2 defined on the partition $p\in P$ have the form

$g(x) = 1/\alpha_0^2 -$
$(a_j \cosh rx + b_j \cosh sx + c_j \sinh rx + d_j \sinh sx),$

for all $x\in I_j$ $(j=0,1,\ldots,n)$ where the roots $\pm r, \pm s\,(r,s>0)$ of

$$\alpha_0^2 - \alpha_1^2m^2 + \alpha_2^2m^4 = 0,$$

are assumed to be distinct and real, and a_j, b_j, c_j and d_j are the spline coefficients.

In each subinterval I_j we denote

$$C_r = \cosh r\omega_j,\ S_r = \sinh r\omega_j,$$

where $\omega_j = \frac{h_j}{2}$, $0 \leqslant j \leqslant n-1$, and $\omega_n = -\frac{h_n}{2}$, and similarly for C_s and S_s.

5.1 The Optimal Formula for a Fixed Mesh

THEOREM II

Let p_2 be a partition from P. Denote by $\mathfrak{Q}_{p_2}$ the subset of $\mathfrak{Q}(n,2)$ containing all the quadrature formulae defined on the partition p_2. The optimal quadrature formula $Q_n^*(f)$ in $\mathfrak{Q}_{p_2}$ over H_2 is given by the weights

$$C_j = +\,\alpha_2^2R_{j3}^*,\ D_j = -\,\alpha_2^2R_{j2}^*$$

where the spline g^* is defined by

(1) $a_j^* = \frac{sS_s}{\alpha_0{}^2T_1}$, $b_j^* = \frac{-rS_r}{\alpha_0{}^2T_1}$,

$T_1 = sC_rS_s - rS_rC_s$,

$c_j^* = d_j^* = 0$, $(j=1,\ldots,n-1)$:

(2) $a_j^* = \frac{r^2C_r - s^2C_s}{r\alpha_0{}^2T_2}$; $b_j^* = -\frac{r^2}{s^2}\ a_j^*$,

$c_j^* = \frac{-r(S_r - \frac{r}{s}S_s)}{\alpha_0{}^2T_2}$, $d_j^* = -\frac{s}{r}\,c_j$,

where $T_2 = \frac{1}{r}(C_r - \frac{r^2}{s^2}C_s)(r^2C_r - s^2C_s)$

$-r(S_r - \frac{s}{r}S_s)(S_r - \frac{r}{s}S_s)$,

$(j=0$ and $n)$.

Further $g^*(x_j) = g^{*\prime}(x_j) = 0$, $j=1,\ldots,n$.

PROOF: We will minimize

$$\|g\|^2 = \sum_{j=0}^{n} \int_{I_j} \alpha_0{}^2g^2(x) + \alpha_1{}^2g'^2(x) + \alpha_2{}^2g''^2(x)\ dx, \qquad (5.0)$$

with respect to the spline coefficients a_j, b_j, c_j and d_j.

Denote

$$M_j = \int_{I_j} \alpha_0{}^2g^2(x) + \alpha_1{}^2g'^2(x) + \alpha_2{}^2g''^2(x)\ dx,$$

and consider first that $1 \leq j \leq n-1$. By expanding directly using the relations $r^2s^2 = \frac{\alpha_0{}^2}{\alpha_2{}^2}$ and $r^2+s^2 = \frac{\alpha_1{}^2}{\alpha_2{}^2}$,

and integrating, we find that

$$M_j = 2\alpha_1^2\{r(a_j^2 + c_j^2)S_rC_r + s(b_j^2 + d_j^2)S_sC_s\}$$
$$+ 4\alpha_0\alpha_2\{(ra_jb_j + sc_jd_j)C_rS_s + (sa_jb_j + rc_jd_j)S_rC_s\}$$
$$- 4\{a_j \frac{S_r}{r} + b_j \frac{S_s}{s}\} + \frac{h_j}{\alpha_0^2} .$$

The system of normal equations

$$ra_j\alpha_1^2S_rC_r + \alpha_0\alpha_2b_j(rC_rS_s + sS_rC_s) = \frac{S_r}{r}$$

$$sb_j\alpha_1^2S_sC_s + \alpha_0\alpha_2a_j(rC_rS_s + sS_rC_s) = \frac{S_s}{s}$$

$$rc_j\alpha_1^2S_rC_r + \alpha_0\alpha_2d_j(sC_rS_s + rS_rC_s) = 0$$

$$sd_j\alpha_1^2S_sC_s + \alpha_0\alpha_2c_j(sC_rS_s + rS_rC_s) = 0$$

has a determinant $\Delta_1\Delta_2$ where

$$\Delta_1 = rs\alpha_1^4S_rS_sC_rC_s - \alpha_0^2\alpha_2^2(rC_nS_s + sS_rC_s)^2$$
$$= \frac{rs}{\alpha_2^4S_r^2S_s^2}(r^3-s^3)(rt_r - st_s),$$

$$\left(t_r = \frac{S_r}{C_r}, \quad t_s = \frac{S_s}{C_s}\right)$$

and

$$\Delta_2 = rs\alpha_1^4S_rC_rS_sC_s - \alpha_0^2\alpha_2^2(sC_rS_s + rS_rC_s)^2$$
$$= \frac{rs}{\alpha_2^4C_r^2C_s^2}(r^3-s^3)\left(\frac{r}{t_r} - \frac{s}{t_s}\right).$$

Now since r and s are distinct the product $\Delta_1\Delta_2$ never vanishes and so the unique solution is

$$\left.\begin{aligned} a_j^* &= \frac{sS_s}{\alpha_0{}^2T_1}, \quad b_j^* = \frac{-rS_r}{\alpha_0{}^2T_1}, \\ c_j^* &= d_j^* = 0, \quad \text{where} \quad T_1 = (sC_rS_s - rS_rC_s). \end{aligned}\right\} \qquad (5.1)$$

As for the case $N=1$, M_j is a quadratic function of a_j, b_j, c_j, d_j which has a total differential of second order

$$\begin{aligned} &\Phi(da_j, db_j, dc_j, dd_j) \\ &= 4\{r\alpha_1{}^2S_rC_r(da_j)^2 + \alpha_0\alpha_2(rC_rS_s+sS_rC_s)da_jdb_j \\ &\qquad + s\alpha_1{}^2S_sC_s(db_j)^2\} \\ &+ 4\{r\alpha_1{}^2S_rC_r(dc_j)^2 + \alpha_0\alpha_2(sC_rS_s+rS_rC_s)dc_jdd_j \\ &\qquad + s\alpha_1{}^2S_sC_s(dd_j)^2\}. \end{aligned}$$

This quadratic form is positive definite whenever Δ_1 and Δ_2 are strictly positive and since $x \tanh x$ and $x/\tanh x$ are both monotonic increasing functions for $x > 0$, The solutions (5.1) will define a minimum whenever r and s are distinct and h is positive. Thus the extremal defined by the normal equations is a minimum.

From (5.1) we see that, in the inside intervals, the spline defined by the normal equations is a symmetric function of its argument h. By substitution using (5.1) we have

$$\begin{aligned} g^{*\prime}\left(\frac{h_1}{2}-\right) &= -(ra_j^*S_r + sb_j^*S_s), \\ &= -\left\{\frac{\alpha_1{}^2}{rs}(sS_rC_s - rC_rS_s) - \alpha_0\alpha_2T_1\left[\frac{1}{r^2} + \frac{1}{s^2}\right]\right\}, \\ &= -\left\{\frac{\alpha_1{}^2\alpha_2T_1}{\alpha_0} - \frac{\alpha_1{}^2\alpha_2T_1}{\alpha_0}\right\}, \\ &= 0. \end{aligned}$$

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Similarly

$$g^*\left(\frac{h_1}{2}-\right) = 1/\alpha_0^2 - (a_j^* C_r + b_j^* C_s),$$

$$= \frac{\alpha_0 \alpha_2 T_1}{\alpha_1^2}\left(\frac{b_j^*}{rS_r} + \frac{a_j^*}{sS_s}\right),$$

$$= 0.$$

Then from the symmetry of g^* and the anti-symmetry of $g^{*\prime}$, it follows that

$$g^*(x_j) = g^{*\prime}(x_j) = 0 \qquad \text{each } j=1,\ldots,n.$$

This calculation verifies the continuity of g^* and $g^{*\prime}$ for the points $x_2, x_3, \ldots, x_{n-1}$ but, more than that, it gives an alternative system for the spline coefficients in the intervals I_0 and I_n. Of the four coefficients in I_0, two are determined by the end point condition (2.3) with $N=2$ and the other two may now be found explicitly from the two relations just derived. Clearly from the symmetry considerations the situation is the same for I_n. The system in I_0 and I_n is, in fact,

$$\begin{bmatrix} C_r & C_s & S_r & S_s \\ rS_r & sS_s & rC_r & sC_s \\ r^2 & s^2 & 0 & 0 \\ 0 & 0 & s & r \end{bmatrix} \begin{bmatrix} a_j \\ b_j \\ c_j \\ d_j \end{bmatrix} = \begin{bmatrix} 1/\alpha_0^2 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

for $j=0$ and n and this system has solution

$$\left.\begin{aligned} a_j^* &= \frac{r^2C_r - s^2C_s}{r\alpha_0^{\,2}T_2}, \quad b_j^* = -\frac{r^2}{s^2}\,a_j^*, \\ c_j^* &= \frac{r(S_r - \frac{r}{s}\,S_s)}{\alpha_0^{\,2}T_2}, \quad d_j^* = -\frac{s}{r}\,c_j^*, \end{aligned}\right\} \qquad (5.3)$$

where

$$T_2 = \frac{1}{r}\,(C_r - \frac{r^2}{s^2}\,C_s)(r^2C_r - s^2C_s)$$

$$- \; r(S_r - \frac{s}{r}\,S_s)(S_r - \frac{r}{s}\,S_s).$$

Now because g^* is determined in I_0 and I_n by the continuity conditions and the normal equations for the intervals I_1 up to I_{n-1}, and since these normal equations define a minimum on each interval, we know that g^* does indeed minimize (5.0).

This completes the proof of THEOREM II.

5.2 The Optimal Mesh Distribution

We are now in a position to determine the distribution of mesh points which will minimize the error of approximation. In part (1) of THEOREM III the mesh is described for the case that h_0 and h_n are prescribed and in part (2) the system for the optimal values of h_0 and h_n is given.

THEOREM III

The quadrature formula $Q_n^*(f)$ which is optimal in $\mathfrak{Q}(n,2)$ over H_2 has its weights C_j and D_j given by THEOREM II and its mesh given by

(1) $h_j = \frac{1}{(n-1)} \left[(t_2 - t_1) - \left(\frac{h_0}{2} + \frac{h_n}{2}\right)\right],$

$= \text{constant}, \qquad 1 \leq j \leq n-1.$

(2) $h_0 = h_n,$

and $\int_{I_0} \frac{d}{dh_0} g^*(x)\,dx = \int_{I_1} \frac{d}{dh_1} g^*(x)\,dx,$

where g^* is the spline defined in THEOREM II.

PROOF: As for N=1 we define a function

$$\omega = \omega(h_0, h_1 \ldots, h_n),$$
$$= \|g^*\|^2 - \theta \left(\sum_{j=0}^{n}{}'' h_j - (t_2 - t_1)\right), \quad \theta \text{ real.}$$

In THEOREM II it was shown that

$$g^*(x_j) = g^{*\prime}(x_j) = 0, \qquad (j=1,\ldots,n),$$

and, applying lemma 3 to g^*, we have

$$\omega = \int_{t_1}^{t_2} g^*(x)\,dx - \theta \left(\sum_{j=0}^{n}{}'' h_j - (t_2 - t_1)\right).$$

Once again from the form of ω over each subinterval I_j, the normal equations $\frac{d\omega}{dh_j} = 0$ for each j define a minimum point for $\|g^*\|^2$ under the constraints

$$\sum_{j=0}^{n}{}'' h_j = t_2 - t_1 , \; h_j \geq 0.$$

(1) Suppose first that h_0 and h_n are prescribed. Then in $1 \leq j \leq n-1$ the normal equations are

$$\frac{d}{dh_j} \int_{-\frac{h_j}{2}}^{\frac{h_j}{2}} g^*(x)\, dx = \theta. \tag{5.4}$$

Now g^*, for $x \in I_j$, is a function of the mesh interval h_j only. Therefore all the equations (5.4) have exactly the same form and each one is independent of j and we can say

$$h_j = \frac{1}{(n-1)} \left[(t_2 - t_1) - \frac{(h_0 + h_n)}{2} \right], \tag{5.5}$$

$$= \text{constant for all } j=1,\ldots,n-1.$$

(2) Suppose then that h_0 and h_n are no longer fixed. As when $N=1$ we will write $g^*(h_j;x) = g^*(x)$ to indicate that the coefficients of g^* are functions of h_j when $x \in I_j$.

Setting $\frac{d\omega}{dh_0} = \frac{d\omega}{dh_n} = 0$ yields

$$\frac{d}{dh_0} \int_0^{\frac{h_0}{2}} g^*(h_0;x)\, dx = \frac{d}{dh_n} \int_{-\frac{h_n}{2}}^{0} g^*(-h_n;x)\, dx = \frac{\theta}{2}.$$

Differentiating we get

$$\tfrac{1}{2}g^*\left(h_o;\frac{h_o}{2}\right) + \int_0^{\frac{h_o}{2}} \frac{d}{dh_o}\, g^*(h_o:x)\; dx$$

$$= -\tfrac{1}{2}g^*\left(-h_n;\; -\frac{h_n}{2}\right) + \int_{\frac{-h_n}{2}}^{0} \frac{d}{dh_n}\, g^*(-h_n;x)\; dx = \frac{\theta}{2}\, .$$

But in I_o and I_n, a_j^* and b_j^* are even functions of their arguments and c_j^* and d_j^* are odd functions. Then as

$$g^*\left(h_o;\, \frac{h_o}{2}\right) = g^*\left(-h_n;\; -\frac{h_n}{2}\right) = 0,$$

we may replace the above relation by

$$\int_0^{\frac{h_o}{2}} \frac{d}{dh_o}\, g^*(h_o;x)\; dx = \int_0^{\frac{h_n}{2}} \frac{d}{dh_n}\, g^*(h_n;x)\; dx = \frac{\theta}{2}\, ,$$

and, immediately,

$$h_o = h_n\, . \tag{5.6}$$

Differentiating in (5.4), and noting again that $g^*\left(\pm\, \frac{h_j}{2}\right) = 0$, we find that the relation

$$\int_0^{\frac{h_o}{2}} \frac{d}{dh_o}\, g^*(h_o;x)\; dx = \int_0^{\frac{h_1}{2}} \frac{d}{dh_1}\, g^*(h_1;x)\; dx, \tag{5.7}$$

which along with (5.5) and (5.6) gives us a complete characterization of the optimal mesh. This completes the proof of THEOREM III.

5.3 The Weights to the Derivative Values

__COROLLARY__ 1: For the optimal formula in $\mathcal{Q}(n,2)$ over H_2 the derivative weights vanish,

i.e. $D_j = 0$, $j=1,\ldots,n$,

and an alternative system for the mesh distribution is given by (5.5), (5.6) and $R^*_{12} = 0$, where g^* is the spline defined in __THEOREM II__.

__PROOF__: From relation (3.6) with $N=2$

$$D_j = -\alpha_2^2 \; R^*_{j2},$$

$$= -\alpha_2^2(g^{*\prime\prime}(x_j -) - g^{*\prime\prime}(x_j +)).$$

But in $1 \leq j \leq n-1$

$$g^{*\prime\prime}\left(+ \frac{h_j}{2} -\right) = g^{*\prime\prime}\left(- \frac{h_j}{2} +\right) = - (r^2 a^*_j C_r + s^2 b^*_j C_s).$$

Substituting for a^*_j and b^*_j from (5.1) with all the h_j equal, shows that $g^{*\prime\prime}$ is continuous at all the points $x_2,\ldots,x_{n-1}$, whence $D_2 = D_3 = \cdots = D_{n-1} = 0$.

Because of symmetry it will suffice to show that $D_1 = 0$.

From __THEOREM II__

$$aC_r + bC_s = 1/\alpha_0{}^2, \tag{5.8}$$

$$raS_r + sbS_s = 0 \quad , \tag{5.9}$$

where $a = a^*_1$, $b = b^*_1$ and, eliminating b^*_0 and d^*_0 by

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the conditions (2.3) with $N=2$,

$$a_0\left(C_{r_0} - \frac{r^2}{s^2} C_{s_0}\right) + c_0\left(S_{r_0} - \frac{s}{r} S_{s_0}\right) = 1/\alpha_0^2, \qquad (5.10)$$

$$ra_0\left(S_{r_0} - \frac{r}{s} S_{s_0}\right) + \frac{c_0}{r}\left(r^2 C_{r_0} - s^2 C_{s_0}\right) = 0 , \qquad (5.11)$$

where $a_0 = a_0^*$, $c_0 = c_0^*$ and $C_{r_0} = \cosh \frac{rh_0}{2}$, etc. ((5.8) and (5.9) result from $g^*(x_1 +) = g^{*\prime}(x_1 +) = 0$ and (5.10), (5.11) from $g^*(x_1 -) = g^{*\prime}(x_1 -) = 0$). We will use the above equations to show that for the optimal values of h_0 and h_1, $R_{12}^* = 0$.

The minimum condition (5.7) when integrated becomes

$$\frac{S_r}{r}\frac{da}{dh_1} + \frac{S_s}{s}\frac{db}{dh_1} = \frac{da_0}{dh_0}\left(\frac{S_{r_0}}{r} - \frac{r^2}{s^2} S_{s_0}\right) + \frac{dc_0}{dh_0}\frac{\left(C_{r_0} - C_{s_0}\right)}{r} . \qquad (5.12)$$

If we differentiate (5.8) with respect to h_1 we get

$$C_r \frac{da}{dh_1} + C_s \frac{db}{dh_1} + \tfrac{1}{2}(raS_r + sbS_s) = 0,$$

and since
$$g^{*\prime}\left(\frac{h_1}{2}\right) = 0,$$

$$C_r \frac{da}{dh_1} + C_s \frac{db}{dh_1} = 0. \qquad (5.13)$$

Similarly, differentiating (5.9) with respect to h_1, we have

$$\tfrac{1}{2}(r^2 aC_r + s^2 bC_s) + r\frac{da}{dh_1} S_r + s\frac{db}{dh_1} S_s = 0,$$

or

$$r\,\frac{da}{dh_1}\,S_r + s\,\frac{db}{dh_1}\,S_s = \tfrac{1}{2}g^{*\prime\prime}\left(\frac{h_1}{2}\right). \tag{5.14}$$

Solving (5.13) and (5.14) for $\frac{da}{dh_1}$, $\frac{db}{dh_1}$ we find

$$\frac{da}{dh_1} = \frac{-1}{2T_1}\,g^{*\prime\prime}\left(\frac{h_1}{2}+\right)C_s,\quad \frac{db}{dh_1} = \frac{1}{2T_1}\,g^{*\prime\prime}\left(\frac{h_1}{2}+\right)C_r,$$

where $T_1 = sC_rS_s - rS_rC_s$.

By differentiating (5.10) and (5.11) with respect to h_0 and solving the resulting system we get

$$\frac{da_0}{dh_0} = \frac{1}{2T_2}\,g^{*\prime\prime}\left(\frac{h_0}{2}-\right)\left(S_{r_0} - \frac{s}{r}\,S_{s_0}\right),$$

$$\frac{db_0}{dh_0} = -\frac{1}{2T_2}\,g^{*\prime\prime}\left(\frac{h_0}{2}-\right)\left(C_{r_0} - \frac{r^2}{s^2}\,C_{s_0}\right),$$

where

$$T_2 = \left(C_{r_0} - \frac{r^2}{s^2}\,C_{s_0}\right)\frac{\left(r^2C_{r_0} - s^2C_{s_0}\right)}{r}$$

$$-r\left(S_{r_0} - \frac{r}{s}\,S_{s_0}\right)\left(S_{r_0} - \frac{s}{r}\,S_{s_0}\right).$$

Equation (5.12) then becomes

$$\frac{g^{*\prime\prime}\left(\frac{h_1}{2}+\right)}{rs}\left[\frac{rC_rS_s - sS_rC_s}{sC_rS_s - rS_rC_s}\right]$$

$$= \frac{g^{*\prime\prime}\left(\frac{h_0}{2}-\right)}{T_2}\left[\left(C_{r_0} - \frac{r^2}{s^2}\,C_{s_0}\right)\frac{\left(C_{r_0} - C_{s_0}\right)}{r}\right.$$

$$\left. - \left(S_{r_0} - \frac{s}{r}\,S_{s_0}\right)\left(\frac{S_{r_0}}{r} - \frac{r^2}{s^3}\,S_{s_0}\right)\right]. \tag{5.15}$$

By elementary algebra it can be seen that

$$\left\{\left(C_{r_0} - \frac{r^2}{s^2} C_{s_0}\right) \frac{\left(C_{r_0} - C_{s_0}\right)}{r} - \left(S_{r_0} - \frac{s}{r} S_{s_0}\right)\left(\frac{S_{r_0}}{r} - \frac{r^2}{s^3} S_{s_0}\right)\right\}$$

$$= \frac{1}{r^2 s^2}\left\{r\left(C_{r_0} - C_{s_0}\right)\left(r^2 C_{r_0} - s^2 C_{s_0}\right) - \left(r^3 S_{r_0} - s^3 S_{s_0}\right)\left(S_{r_0} - \frac{r}{s} S_{s_0}\right)\right\}$$

(5.16)

and so we can replace the term in square brackets on the right hand side of (5.15) by the whole of the right hand side of (5.16). But by substitution of the spline coefficients we see that

$$g^{*\prime\prime}\left(-\frac{h_1}{2}+\right) = \frac{-rs}{\alpha_0^2}\left[\frac{rC_r S_s - sS_r C_s}{sC_r S_s - rS_r C_s}\right], \tag{5.17}$$

and

$$g^{*\prime\prime}\left(\frac{h_0}{2}-\right) = \frac{-1}{\alpha_0^2 T_2}\Big[r\left(C_{r_0} - C_{s_0}\right)\left(r^2 C_{r_0} - s^2 C_{s_0}\right)$$

$$- \left(r^3 S_{r_0} - s^3 S_{s_0}\right)\left(S_{r_0} - \frac{r}{s} S_{s_0}\right)\Big], \tag{5.18}$$

and so (5.15) becomes

$$\left[g^{*\prime\prime}\left(-\frac{h_1}{2}+\right)\right]^2 = \left[g^{*\prime\prime}\left(\frac{h_0}{2}-\right)\right]^2. \tag{5.19}$$

Using the relation $\alpha_0^2/\alpha_2^2 = r^2 s^2$ we can rewrite (5.17) as

$$g^{*\prime\prime}\left(-\frac{h_1}{2}+\right) = \frac{1}{\alpha_2^2}\left[\frac{\frac{t_r}{r} - \frac{t_s}{s}}{st_s - rt_r}\right],$$

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where we have denoted $t_r = \frac{S_r}{C_r}$ and $t_s = \frac{S_s}{C_s}$.

From the properties of tanh x it follows that $g^{*\prime\prime}\left(-\frac{h_1}{2}+\right) > 0$ for all $h_1 > 0$ and $r,s > 0$ and distinct. Similarly we can rewrite (5.18) as

$$g^{*\prime\prime}\left(\frac{h_0}{2}-\right) = \frac{-1}{rs^2\alpha_2{}^2T_2}\left[(r^2+s^2)(1-C_rC_s) + (r^4+s^4)\frac{S_r}{r}\frac{S_s}{s}\right], \tag{5.20}$$

$$= \frac{-1}{rs^2\alpha_2{}^2T_2}\left[(r^2+s^2) + \frac{1}{2rs}C_{r+s}((r^4+s^4)-rs(r^2+s^2)) - \frac{1}{2rs}C_{r-s}((r^4+s^4)+rs(r^2+s^2))\right]$$

$$= \frac{-1}{rs^2\alpha_2{}^2T_2}\left[(r^2+s^2) + \frac{1}{2rs}\sum_{j=0}^{\infty}\frac{(\frac{1}{2}h_0)^{2j}}{(2j)!}\{(r+s)^{2j}(r^3-s^3)(r-s)-(r-s)^{2j}(r^3+s^3)(r+s)\}\right].$$

Further we can write

$$rs^2T_2 = 2r^2s^2 + rs(r^2+s^2)S_rS_s - (r^4+s^4)C_rC_s$$

$$= 2r^2s^2 + \tfrac{1}{2}C_{r+s}(rs(r^2+s^2)-(r^4+s^4)) - \tfrac{1}{2}C_{r-s}(rs(r^2+s^2)+(r^4+s^4))$$

$$= 2r^2s^2 - \tfrac{1}{2}\left[\sum_{j=0}^{\infty}\frac{(\frac{1}{2}h_0)^{2j}}{(2j)!}((r+s)^{2j}(r^3-s^3)(r-s)+(r-s)^{2j}(r^3+s^3)(r+s))\right] \tag{5.21}$$

Now since, for $j = 1,2\ldots,$

$$(r+s)^{2j}(r^3-s^3)(r-s)-(r-s)^{2j}(r^3+s^3)(r+s)$$
$$= (r^2-s^2)^2[(r+s)^{2j-2}(r^2+s^2+rs)-(r-s)^{2j-2}(r^2+s^2-rs)]$$

is always positive $\left(r, s > 0,\right.$ and distinct$\left.\right)$ it follows that $rs^2T_2 < 0$ and hence that $g^{*\prime\prime}\left(-\frac{h_0}{2}+\right) > 0$.

Thus (5.19) implies that $R^*_{12} = 0$ and the result is proved.

6. Convergence of the Optimal Formulae

Definition: (1) Let $\{n_\ell\}_{\ell=1}^{\infty}$ be an increasing sequence of positive numbers and let $\pi = \{p_\ell\}_{\ell=1}^{\infty}$ be a sequence of partitions each from P, and such that p_ℓ has n_ℓ points.

Let $\{Q_\ell(f)\}_{\ell=1}^{\infty}$,

$$Q_\ell(f) = \sum_{j=1}^{n_\ell} \sum_{i=1}^{N} A_{ij}^{(\ell)} f^{(i-1)}(x_j^{(\ell)}),$$

be a sequence of quadrature formulae such that $Q_\ell(f)$ is defined on p_ℓ. We say that $\{Q_\ell(f)\}$ converges to $I(f)$ if

$$\lim_{\ell\to\infty} \|I - Q_\ell\|_{H_N^*} = 0.$$

(2) Let p be from P. We define the norm of p, denoted $|p|$ by

$$|p| = \max_{0\leq j\leq n} h_j.$$

<u>THEOREM IV</u>: Suppose that $\pi = \{p_\ell\}_{\ell=1}^{\infty}$ satisfies $\lim_{\ell\to\infty}|p_\ell| = 0$. Let $\tilde{Q}_{p_\ell} \subset \tilde{Q}(n_\ell,N)$ be the set of all quadrature formulae defined on p_ℓ and let $Q^*_{p_\ell}$ be the optimal formula in $\tilde{Q}_{p_\ell}$ over H_N. Then for $N=1$ and 2

(1) $\{Q^*_{p_\ell}\}$ converges to $I(f)$ as $\ell\to\infty$

(2) There exists a constant K, independent of ℓ such that for ℓ sufficiently large $\|E^*_{p_\ell}\| = \|I-Q^*_{p_\ell}\| < K|p_\ell|^N$

<u>Proof</u>: For N=1 and 2 the form of the coefficients of g^* is such that we may write

$$||E^*||^2 = \frac{1}{\alpha_N^2}\,\xi_1\left(\frac{\alpha_0}{\alpha_N},\frac{\alpha_1}{\alpha_N},\ldots,\frac{\alpha_{N-1}}{\alpha_N}\right).$$

From the definition of $||f||$ we can also put

$$||f||^2 = \alpha_N^2\,\xi_2\left(\frac{\alpha_0}{\alpha_N},\frac{\alpha_1}{\alpha_N},\ldots,\frac{\alpha_{N-1}}{\alpha_N}\right),$$

and so the bound $||E^*||\,||f||$ on $|E^*(f)|$ can be considered as a function only of the N ratios

$$\alpha_0/\alpha_N,\alpha_1/\alpha_N,\ldots,\alpha_{N-1}/\alpha_N.$$

We therefore lose no generality by setting $\alpha_N = 1$.

(i) Consider first the case N=1.

From lemma 4 we may write for $p_\ell\in\pi$

$$||E^*_{p_\ell}||^2 = \alpha_0^{-2}[(t_2-t_1) - \sum_{j=1}^{n_\ell} C_j^{(\ell)}], \qquad (6.0)$$

where $C_j^{(\ell)} = -(g^{*\prime}(\tfrac{1}{2}h_{j-1}^{(\ell)}-)-g^{*\prime}(-\tfrac{1}{2}h_j^{(\ell)}+))$,

are the optimal weights for the partition p_ℓ and where the index ℓ denotes the dependence of the mesh intervals (and hence the weights $C_j^{(\ell)}$) on p_ℓ.

Let us define

$$\varphi_j^{(\ell)}(h_j^{(\ell)}) = \tfrac{1}{2}h_j^{(\ell)}+g^{*\prime}(-\tfrac{1}{2}h_j^{(\ell)}+) \qquad (6.1)$$

$$= \tfrac{1}{2}h_j^{(\ell)} - \frac{1}{r}\tanh\frac{1}{2}rh_j^{(\ell)}$$

where $r=\alpha_0$ since we now have $\alpha_1=1$.

Thus

$$C_j^{(\ell)} = -[\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})+\varphi_j^{(\ell)}(h_j^{(\ell)})-\tfrac{1}{2}(h_{j-1}^{(\ell)}+h_j^{(\ell)})] \quad \text{each } j. \tag{6.2}$$

We may write

$$\|E^*_{p_\ell}\|^2 = 2\alpha_0^{-2} \sum_{j=0}^{n_\ell}{}'' \varphi_j^{(\ell)}(h_j^{(\ell)})$$

by collecting the terms in (6.0).

It is clear from the properties of tanh x that for ℓ sufficiently large

$$\varphi_j^{(\ell)}(h_j^{(\ell)}) < \frac{1}{3.2^3}\alpha_0^2(h_j^{(\ell)})^3. \tag{6.3}$$

Therefore

$$\|E^*_{p_\ell}\|^2 < \frac{1}{3.2^3}\left\{2\sum_{j=0}^{n_\ell}{}''(h_j^{(\ell)})^3\right\}$$

$$\leqslant \frac{1}{12}(t_2-t_1)|p_\ell|^2$$

and so setting $K = \sqrt{\frac{1}{12}(t_2-t_1)}$ we have $\|E^*_{p_\ell}\| < K|p_\ell|$

as required for $N=1$.

(ii) Consider now the case $N=2$. Once again

$$\|E^*_{p_\ell}\|^2 = \alpha_0^{-2}[(t_2-t_1) - \sum_{j=1}^{n_\ell} C_j^{(\ell)}]$$

but in this case

$$C_j^{(\ell)} = g^{*'''}(\tfrac{1}{2}h_{j-1}^{(\ell)}-)-g^{*'''}(-\tfrac{1}{2}h_j^{(\ell)}+) \quad \text{for each } j. \tag{6.4}$$

From the symmetry of g^* and the antisymmetry of its odd derivatives we have

$$\|E^*_{p_\ell}\|^2 = \alpha_0^{-2}[(t_2-t_1) - 2\sum_{j=0}^{n_\ell}{}'' g^{*'''}(\tfrac{1}{2}h_j^{(\ell)}-)].$$

Let us define as before

$$\varphi_j^{(\ell)}(h_j^{(\ell)}) = \tfrac{1}{2}h_j^{(\ell)} - g^{*'''}(\tfrac{1}{2}h_j^{(\ell)}-) \quad \text{each} \quad j=0,\ldots,n_\ell. \quad (6.5)$$

Then since T_2 (theorem II) does not vanish if r and s are distinct we may say that for each j $g^{*'''}(\frac{1}{2}h_j^{(\ell)}-)$ is an analytic function of $h_j^{(\ell)}$ in the neighbourhood of the point $h_j^{(\ell)} = 0$. The first terms of the Maclaurin series in $h_j^{(\ell)}$ for $g^{*'''}(\frac{1}{2}h_j^{(\ell)})$ are

$$g^{*'''}(\tfrac{1}{2}h_j^{(\ell)}-) = \tfrac{1}{2}h_j^{(\ell)}\{1 + 0.h_j^{(\ell)^2} - K_j\alpha_0^2 h_j^{(\ell)^4} + \ldots\}, \quad (6.6)$$

where $K_0 = K_n = \dfrac{6}{5!2^4}$, $K_j = \dfrac{8}{3.5!2^4}$ $\quad 1 \leqslant j \leqslant n-1$, and so K_j is independent of ℓ. Then

$$\varphi_j^{(\ell)}(h_j^{(\ell)}) < K_j\alpha_0^2(h_j^{(\ell)})^5 \quad (6.7)$$

if ℓ is sufficiently large. Now $\sum_{j=0}^{n_\ell}{}'' h_j^{(\ell)} = t_2-t_1$ for any ℓ and so

$$\begin{aligned}\|E^*_{p_\ell}\|^2 &= 2\alpha_0^{-2} \sum_{j=0}^{n_\ell}{}''\varphi_j^{(\ell)}(h_j^{(\ell)}) \\ &< 2\alpha_0^{-2} \sum_{j=0}^{n_\ell}{}'' K_j\alpha_0^2(h_j^{(\ell)})^5 \\ &\leqslant 2K_{max}(t_2-t_1)|p_\ell|^4\end{aligned}$$

where $K_{max} = \max_j K_j$ and ℓ is sufficiently large.

Then putting $K = \sqrt{2K_{max}(t_2-t_1)}$ we have

$\|E^*_{p_\ell}\| < K|p_\ell|^2$ as required for $N=2$, and the theorem is proved.

Thus we are assured that given <u>any</u> sequence π of partitions whose largest mesh intervals tend to zero, the sequence of optimal formulae defined on these partitions will converge to the integral at least as quickly as the N^{th} power of the largest mesh length, when $n = 1$ or 2.

7. The Optimal Formulae and The Midpoint Rule.

Let us construct quadrature formulae

$$M^{(1)}(f) = \sum_{j=1}^{n} U_j^{(1)} f(x_j)$$

and

$$M^{(2)}(f) = \sum_{j=1}^{n} U_j^{(2)} f(x_j) + V_j^{(2)} f'(x_j)$$

which are defined on an arbitrary mesh and which are exact for the constant function $f(x) = c$. Further let $M^{(2)}$ be exact for the line $f(x) = x$. $M^{(1)}$ and $M^{(2)}$ can each be considered as a composite rule arising from a one point formula in which the point, x_j, is used as the sampling point for the function in the sub-interval $S_j = (\frac{1}{2}(x_{j-1}+x_j), \frac{1}{2}(x_j+x_{j+1}))$, $j=2,\ldots,n-1$, and x_1 and x_n are used as the sampling points for the intervals

$$S_1 = (t_1, \tfrac{1}{2}(x_1+x_2)) \text{ and } S_n = (\tfrac{1}{2}(x_{n-1}+x_n), t_2)$$

respectively.

Denoting the errors of $M^{(1)}$ and $M^{(2)}$ by $E^{(1)}$ and $E^{(2)}$ then on each subinterval S_j the requirement

$$E^{(1)}(c) = E^{(2)}(c) = 0 \tag{7.1}$$

is satisfied if

$$\int_{S_j} c\,dx = cU_j^{(1)} = cU_j^{(2)}$$

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whence $\frac{1}{2}c(x_{j+1}-x_{j-1}) = \frac{1}{2}c(h_{j-1}+h_j) = U_j^{(1)}c = U_j^{(2)}c$

or $$U_j^{(1)} = U_j^{(2)} = \tfrac{1}{2}(h_{j-1}+h_j) \quad \text{each } j.$$

Let us therefore denote the weights

$$U_j^{(1)} = U_j^{(2)} = U_j, \quad V_j^{(2)} = V_j.$$

Clearly (7.1) is satisfied on the whole interval (t_1, t_2).

Similarly the requirement

$$E^{(2)}(x) = 0 \tag{7.2}$$

on each subinterval leads to

$$\int_{\frac{1}{2}(x_{j-1}+x_j)}^{\frac{1}{2}(x_j+x_{j+1})} x\,dx = U_j x_j + V_j.$$

Thus $V_j = \frac{1}{8}(h_j^2 - h_{j-1}^2) = \frac{1}{2}((\frac{1}{2}h_j)^2-(\frac{1}{2}h_{j-1})^2)$ for each j.

Once again (7.2) holds on the whole of (t_1, t_2).

Since these quadrature formulae, for the case that all the h_j are equal, collapse to the well-known midpoint rule

$$M(f) = h \sum_{j=1}^{n} f(x_j),$$

x_j and h defined by $h = \dfrac{t_2-t_1}{n}$,

$$x_j = t_1 + (j-\tfrac{1}{2})h, \; j=1,\ldots,n,$$

we will call them the Generalized Midpoint Rules (G.M.R.).

<u>THEOREM V</u>: Let $\left\{Q^{*}_{p_\ell}\right\}_{\ell=1}^{\infty}$ be defined as in theorem IV and let $\left\{M^{(N)}_{p_\ell}\right\}_{\ell=1}^{\infty}$ be the sequence of G.M.R.'s each defined on the partition p_ℓ.

Then (1) for $N=1$ and 2 there exist constants $\kappa_0^{(1)}$ and $\kappa_0^{(2)}$, independent of ℓ, such that for ℓ sufficiently large

$$0 < 1 - \frac{C_j^{(\ell)}}{U_j^{(\ell)}} < \kappa_0^{(N)} |p_\ell|^{2N}. \qquad (7.3)$$

(2) Further, for the case $N=2$ there exists a constant $\kappa_1^{(2)}$, independent of ℓ, such that for $j=2,\ldots,n_\ell-1$,

(a) If $V_j^{(\ell)} = 0$ then $D_j^{(\ell)} = 0$, and

(b) If $V_j^{(\ell)} \neq 0$

$$0 < 1 - \frac{D_j^{(\ell)}}{\frac{2}{3}V_j^{(\ell)}} < \kappa_1^{(2)} |p_\ell|^{N}. \qquad (7.4)$$

<u>Proof</u>: Consider first the case $N=1$.

From (6.2) we may write

$$\frac{C_j^{(\ell)}}{U_j^{(\ell)}} = 1 - \frac{\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)}) + \varphi_j^{(\ell)}(h_j^{(\ell)})}{\frac{1}{2}(h_{j-1}^{(\ell)} + h_j^{(\ell)})} \qquad \text{each } j.$$

Then using (6.3), if ℓ is sufficiently large we can say

$$\frac{\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)}) + \varphi_j^{(\ell)}(h_j^{(\ell)})}{\frac{1}{2}(h_{j-1}^{(\ell)} + h_j^{(\ell)})} < \frac{\alpha_0^2}{3.2^3} \cdot \frac{(h_{j-1}^{(\ell)})^3 + (h_j^{(\ell)})^3}{\frac{1}{2}(h_{j-1}^{(\ell)} + h_j^{(\ell)})}$$

$$\leqslant \kappa_0^{(1)} |p_\ell|^{2N},$$

where $\kappa_0^{(1)} = \frac{\alpha_0^2}{12}$. Thus (7.3) holds if ℓ is sufficiently large and $C_j^{(\ell)}$ tends to $U_j^{(\ell)}$ from below with the rate of $|p_\ell|^{2N}$ ar required.

Consider now if $N=2$. With φ_j defined by (6.5) we can write

$$C_j^{(\ell)} = \tfrac{1}{2}(h_{j-1}^{(\ell)}+h_j^{(\ell)}) - (\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})+\varphi_j^{(\ell)}(h_j^{(\ell)}))$$

Then

$$\frac{C_j(\ell)}{U_j(\ell)} = 1 - \frac{2(\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})+\varphi_j^{(\ell)}(h_j^{(\ell)}))}{(h_{j-1}^{(\ell)} + h_j^{(\ell)})}$$

and using (6.6) and (6.7) we may say that if ℓ is sufficiently large

$$\frac{\varphi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})+\varphi_j^{(\ell)}(h_j^{(\ell)})}{(h_{j-1}^{(\ell)}+h_j^{(\ell)})} < K_{max}\alpha_0^2 \frac{(h_{j-1}^{(\ell)})^5+(h_j^{(\ell)})^5}{h_{j-1}^{(\ell)}+h_j^{(\ell)}} \qquad (7.5)$$

$$\leqslant K_{max}\alpha_0^2 |p_\ell|^4$$

$$= \kappa_0^{(2)} |p_\ell|^{2N},$$

where $\kappa_0^{(2)} = K_{max}\alpha_0^2$, as required.

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2 (a) We note first that $V_j^{(\ell)} = 0$ implies that $h_{j-1}=h_j$. Then by using the argument of the proof to Corollary 1 in section (5.3) we have immediately $V_j=0$ implies $D_j=0$.

(b) The spline $g^{*''}(\frac{1}{2}h_j^{(\ell)}-)$ is an even function of h_j which is an analytic function of h_j in the neighbourhood of the point $h_j=0$. The first terms of the Maclaurin series for $g^{*''}(\frac{1}{2}h_j^{(\ell)}-)$ are

$$g^{*''}(\tfrac{1}{2}h_j^{(\ell)}-) = \tfrac{1}{3}(\tfrac{1}{2}h_j^{(\ell)})^2 - \frac{8\alpha_1^{\,2}}{3.5!}(\tfrac{1}{2}h_j^{(\ell)})^4+\dots .$$

We define for $j=1,2,\dots,n_\ell-1$,

$$\psi_j^{(\ell)}(h_j^{(\ell)}) = \tfrac{1}{3}(\tfrac{1}{2}h_j^{(\ell)})^2 - g^{*''}(\tfrac{1}{2}h_j^{(\ell)}-).$$

Then

$$\begin{aligned} D_j^{(\ell)} &= -(g^{*''}(\tfrac{1}{2}h_{j-1}^{(\ell)}-)-g^{*''}(-\tfrac{1}{2}h_j^{(\ell)}+)) \\ &= -(g^{*''}(\tfrac{1}{2}h_{j-1}^{(\ell)}-)-g^{*''}(\tfrac{1}{2}h_j^{(\ell)}-)) \\ &= -\Big\{\tfrac{1}{3}((\tfrac{1}{2}h_{j-1}^{(\ell)})^2-(\tfrac{1}{2}h_j^{(\ell)})^2) \\ &\qquad -(\psi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})-\psi_j^{(\ell)}(h_j^{(\ell)}))\Big\}, \end{aligned}$$

and

$$\frac{D_j^{(\ell)}}{\frac{2}{3}V_j^{(\ell)}} = \left\{1 - \frac{\psi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})-\psi_j^{(\ell)}(h_j^{(\ell)})}{\frac{1}{3}((\frac{1}{2}h_{j-1}^{(\ell)})^2-(\frac{1}{2}h_j^{(\ell)})^2)}\right\}.$$

But $(\frac{1}{2}h_{j-1}^{(\ell)})^2-(\frac{1}{2}h_j^{(\ell)})^2$ divides $\psi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})-\psi_j^{(\ell)}(h_j^{(\ell)})$

exactly and so we may say, using the property

$$\psi_j^{(\ell)}(h_j^{(\ell)}) < \frac{8\alpha_1^2}{3.5!2^4}(h_j^{(\ell)})^4,$$

for ℓ sufficiently large, that

$$\frac{\psi_{j-1}^{(\ell)}(h_{j-1}^{(\ell)})-\psi_j^{(\ell)}(h_j^{(\ell)})}{\frac{1}{3}((\frac{1}{2}h_{j-1}^{(\ell)})^2-(\frac{1}{2}h_j^{(\ell)})^2)} < \frac{8\alpha_1^2}{5!2^4} \cdot |p_\ell|^2$$

$$= \kappa_1^{(2)}|p_\ell|^N$$

where $\kappa_1^{(2)} = \frac{\alpha_1^2}{2.5!}$ and $D_j^{(\ell)}$ tends to $\frac{2}{3}V_j^{(\ell)}$ with the rate of $|p_\ell|^N$ as required.

Let us denote the optimal quadrature formula for the case N = 1(2) by the mnemonic OQF1(2), and let us denote the corresponding optimal mesh by OM1(2).

We may note here that if we use the OQF2 and the G.M.R. each on the mesh OM1 then the G.M.R. reduces to the midpoint rule and does not use derivative values at x_1 and x_n while the OQF2 <u>does</u> use the derivative values at these points. If however we use the G.M.R. and OQF2 each on OM2, the OQF2 uses no derivatives at x_1 and x_n and the G.M.R. does. These weights, when they do not vanish, will be seen to be small. However it is clear that each rule, used on a semi equidistant mesh (i.e. defined by (5.5), (5.6) and $h_\bullet$ = constant) which is not optimal for that rule, uses derivative values to overcome the so called boundary effect. That is to overcome what may be considered as a jump discontinuity in the integrand at the endpoints t_1 and t_2. It would seem that on its own optimal mesh each formula can take account of this jump without the use of derivative values.

But there are two points about the weights D_j and V_j which remain unclear. Firstly, the author could not see what relation these weights bear to each other at the end points x_1 and x_n, and secondly the author did not discover the reason for the multiplier $\frac{2}{3}$ in the relation (7.4).

7.1 The case $\alpha_0 = 0$

We can find the weights to the optimal formula when $\alpha_0 = 0$ as a simple consequence of theorem IV. We note first that relation (7.3) applies to both cases N=1 and 2.

From section (7.0) we have $\kappa_0^{(1)} = \dfrac{\alpha_0^2}{12}$ and $\kappa_0^{(2)} = K_{max}\alpha_0^2$ whence taking the limit as $\alpha_0 \to 0$ in (7.3) shows that for $\alpha_0 = 0$ the optimal formula has $C_j = U_j$, $j = 1,\ldots,n$.

The weights to the derivative values are defined as before by the jumps R^*_{j2} in the second derivative at the mesh points.

Now since $\pm r, \pm s$ are the roots of $\alpha_0^2 - \alpha_1^2 m^2 + m^4 = 0$ we see that when $\alpha_0 \to 0$, $r \to 0$ and $s \to \alpha_1$ so that letting $r \to 0$ and $s \to \alpha_1$ in (5.17) gives

$$\lim_{\alpha_0\to 0} g^{*\prime\prime}(\tfrac{1}{2}h_j-) = \tfrac{1}{2}h_j(\alpha_1 \tanh \tfrac{1}{2}\alpha_1 h_j)^{-1} - 1/\alpha_1^2$$

$$j = 1,\ldots,n-1.$$

For I_0 and I_n we have, using (5.21), that

$$\lim_{\alpha_0\to 0} rs^2T_2 = -\alpha_1^4 \cosh \tfrac{1}{2}\alpha_1 h_j, \quad j = 0 \text{ and } n,$$

and so from (5.20)

$$\lim_{\alpha_0\to 0} g^{*\prime\prime}(\tfrac{1}{2}h_j-) = \frac{\tfrac{1}{2}h_j}{\alpha_1} \tanh \tfrac{1}{2}\alpha_1 h_j - \frac{1}{\alpha_1^2} + \frac{1}{\alpha_1^2 \cosh \tfrac{1}{2}\alpha_1 h_j},$$

$$j = 0 \text{ and } n.$$

Then $D_j = -R^*_{j2} = -(g^{*\prime\prime}(\tfrac{1}{2}h_{j-1}-) - g^{*\prime\prime}(\tfrac{1}{2}h_j))$ as before and the optimal mesh is given by (5.5), (5.6) and $R^*_{12} = D_1 = 0$: i.e.

$$\tfrac{1}{2}h_1(\alpha_1 \tanh \tfrac{1}{2}\alpha_1 h_1)^{-1} = \frac{\tfrac{1}{2}h_0}{\alpha_1}\tanh \tfrac{1}{2}\alpha_1 h_0 + \frac{1}{\alpha_1^2 \cosh \tfrac{1}{2}\alpha_1 h_0}$$

or

$$\frac{1}{\cosh \tfrac{1}{2}\alpha_1 h_0} + \tfrac{1}{2}\alpha_1 h_0 \tanh \tfrac{1}{2}\alpha_1 h_0 = \frac{\tfrac{1}{2}\alpha_1 h_1}{\tanh \tfrac{1}{2}\alpha_1 h_1}.$$

Thus all the cases of interest for $N \leq 2$ have been considered: viz.

(a)	$\alpha_0, \alpha_1 \neq 0$	(N=1)	OQF1
(b)	$\alpha_0 = 0, \alpha_1 \neq 0$	(N=1)	Midpoint Formula
(c)	$\alpha_0, \alpha_1, \alpha_2 \neq 0$	(N=2)	OQF2
(d)	$\alpha_0 = 0, \alpha_1, \alpha_2 \neq 0$	(N=2)	G.M.R.
(e)	$\alpha_0 = \alpha_1 = 0, \alpha_2 \neq 0$	(N=2)	Krylov Formula with $q=2$.

For completeness we include here the weights and mesh of the Krylov formula (corresponding to case (e)) for the interval

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(0,1). This formula is easily obtained by setting $p=2$ in (1.6), (1.7) and (1.8). In the present notation these are

$$h_0 = h_n = h\sqrt{\frac{2}{3}},$$

$$h_j = h = (n + \sqrt{\frac{2}{3}} - 1)^{-1} = \text{constant}, \quad j=1,\ldots,n-1,$$

$$C_j = h, \quad j=2,\ldots,n-1$$

$$C_1 = C_n = \tfrac{1}{2}h(1 + \sqrt{\frac{2}{3}}).$$

It is interesting that a second order approximation to the solution of $R^{*}_{12} = 0$ (i.e. equating the Maclaurin series in h_0, h_1 for $g^{*\prime\prime}(\tfrac{1}{2}h_0-)$ and $g^{*\prime\prime}(\tfrac{1}{2}h_1-)$ respectively, and ignoring fourth and higher order terms) also yields $h_0 = h_1\sqrt{\frac{2}{3}}$, independently of α_0 and α_1. Thus this serves as a starting value for the numerical (iterative) solution of $R^{*}_{12} = 0$ (see chapter 9).

8. The Optimal Closed Formula

A quadrature formula in which the values of the function and its derivatives at the end points of the interval of integration are used is called a closed formula. The optimal n-point closed formula is easily obtained from THEOREM III where it was shown that if h_0 and h_n are prescribed, the remaining intervals $h_1, h_2, \ldots, h_{n-1}$ have equal length. The closed formula then is the case for which $h_0 = h_n = 0$.

COROLLARY 2: Let $\tilde{Q}_{p_3}$ be the subset of $\tilde{Q}(n,2)$ containing those quadrature formulae whose partitions have $x_1 = t_1$ and $x_n = t_2$. Then the quadrature formula $Q_n^*(f)$ which is optimal in $\tilde{Q}_{p_3}$ over H_2 is characterized by

(1) $$2C_1 = 2C_n = C_j = \frac{2(r^2-s^2)\,t_r\,t_s}{rs(rt_r-st_s)}, \qquad j=2,\ldots,n-1,$$

(2) $$D_j = 0, \qquad j=2,\ldots,n-1,$$

$$D_1 = D_n = \frac{1}{rs}\left(\frac{rt_s-st_r}{st_s-rt_r}\right), \qquad \text{and}$$

(3) $$h_j = \frac{t_2 - t_1}{n-1}, \qquad j=0,\ldots,n$$

where we have denoted

$$t_r = \frac{S_r}{C_r} \quad \text{and} \quad t_s = \frac{S_s}{C_s}.$$

PROOF: From THEOREM III part (1) we have, putting

$h_o = h_n = 0$

$$h_j = \frac{t_2 - t_1}{n-1}, \qquad 1 \leqslant j \leqslant n-1.$$

As before $D_j = 0,$ $\qquad 2 \leqslant j \leqslant n-1,$

and $\qquad C_j = \alpha_2{}^2 R^*_{j3},$

$$= -2\alpha_2{}^2(r^3 a_j S_r + s^3 b_j S_s), \qquad 2 \leqslant j \leqslant n-1,$$

$$= \frac{(r^2 - s^2)t_r t_s}{rs(rt_r - st_s)} .$$

From THEOREM II part (2) we can see that, since the spline coefficients in I_o and I_n are continuous functions of the mesh lengths h_o and h_n,

$$\lim_{h_o \to 0} g^{*'''}\left(\frac{h_o}{2} -\right) = \lim_{h_n \to 0} -g^{*'''}\left(-\frac{h_n}{2} +\right) = 0,$$

whence

$$C_n = C_1 = \alpha_2{}^2 R^*_{13}$$

$$= -\alpha_2{}^2 g^*\left(-\frac{h_1}{2} +\right),$$

$$= -\alpha_2{}^2(r^3 a_1 S_r + s^3 b_1 S_s),$$

$$= \tfrac{1}{2}C_j, \qquad 2 \leqslant j \leqslant n-1,$$

since all the h_j are equal.

Similarly

$$\lim_{h_o \to 0} g^{*''}\left(\frac{h_o}{2} -\right) = \lim_{h_n \to 0} -g^{*''}\left(-\frac{h_n}{2} +\right) = 0,$$

and so

.2

$$D_n = D_1 = -\alpha_2{}^2 g^{*\prime\prime}\left(-\frac{h_1}{2}+\right)$$

$$= \alpha_2{}^2(r^2 a_1 C_r + s^2 b_1 C_s),$$

$$= \frac{1}{rs}\begin{pmatrix} rt_s - st_r \\ \hline st_s - rt_r \end{pmatrix} .$$

9. Numerical Considerations

9.1 Round off Properties of the Optimal Formula

In section 7 we showed that the weights C_j of the optimal formula on an arbitrary mesh tend to the weights U_j of the G.M.R. $M^{(1)}$ from below. In this section we show that these weights are also positive.

For $N=1$ we have

$$C_j^* = \frac{1}{r}(\tanh \tfrac{1}{2}rh_{j-1} + \tanh \tfrac{1}{2}rh_j)$$

and the result is immediate since $\tanh x > 0$ if $x > 0$.

For the case $N=2$ we can write

$$g^{*\prime\prime\prime}(\tfrac{1}{2}h_j-) = \frac{r^2-s^2}{rs^2T_2}\left(\frac{s^2}{r}C_sS_r - \frac{r^2}{s}C_rS_s\right),\ j=0 \text{ and } n.$$

and

$$g^{*\prime\prime\prime}(\tfrac{1}{2}h_j-) = -\frac{(r^2-s^2)}{T_1}\frac{S_rS_s}{rs} \quad j=1,2,\ldots,n-1,$$

and since

$$\text{sign}\left(\frac{s^2}{r}C_sS_r - \frac{r^2}{s}C_rS_s\right) = \text{sign}(s-r),$$

and $T_2 < 0$ we have

$$g^{*\prime\prime\prime}(\tfrac{1}{2}h_j-) > 0, \quad j=0 \text{ and } n.$$

Similarly sign (T_1) = sign$(s-r)$ and so

$$g^{*\prime\prime\prime}(\tfrac{1}{2}h_j-) > 0, \quad j=1,\ldots,n-1.$$

Using (6.4) we can write

$$C_j^* = g^{*\prime\prime\prime}(\tfrac{1}{2}h_{j-1}-)+g^{*\prime\prime\prime}(\tfrac{1}{2}h_j-) \quad \text{and so}$$

the weights C_j satisfy

$$0 < C_j < \tfrac{1}{2}(h_{j-1}+h_j) \quad \text{all} \quad j.$$

Thus if the optimal Formula is used with the optimal mesh (i.e. all D_j's = 0) then we may say that the optimal formula, while best in the sense of the norm for H_1 or H_2 is well suited to automatic computation because it keeps the roundoff error from accumulating unduly. By comparison the high order Newton-Cotes formulae, which have the highest possible order of precision on a fixed ("equally spaced") mesh are of little practical use because they have both positive and negative coefficients.

9.2 The numerical computation of the optimal mesh.

The system of equations (5.5), (5.6) and $R_{12}^* = 0$, given in Corollary I to theorem III is non-linear and affords no easy explicit solution. However for given n, t_1, and t_2 we can set $h_0+(n-1)h_1 = t_2-t_1$ and consider the equation, $R_{12}^* = g^{*\prime\prime}(\tfrac{1}{2}h_0-)-g^{*}(\tfrac{1}{2}h_1-) = 0$, defining h_0 and h_1, as an equation in the single variable $\rho = h_0/h_1$. By differentiating (5.17) and (5.20) with respect to h_j it can be seen that for all j, $\frac{d}{dh_j}g^{*\prime\prime}(\tfrac{1}{2}h_j)> 0$, whence $g^{*\prime\prime}(\tfrac{1}{2}h_j)$ is a monotone increasing function of h_j. Then while $h_0+(n-1)h_1 = t_2-t_1$, $g^{*\prime\prime}(\tfrac{1}{2}h_0)$ will be a monotone

.2

increasing function of ρ and $g^{*\prime\prime}(\frac{1}{2}h_1)$ will be a monotone decreasing function of ρ. The equation therefore lends itself to solution by any of the standard iterative procedures.

In our calculations of ρ_0, the optimal ratio h_0/h_1, the secant method proved to be the simplest and converged rapidly for all values of $\alpha_0{}^2, \alpha_1{}^2$ chosen.

For the purposes of comparison the function $g^*(x)$ and its first two derivatives are shown in Fig.I. Fig.I.1 shows the optimal spline for $\rho < \rho_0$, Fig.I.2 shows $\rho=\rho_0$ and Fig.I.3 shows $\rho > \rho_0$. Only the first two intervals I_0, I_1 are shown. For $\rho \neq \rho_0$ the weights D_j are given by the magnitude of the difference $g^{*\prime\prime}(\frac{1}{2}h_1-)-g^{*\prime\prime}(\frac{1}{2}h_0-)$. In Figs.II.1 up to II.5 the optimal spline and its derivatives are shown on the first two intervals, of the optimal 3 point mesh for varying $\alpha_0{}^2$, $\alpha_1{}^2$. In all cases $\alpha_2{}^2 = 1$ and $t_1=0$, $t_2=1$. The most striking feature of the graphs is the difference between the function's deviation from the axis and the deviation of the two derivatives. This difference is large even when $\alpha_0{}^2=1$ and $\alpha_1{}^2=100$ when one might expect, since the weights to $\int_0^1 g^{*2}(x)dx$ and $\int_0^1 g^{*\prime\prime 2}(x)dx$ are equal, that the areas under the curves $g^{*\prime\prime}$ and g^* might be comparable. They are not comparable however because the optimal spline satisfies

.3

$$\int_0^1 \alpha_0{}^2 g^{*2}(x)+\alpha_1{}^2 g^{*\prime 2}(x)+g^{*\prime\prime 2}(x)\,dx = \int_0^1 \overset{*}{g}(x)\,dx \quad (9.1)$$

and so g^* represents, in a sense, the function defining a point of equilibrium between the L.H.S. and the R.H.S. of (9.1). Within this limitation however, the effect of weighting one of the integrals in the norm more heavily than the other two can be seen to affect the corresponding function by allowing it to "deviate less" from the axis. To better illustrate the function g^* itself we show, in Figs.II.4 and, II.5, the functions g^* and $g^{*\prime}$ on a magnified scale. In both Fig. I and Fig. II the x scale has been approximately normalized.

9.3 Data for the Optimal Formulae (N=2)

In table I we give, for various values of n, $\alpha_0{}^2$ and $\alpha_1{}^2$, the value of ρ_0 and the products nC_1 and nC_2 for the interval $(0,1)$. From this table the corresponding value of $||E^*||$ can easily be computed from the formula

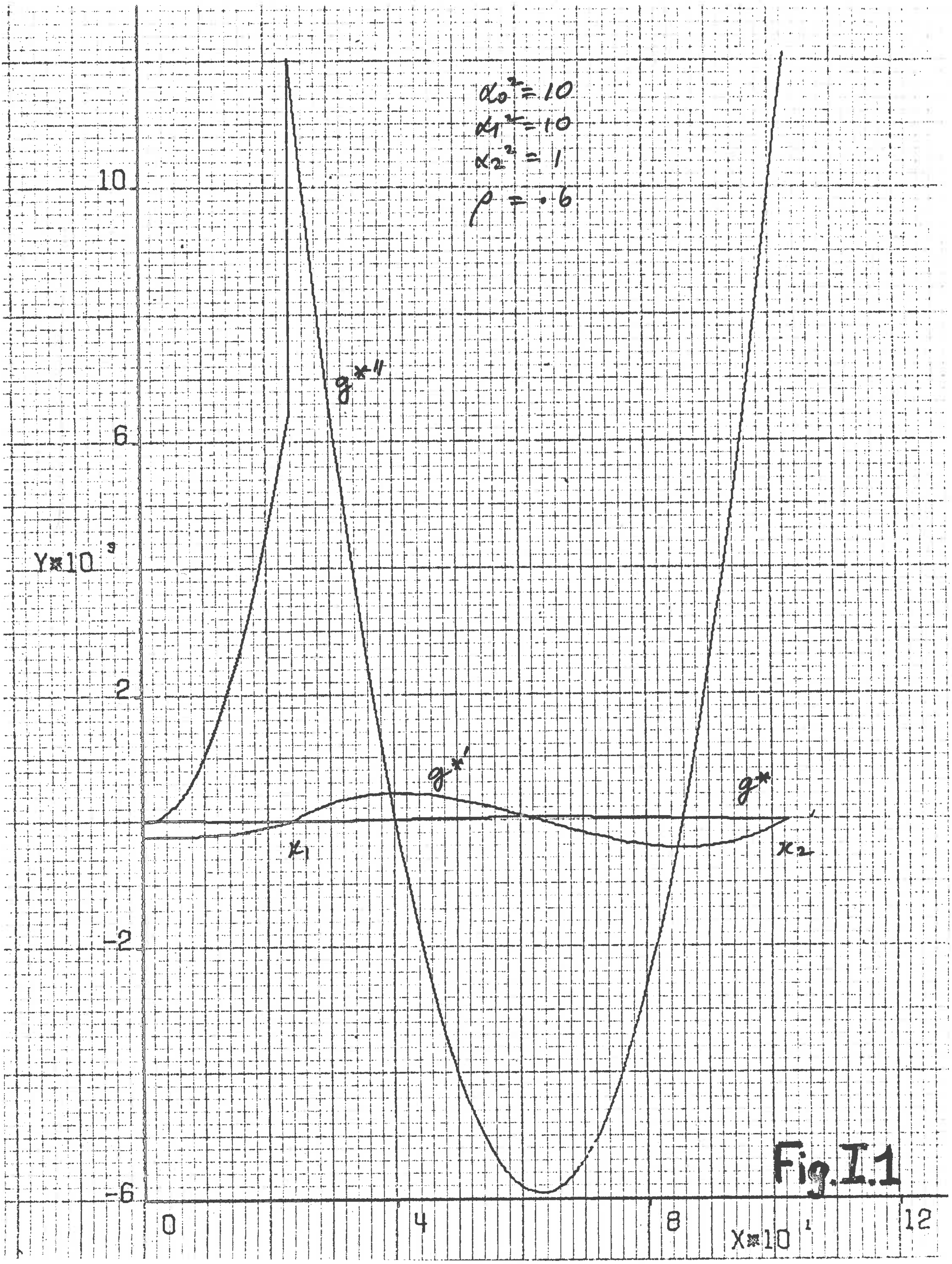
$$||E^*|| = \left\{\frac{1}{\alpha_0{}^2}[1-2C_1-(n-2)C_2]\right\}^{\frac{1}{2}}.$$

9.4 Numerical Comparison of the Optimal Formulae

To demonstrate the formulae developed above, the OQF1, OQF2 and G.M.R. were applied to functions whose integrals could be computed exactly and they were compared

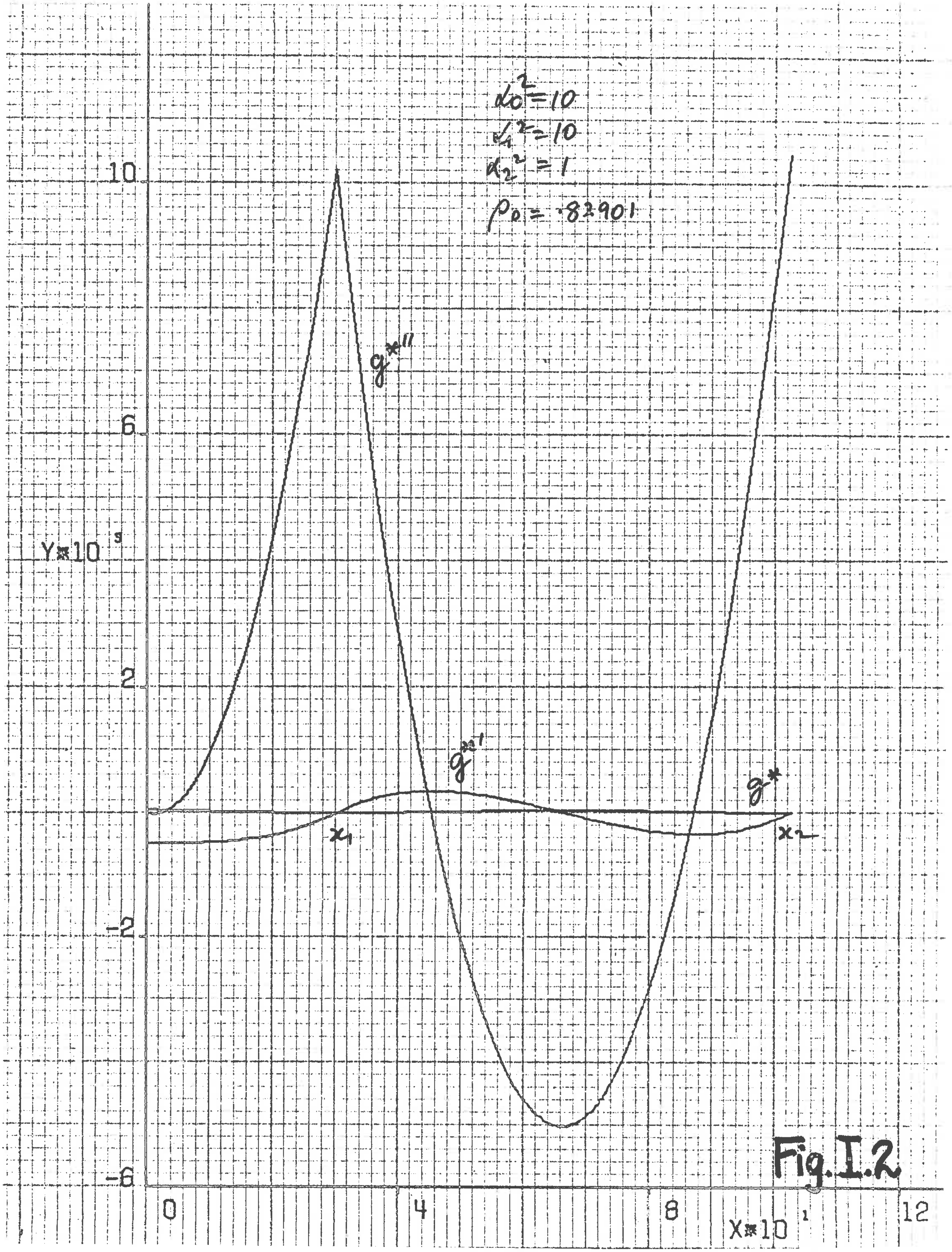
.4

with the Trapezoidal Rule and the Midpoint Rule (itself an optimal formula). Table II shows the errors of the formulae for varying values of n and α_0^2, α_1^2 (such that r and s are distinct and positive). Tables II.9 and II.10 show the optimal formulae applied to two functions <u>not</u> in H_1.



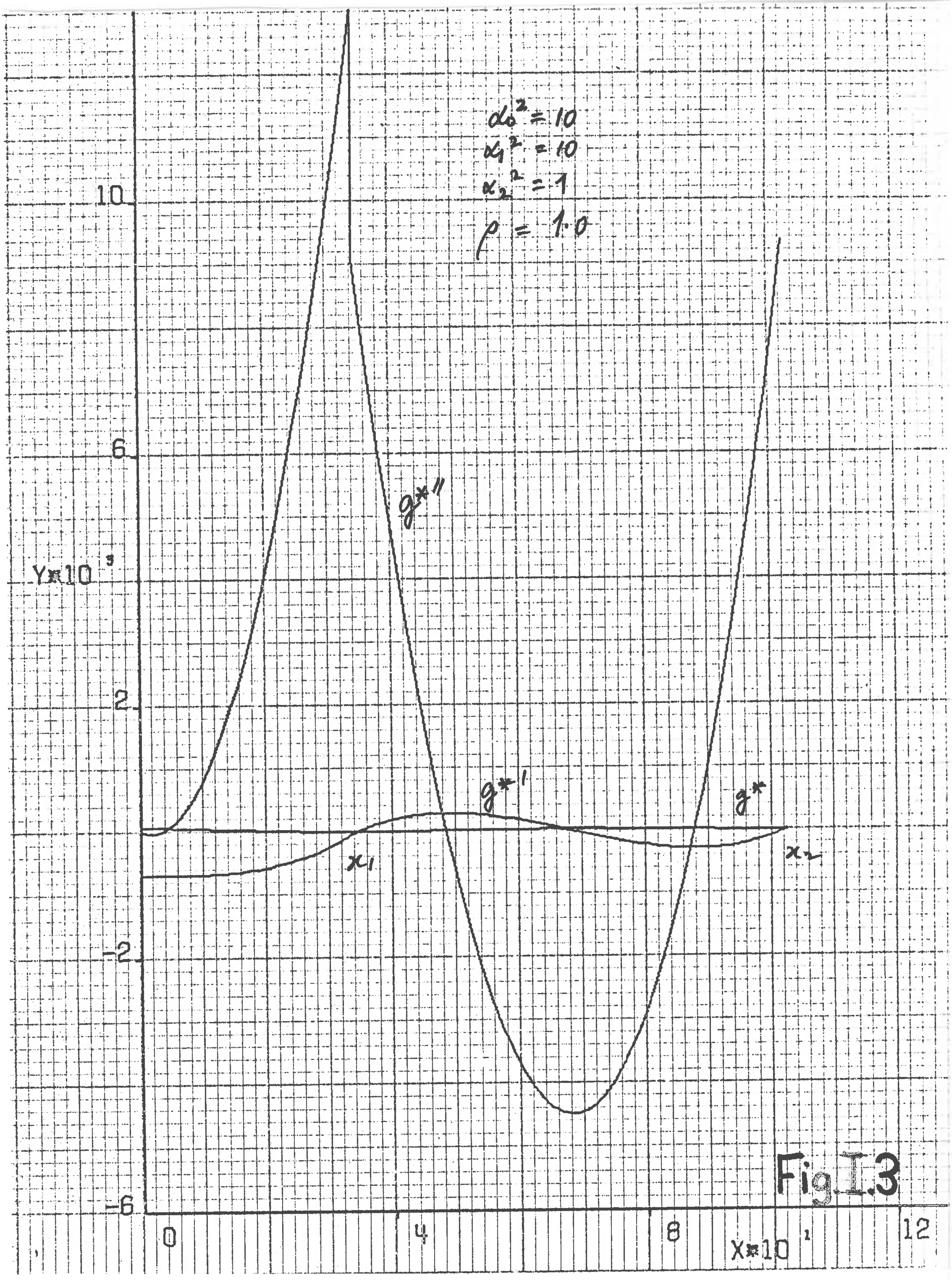
$\alpha_0^2 = 10$
$\alpha_1^2 = 10$
$\alpha_2^2 = 1$
$\rho = .6$
10
6
2
-2
-6
Y*10
$g^{*''}$
$g^{*'}$
g^*
x_1
x_2
0
4
8
12
X*10

Fig.I.1



$\alpha_0^2=10$
$\alpha_1^2=10$
$\alpha_2^2=1$
$\rho_0=\cdot 827901$
10
6
2
-2
-6
Y*10 5
g*''
g*'
g*
x_1
x_2
0
4
8
12
X*10 1

Fig. I.2



$\alpha_0^2 = 10$
$\alpha_1^2 = 10$
$\alpha_2^2 = 1$
$\rho = 1.0$
10
6
2
-2
-6
Y*10
g*''
g*'
g*
x1
x2
0
4
8
12
X*10

Fig. I.3

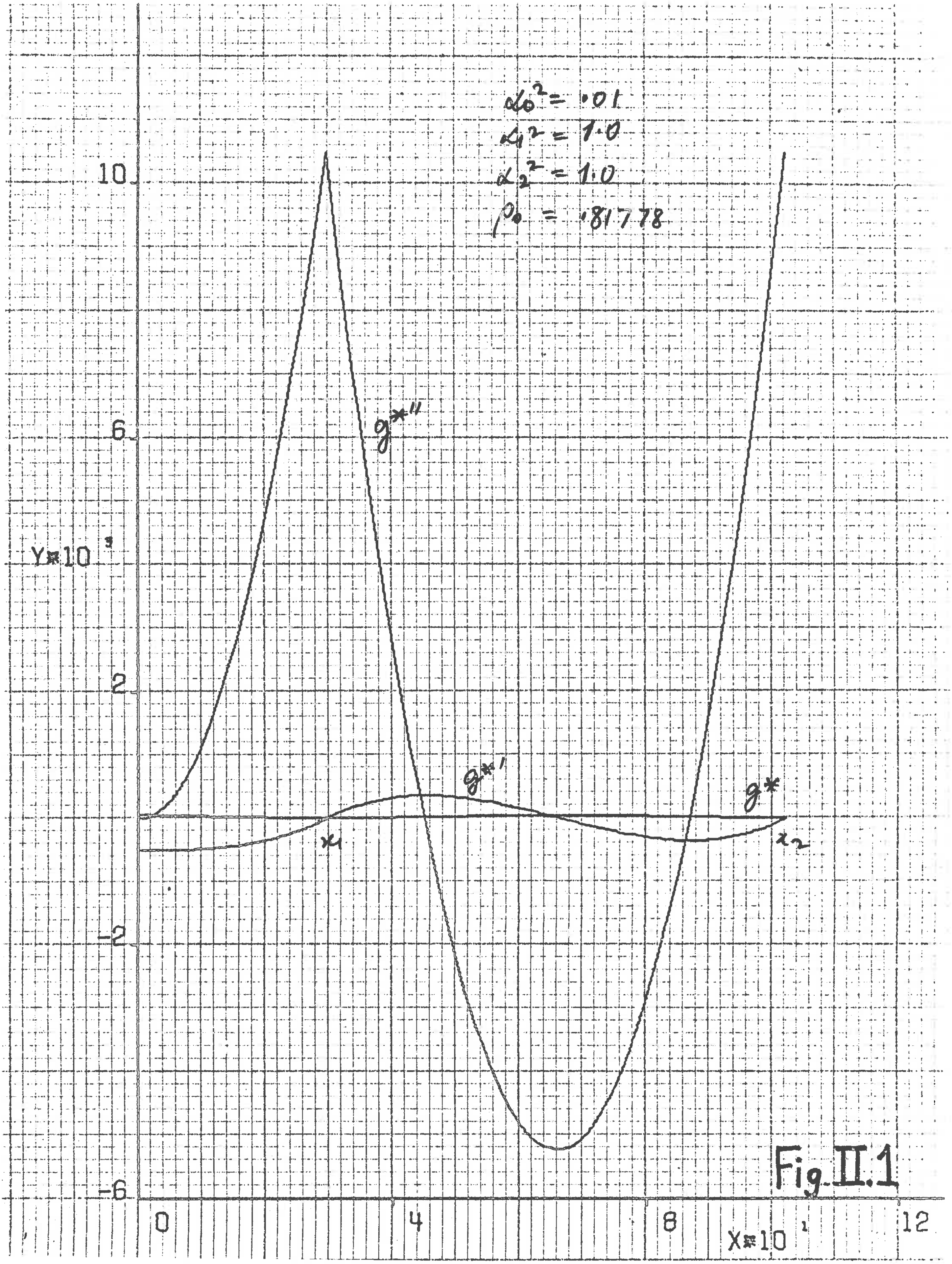
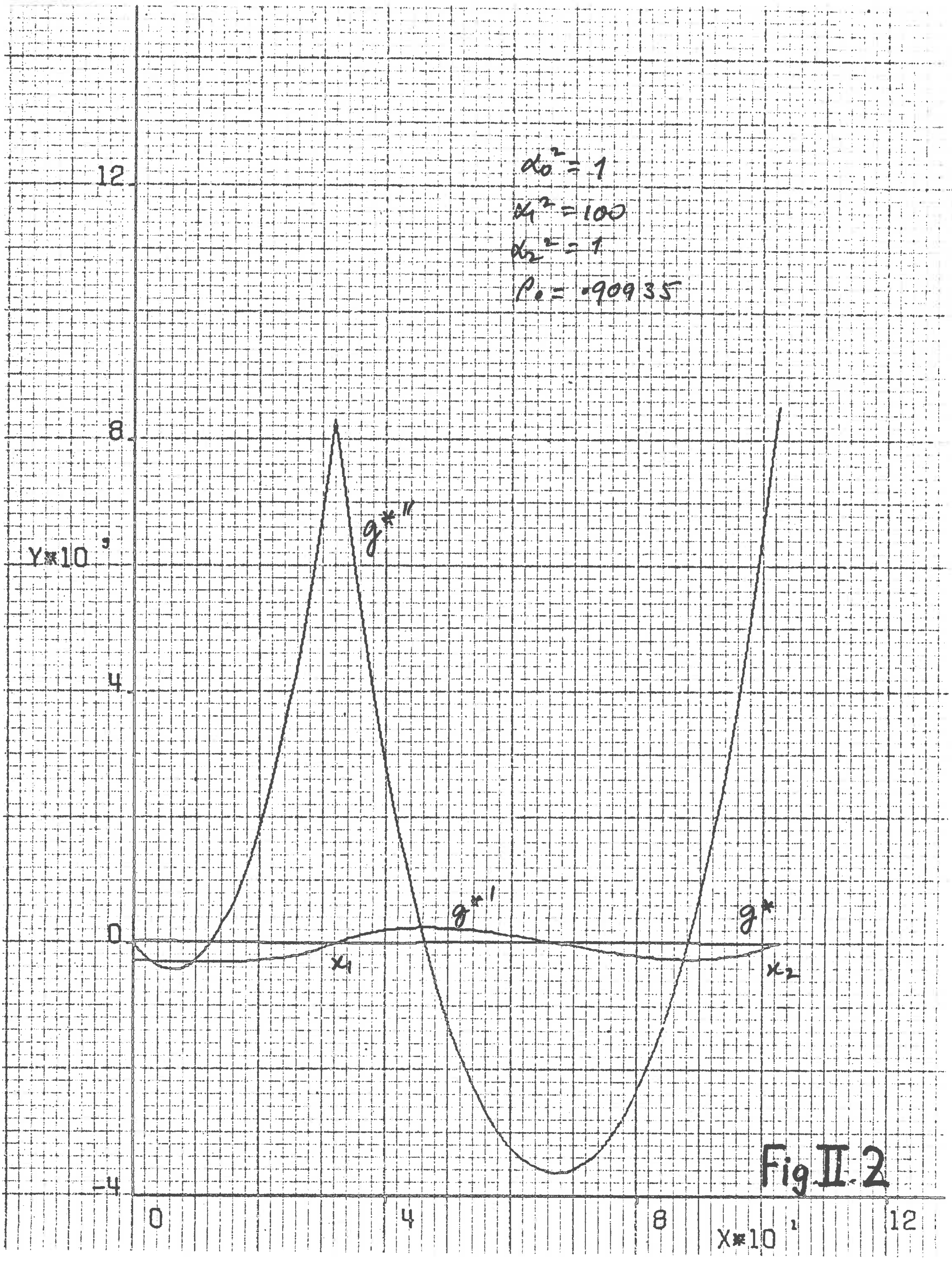
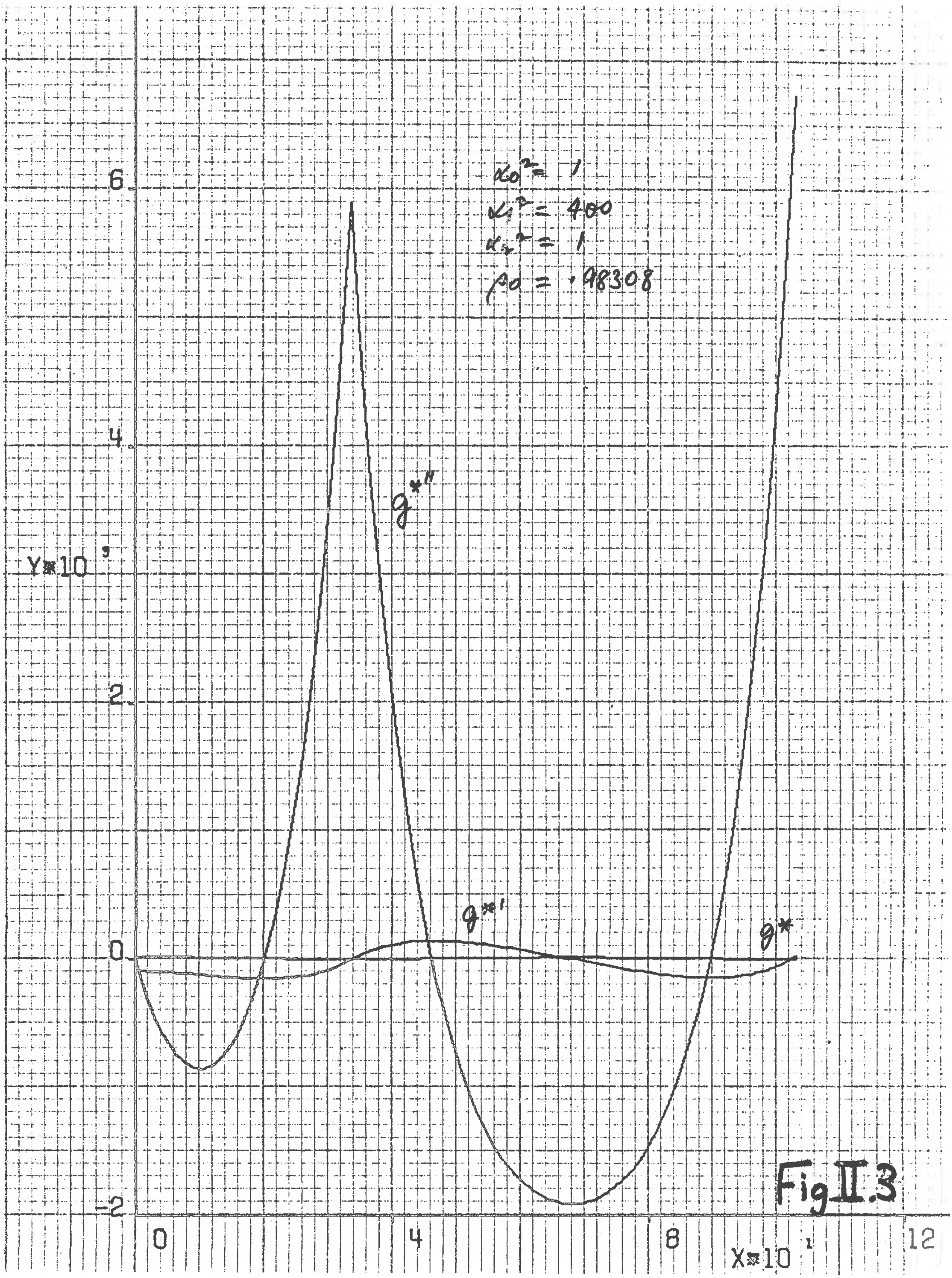

$\alpha_0^2 = \cdot 01$
$\alpha_1^2 = 1 \cdot 0$
$\alpha_2^2 = 1 \cdot 0$
$\rho_0 = \cdot 81778$
10
6
2
-2
-6
Y*10³
$g^{*''}$
$g^{*'}$
g^*
x_1
x_2
0
4
8
12
X*10¹

Fig. II.1



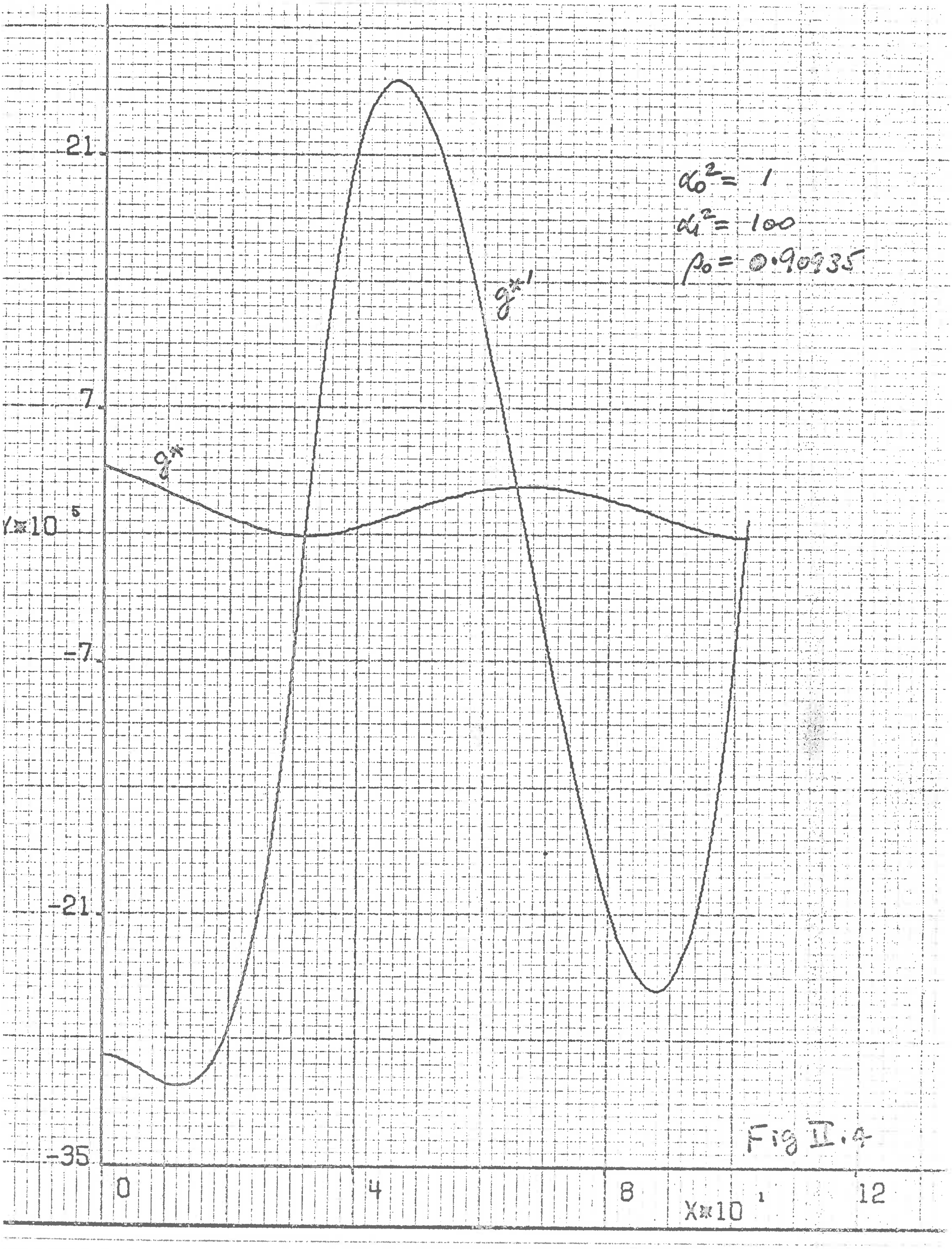
$\alpha_0^2 = 1$
$\alpha_1^2 = 100$
$\alpha_2^2 = 1$
$\rho_0 = .909\,35$
12
8
4
0
-4
Y*10
0
4
8
12
X*10
$g^{*''}$
$g^{*'}$
g^*
x_1
x_2

Fig II.2



$\alpha_0^2 = 1$
$\alpha_1^2 = 400$
$\alpha_2^2 = 1$
$\rho_0 = .98308$
$g^{*''}$
$g^{*'}$
g^{*}
Y*10
X*10
0
4
8
12
6
4
2
0
-2

Fig II.3



21
7
-7
-21
-35
Y*10 5
0
4
8
12
X*10 1
$\alpha_0^2 = 1$
$\alpha_1^2 = 100$
$\rho_0 = 0.90935$
g^*
$g^{*'}$

Fig II.4

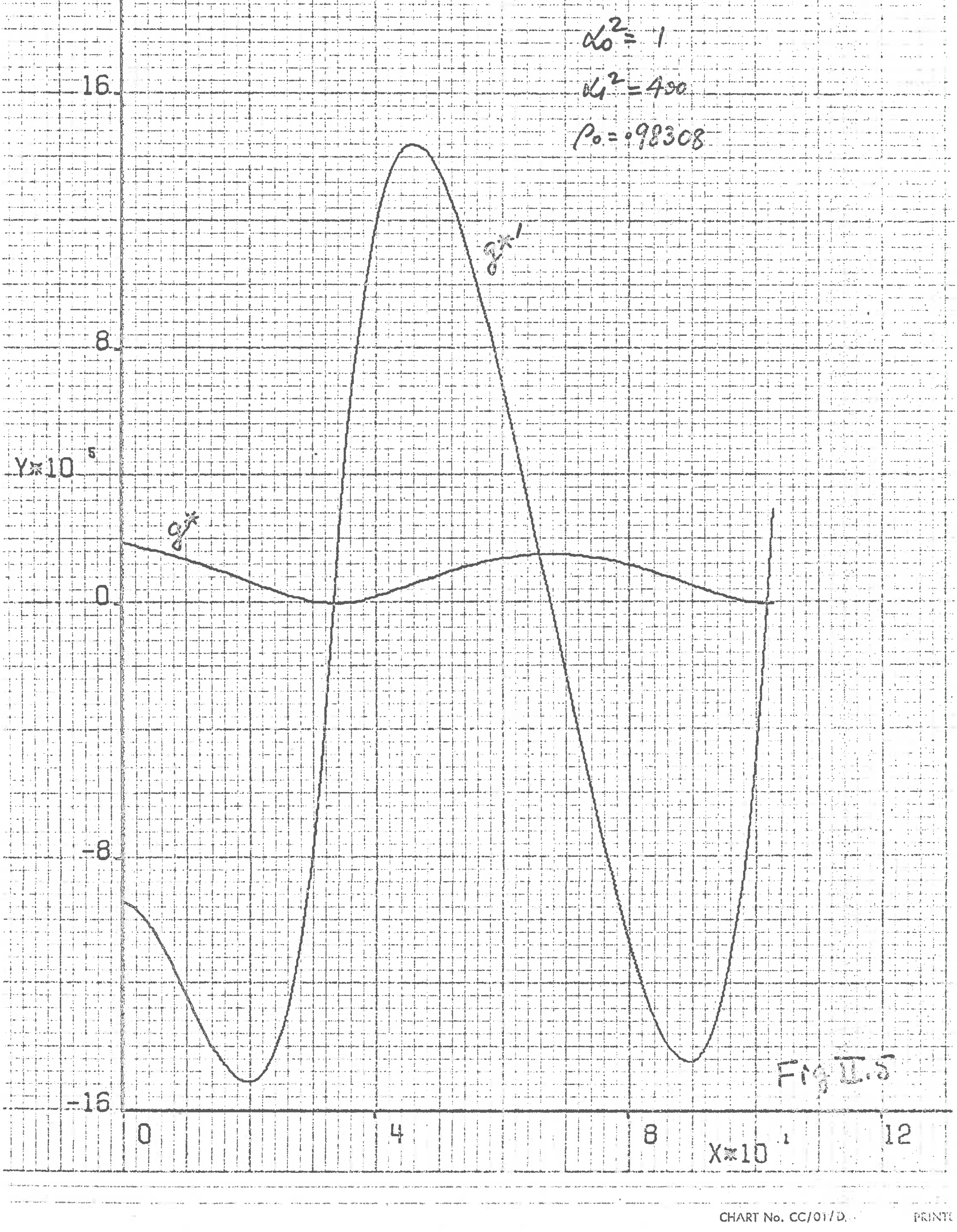


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Table I. Data for the Optimal Formulae (N=2).

3 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81739557	.96759127	1.06481086
.10	1.00	.81777971	.96766385	1.06466570
.20	1.00	.81777985	.96766175	1.06466331
.20	1.50	.81841862	.96778241	1.06442203
.20	2.00	.81905556	.96790267	1.06418154
.20	2.50	.81969067	.96802252	1.06394185
.20	3.00	.82032396	.96814198	1.06370296
.40	1.50	.81841891	.96777822	1.06441725
.40	2.00	.81905585	.96789848	1.06417678
.40	2.50	.81969097	.96801835	1.06393710
.60	2.00	.81905614	.96789430	1.06417201
.60	2.50	.81969126	.96801417	1.06393235
.60	3.00	.82032455	.96813365	1.06369348
.80	2.00	.81905644	.96789012	1.06416725
.80	2.50	.81969156	.96801000	1.06392760
1.00	2.50	.81969185	.96800582	1.06392285
1.00	3.00	.82032514	.96812531	1.06368400
1.20	2.50	.81969214	.96800165	1.06391809
1.40	2.50	.81969244	.96799747	1.06391334
1.40	3.00	.82032573	.96811698	1.06367452
1.80	3.00	.82032632	.96810865	1.06366504

4 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81698663	.95205230	1.04794640
.10	1.00	.81719634	.95210987	1.04788882
.20	1.00	.81719639	.95210926	1.04788813
.20	1.50	.81754551	.95220509	1.04779230
.20	2.00	.81789413	.95230077	1.04769662
.20	2.50	.81824227	.95239630	1.04760110
.20	3.00	.81858990	.95249167	1.04750573
.40	1.50	.81754559	.95220387	1.04779091
.40	2.00	.81789422	.95229955	1.04769523
.40	2.50	.81824235	.95239508	1.04759971
.60	2.00	.81789431	.95229833	1.04769384
.60	2.50	.81824244	.95239386	1.04759832
.60	3.00	.81859007	.95248924	1.04750296
.80	2.00	.81789439	.95229712	1.04769246
.80	2.50	.81824252	.95239264	1.04759694
1.00	2.50	.81824261	.95239143	1.04759555
1.00	3.00	.81859025	.95248680	1.04750019
1.20	2.50	.81824270	.95239021	1.04759416
1.40	2.50	.81824278	.95238899	1.04759278
1.40	3.00	.81859042	.95248437	1.04749742
1.80	3.00	.81859059	.95248194	1.04749465

Table I. Data for the Optimal Formulae (N=2) (continued)

6 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81670768	.93697718	1.03151123
.10	1.00	.81679810	.93700925	1.03149519
.20	1.00	.81679811	.93700914	1.03149507
.20	1.50	.81694874	.93706256	1.03146835
.20	2.00	.81709929	.93711595	1.03144166
.20	2.50	.81724975	.93716931	1.03141498
.20	3.00	.81740013	.93722263	1.03138832
.40	1.50	.81694875	.93706234	1.03146810
.40	2.00	.81709930	.93711573	1.03144141
.40	2.50	.81724977	.93716909	1.03141473
.60	2.00	.81709932	.93711551	1.03144116
.60	2.50	.81724978	.93716887	1.03141448
.60	3.00	.81740016	.93722219	1.03138782
.80	2.00	.81709933	.93711529	1.03144090
.80	2.50	.81724980	.93716865	1.03141422
1.00	2.50	.81724981	.93716842	1.03141397
1.00	3.00	.81740019	.93722175	1.03138731
1.20	2.50	.81724983	.93716820	1.03141372
1.40	2.50	.81724985	.93716798	1.03141347
1.40	3.00	.81740023	.93722131	1.03138681
1.80	3.00	.81740026	.93722086	1.03138630

8 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81661349	.92961661	1.02346108
.10	1.00	.81666358	.92963628	1.02345452
.20	1.00	.81666358	.92963625	1.02345449
.20	1.50	.81674705	.92966903	1.02344356
.20	2.00	.81683049	.92970180	1.02343263
.20	2.50	.81691390	.92973457	1.02342171
.20	3.00	.81699729	.92976732	1.02341079
.40	1.50	.81674705	.92966896	1.02344348
.40	2.00	.81683049	.92970174	1.02343256
.40	2.50	.81691391	.92973450	1.02342163
.60	2.00	.81683050	.92970167	1.02343248
.60	2.50	.81691391	.92973443	1.02342156
.60	3.00	.81699730	.92976719	1.02341064
.80	2.00	.81683050	.92970160	1.02343240
.80	2.50	.81691392	.92973437	1.02342148
1.00	2.50	.81691392	.92973430	1.02342140
1.00	3.00	.81699731	.92976705	1.02341049
1.20	2.50	.81691393	.92973423	1.02342133
1.40	2.50	.81691393	.92973416	1.02342125
1.40	3.00	.81699732	.92976692	1.02341033
1.80	3.00	.81699733	.92976678	1.02341018

Table I. Data for the Optimal Formulae (N=2) (continued)

12 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81654774	.92237484	1.01552502
.10	1.00	.81656967	.92238427	1.01552314
.20	1.00	.81656967	.92238426	1.01552313
.20	1.50	.81660620	.92239996	1.01551999
.20	2.00	.81664274	.92241566	1.01551685
.20	2.50	.81667926	.92243135	1.01551371
.20	3.00	.81671579	.92244705	1.01551057
.40	1.50	.81660621	.92239995	1.01551998
.40	2.00	.81664274	.92241564	1.01551684
.40	2.50	.81667927	.92243134	1.01551370
.60	2.00	.81664274	.92241563	1.01551682
.60	2.50	.81667927	.92243133	1.01551368
.60	3.00	.81671579	.92244702	1.01551054
.80	2.00	.81664274	.92241562	1.01551681
.80	2.50	.81667927	.92243131	1.01551367
1.00	2.50	.81667927	.92243130	1.01551365
1.00	3.00	.81671579	.92244699	1.01551052
1.20	2.50	.81667927	.92243129	1.01551364
1.40	2.50	.81667927	.92243128	1.01551363
1.40	3.00	.81671579	.92244697	1.01551049
1.80	3.00	.81671579	.92244694	1.01551046

16 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81652514	.91879860	1.01160020
.10	1.00	.81653738	.91880407	1.01159942
.20	1.00	.81653738	.91880407	1.01159941
.20	1.50	.81655777	.91881320	1.01159811
.20	2.00	.81657817	.91882233	1.01159680
.20	2.50	.81659856	.91883146	1.01159550
.20	3.00	.81661895	.91884059	1.01159420
.40	1.50	.81655777	.91881320	1.01159810
.40	2.00	.81657817	.91882233	1.01159680
.40	2.50	.81659856	.91883146	1.01159550
.60	2.00	.81657817	.91882233	1.01159680
.60	2.50	.81659856	.91883146	1.01159549
.60	3.00	.81661895	.91884059	1.01159419
.80	2.00	.81657817	.91882232	1.01159679
.80	2.50	.81659856	.91883145	1.01159549
1.00	2.50	.81659856	.91883145	1.01159548
1.00	3.00	.81661895	.91884058	1.01159418
1.20	2.50	.81659856	.91883144	1.01159548
1.40	2.50	.81659856	.91883144	1.01159547
1.40	3.00	.81661895	.91884057	1.01159417
1.80	3.00	.81661895	.91884056	1.01159416

Table I. Data for the Optimal Formulae (N=2) (continued)

20 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81651477	.91666713	1.00925921
.10	1.00	.81652257	.91667070	1.00925881
.20	1.00	.81652257	.91667070	1.00925881
.20	1.50	.81653556	.91667666	1.00925815
.20	2.00	.81654856	.91668261	1.00925749
.20	2.50	.81656155	.91668857	1.00925682
.20	3.00	.81657454	.91669453	1.00925616
.40	1.50	.81653556	.91667666	1.00925815
.40	2.00	.81654856	.91668261	1.00925748
.40	2.50	.81656155	.91668857	1.00925682
.60	2.00	.81654856	.91668261	1.00925748
.60	2.50	.81656155	.91668857	1.00925682
.60	3.00	.81657454	.91669452	1.00925616
.80	2.00	.81654856	.91668261	1.00925748
.80	2.50	.81656155	.91668857	1.00925682
1.00	2.50	.81656155	.91668856	1.00925682
1.00	3.00	.81657454	.91669452	1.00925615
1.20	2.50	.81656155	.91668856	1.00925681
1.40	2.50	.81656155	.91668856	1.00925681
1.40	3.00	.81657454	.91669452	1.00925615
1.80	3.00	.81657454	.91669451	1.00925615

24 POINTS

α_0^2	α_1^2	ρ_0	nC_1	nC_2
.10	.70	.81650918	.91525210	1.00770435
.10	1.00	.81651457	.91525462	1.00770413
.20	1.00	.81651457	.91525461	1.00770412
.20	1.50	.81652357	.91525880	1.00770374
.20	2.00	.81653257	.91526299	1.00770336
.20	2.50	.81654156	.91526717	1.00770298
.20	3.00	.81655056	.91527136	1.00770260
.40	1.50	.81652357	.91525880	1.00770374
.40	2.00	.81653257	.91526299	1.00770336
.40	2.50	.81654156	.91526717	1.00770298
.60	2.00	.81653257	.91526299	1.00770336
.60	2.50	.81654156	.91526717	1.00770298
.60	3.00	.81655056	.91527136	1.00770260
.80	2.00	.81653257	.91526299	1.00770336
.80	2.50	.81654156	.91526717	1.00770298
1.00	2.50	.81654156	.91526717	1.00770298
1.00	3.00	.81655056	.91527136	1.00770260
1.20	2.50	.81654156	.91526717	1.00770298
1.40	2.50	.81654156	.91526717	1.00770298
1.40	3.00	.81655056	.91527136	1.00770260
1.80	3.00	.81655056	.91527136	1.00770260

Table I.(contd.)Data for the Optimal Formulae ($N=2$, $\alpha_0=0$)

3 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81662521	.96744778	1.06510444
.20	.81675376	.96747209	1.06505583
.30	.81688224	.96749638	1.06500725
.40	.81701064	.96752065	1.06495870
.50	.81713898	.96754491	1.06491019
.60	.81726724	.96756915	1.06486171
.70	.81739543	.96759337	1.06481326
.80	.81752355	.96761758	1.06476484
.90	.81765159	.96764177	1.06471645
1.00	.81777956	.96766595	1.06466810
1.10	.81790746	.96769011	1.06461977
1.20	.81803529	.96771426	1.06457148
1.30	.81816304	.96773839	1.06452322
1.40	.81829072	.96776250	1.06447500
1.50	.81841833	.96778660	1.06442680
1.60	.81854586	.96781068	1.06437864
1.70	.81867332	.96783475	1.06433051
1.80	.81880071	.96785880	1.06428241
1.90	.81892802	.96788283	1.06423434
2.00	.81905527	.96790685	1.06418630

4 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81656664	.95193760	1.04806240
.20	.81663668	.95195683	1.04804317
.30	.81670670	.95197606	1.04802394
.40	.81677671	.95199528	1.04800472
.50	.81684669	.95201450	1.04798550
.60	.81691665	.95203370	1.04796630
.70	.81698659	.95205291	1.04794709
.80	.81705651	.95207210	1.04792790
.90	.81712642	.95209130	1.04790870
1.00	.81719630	.95211048	1.04788952
1.10	.81726616	.95212966	1.04787034
1.20	.81733601	.95214883	1.04785117
1.30	.81740583	.95216800	1.04783200
1.40	.81747564	.95218716	1.04781284
1.50	.81754542	.95220631	1.04779369
1.60	.81761519	.95222546	1.04777454
1.70	.81768493	.95224460	1.04775540
1.80	.81775466	.95226374	1.04773626
1.90	.81782436	.95228287	1.04771713
2.00	.81789405	.95230199	1.04769801

Table I.(contd.) Data for the Optimal Formulae (N=2, $\alpha_0=0$)

6 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81652675	.93691312	1.03154344
.20	.81655691	.93692382	1.03153809
.30	.81658707	.93693452	1.03153274
.40	.81661722	.93694521	1.03152739
.50	.81664738	.93695591	1.03152205
.60	.81667753	.93696660	1.03151670
.70	.81670767	.93697729	1.03151135
.80	.81673782	.93698799	1.03150601
.90	.81676796	.93699867	1.03150066
1.00	.81679809	.93700936	1.03149532
1.10	.81682822	.93702005	1.03148998
1.20	.81685835	.93703074	1.03148463
1.30	.81688848	.93704142	1.03147929
1.40	.81691860	.93705210	1.03147395
1.50	.81694872	.93706278	1.03146861
1.60	.81697884	.93707346	1.03146327
1.70	.81700895	.93708414	1.03145793
1.80	.81703906	.93709482	1.03145259
1.90	.81706917	.93710550	1.03144725
2.00	.81709927	.93711617	1.03144191

8 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81651329	.92957728	1.02347424
.20	.81652999	.92958384	1.02347205
.30	.81654669	.92959040	1.02346987
.40	.81656339	.92959696	1.02346768
.50	.81658009	.92960352	1.02346549
.60	.81659679	.92961008	1.02346331
.70	.81661349	.92961664	1.02346112
.80	.81663019	.92962320	1.02345893
.90	.81664688	.92962976	1.02345675
1.00	.81666358	.92963631	1.02345456
1.10	.81668027	.92964287	1.02345238
1.20	.81669697	.92964943	1.02345019
1.30	.81671366	.92965599	1.02344800
1.40	.81673035	.92966254	1.02344582
1.50	.81674704	.92966910	1.02344363
1.60	.81676373	.92967565	1.02344145
1.70	.81678042	.92968221	1.02343926
1.80	.81679711	.92968876	1.02343708
1.90	.81681380	.92969532	1.02343489
2.00	.81683048	.92970187	1.02343271

Table I:(contd.) Data for the Optimal Formulae ($N=2$, $\alpha_0=0$).

12 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81650389	.92235601	1.01552880
.20	.81651120	.92235915	1.01552817
.30	.81651851	.92236229	1.01552754
.40	.81652582	.92236543	1.01552691
.50	.81653313	.92236857	1.01552629
.60	.81654043	.92237171	1.01552566
.70	.81654774	.92237485	1.01552503
.80	.81655505	.92237799	1.01552440
.90	.81656236	.92238113	1.01552377
1.00	.81656967	.92238427	1.01552315
1.10	.81657697	.92238741	1.01552252
1.20	.81658428	.92239055	1.01552189
1.30	.81659159	.92239369	1.01552126
1.40	.81659890	.92239683	1.01552063
1.50	.81660620	.92239997	1.01552001
1.60	.81661351	.92240311	1.01551938
1.70	.81662082	.92240625	1.01551875
1.80	.81662812	.92240939	1.01551812
1.90	.81663543	.92241253	1.01551749
2.00	.81664274	.92241567	1.01551687

16 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81650066	.91878764	1.01160177
.20	.81650474	.91878946	1.01160151
.30	.81650882	.91879129	1.01160124
.40	.81651290	.91879312	1.01160098
.50	.81651698	.91879494	1.01160072
.60	.81652106	.91879677	1.01160046
.70	.81652514	.91879860	1.01160020
.80	.81652922	.91880042	1.01159994
.90	.81653330	.91880225	1.01159968
1.00	.81653738	.91880408	1.01159942
1.10	.81654146	.91880590	1.01159916
1.20	.81654554	.91880773	1.01159890
1.30	.81654961	.91880956	1.01159863
1.40	.81655369	.91881138	1.01159837
1.50	.81655777	.91881321	1.01159811
1.60	.81656185	.91881503	1.01159785
1.70	.81656593	.91881686	1.01159759
1.80	.81657001	.91881869	1.01159733
1.90	.81657409	.91882051	1.01159707
2.00	.81657817	.91882234	1.01159681

Table I.(contd.) Data for the Optimal Formulae (N=2, α_0=0)

20 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81649918	.91665998	1.00926000
.20	.81650178	.91666117	1.00925987
.30	.81650438	.91666237	1.00925974
.40	.81650698	.91666356	1.00925960
.50	.81650958	.91666475	1.00925947
.60	.81651217	.91666594	1.00925934
.70	.81651477	.91666713	1.00925921
.80	.81651737	.91666832	1.00925908
.90	.81651997	.91666951	1.00925894
1.00	.81652257	.91667070	1.00925881
1.10	.81652517	.91667190	1.00925868
1.20	.81652777	.91667309	1.00925855
1.30	.81653037	.91667428	1.00925841
1.40	.81653297	.91667547	1.00925828
1.50	.81653556	.91667666	1.00925815
1.60	.81653816	.91667785	1.00925802
1.70	.81654076	.91667904	1.00925788
1.80	.81654336	.91668023	1.00925775
1.90	.81654596	.91668142	1.00925762
2.00	.81654856	.91668262	1.00925749

24 POINTS

α_1^2	ρ_0	nC_1	nC_2
.10	.81649838	.91524708	1.00770481
.20	.81650018	.91524792	1.00770473
.30	.81650198	.91524875	1.00770466
.40	.81650378	.91524959	1.00770458
.50	.81650558	.91525043	1.00770451
.60	.81650738	.91525127	1.00770443
.70	.81650918	.91525210	1.00770435
.80	.81651098	.91525294	1.00770428
.90	.81651277	.91525378	1.00770420
1.00	.81651457	.91525462	1.00770413
1.10	.81651637	.91525545	1.00770405
1.20	.81651817	.91525629	1.00770397
1.30	.81651997	.91525713	1.00770390
1.40	.81652177	.91525796	1.00770382
1.50	.81652357	.91525880	1.00770375
1.60	.81652537	.91525964	1.00770367
1.70	.81652717	.91526048	1.00770359
1.80	.81652897	.91526131	1.00770352
1.90	.81653077	.91526215	1.00770344
2.00	.81653257	.91526299	1.00770336

Table II

For all cases $\alpha_2^2=1$ and the values of α_0^2 and α_1^2 are found as follows. For the errors of the OQF1 and OQF2, the corresponding values of α_0^2 and α_1^2 are to be found in columns 1 and 2 respectively. For the errors of the G.M.R. $(\alpha_0=0)$ however, the corresponding value of α_1^2 is found in Column 1 and Column 2 should be ignored. Thus for $\alpha_1^2 = .01$ the error of the G.M.R. in Table II.1 is -.00074181.

Table II.1. Errors in the calculation of $\int_0^1 e^x \, dx$.

4POINTS TRAPEZOIDAL RULE : .01588063
MIDPOINT RULE : -.00446655

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00455580	-.00075627	-.00074181
.06	.50	-.00500192	-.00074959	-.00074253
.10	.70	-.00535860	-.00075294	-.00074311
.10	1.00	-.00535860	-.00075728	-.00074311
.20	1.00	-.00624954	-.00075840	-.00074456
.20	2.00	-.00624954	-.00077285	-.00074456
.20	3.00	-.00624954	-.00078725	-.00074456
.40	1.50	-.00802809	-.00076788	-.00074747
.80	2.00	-.01157192	-.00077957	-.00075326
1.00	2.50	-.01333723	-.00078901	-.00075616
1.00	3.00	-.01333723	-.00079620	-.00075616
2.00	3.00	-.02209843	-.00080738	-.00077061

8POINTS TRAPEZOIDAL RULE : .00292125
MIDPOINT RULE : -.00111816

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00114052	-.00008824	-.00008734
.06	.50	-.00125230	-.00008782	-.00008739
.10	.70	-.00134172	-.00008803	-.00008742
.10	1.00	-.00134172	-.00008830	-.00008742
.20	1.00	-.00156520	-.00008836	-.00008751
.20	2.00	-.00156520	-.00008926	-.00008751
.20	3.00	-.00156520	-.00009016	-.00008751
.40	1.50	-.00201196	-.00008894	-.00008769
.80	2.00	-.00290464	-.00008964	-.00008805
1.00	2.50	-.00335057	-.00009022	-.00008823
1.00	3.00	-.00335057	-.00009067	-.00008823
2.00	3.00	-.00557601	-.00009131	-.00008913

24POINTS TRAPEZOIDAL RULE : .00027067
MIDPOINT RULE : -.00012429

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00012678	-.00000312	-.00000311
.06	.50	-.00013921	-.00000312	-.00000311
.10	.70	-.00014915	-.00000312	-.00000311
.10	1.00	-.00014915	-.00000312	-.00000311
.20	1.00	-.00017400	-.00000312	-.00000311
.20	2.00	-.00017400	-.00000313	-.00000311
.20	3.00	-.00017400	-.00000314	-.00000311
.40	1.50	-.00022371	-.00000313	-.00000311
.80	2.00	-.00032312	-.00000314	-.00000312
1.00	2.50	-.00037282	-.00000314	-.00000312
1.00	3.00	-.00037282	-.00000315	-.00000312
2.00	3.00	-.00062127	-.00000316	-.00000313

Table II.2. Errors in the calculation of $\int_0^1 e^{5x}dx$.

4POINTS TRAPEZOIDAL RULE : 6.52826634
MIDPOINT RULE : -1.83543189

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-1.83687176	-.58928377	-.58431412
.06	.50	-1.84406840	-.58678638	-.58456539
.10	.70	-1.84982248	-.58779733	-.58476638
.10	1.00	-1.84982248	-.58930103	-.58476638
.20	1.00	-1.86419510	-.58932021	-.58526874
.20	2.00	-1.86419510	-.59432205	-.58526874
.20	3.00	-1.86419510	-.59930775	-.58526874
.40	1.50	-1.89288659	-.59186147	-.58627298
.80	2.00	-1.95005547	-.59443690	-.58827954
1.00	2.50	-1.97853340	-.59696990	-.58928185
1.00	3.00	-1.97853340	-.59946058	-.58928185
2.00	3.00	-2.11986862	-.59965160	-.59428376

8POINTS TRAPEZOIDAL RULE : 1.24298198
MIDPOINT RULE : -.47444912

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.47482683	-.07880751	-.07845865
.06	.50	-.47671517	-.07863194	-.07847627
.10	.70	-.47822564	-.07870284	-.07849036
.10	1.00	-.47822564	-.07880850	-.07849036
.20	1.00	-.48200098	-.07880959	-.07852560
.20	2.00	-.48200098	-.07916167	-.07852560
.20	3.00	-.48200098	-.07951357	-.07852560
.40	1.50	-.48954811	-.07898785	-.07859606
.80	2.00	-.50462825	-.07916826	-.07873696
1.00	2.50	-.51216127	-.07934643	-.07880740
1.00	3.00	-.51216127	-.07952235	-.07880740
2.00	3.00	-.54975594	-.07953333	-.07915948

24POINTS TRAPEZOIDAL RULE : .11601857
MIDPOINT RULE : -.05325042

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.05329300	-.00302087	-.00301635
.06	.50	-.05350588	-.00301860	-.00301658
.10	.70	-.05367618	-.00301951	-.00301676
.10	1.00	-.05367618	-.00302088	-.00301676
.20	1.00	-.05410193	-.00302089	-.00301722
.20	2.00	-.05410193	-.00302545	-.00301722
.20	3.00	-.05410193	-.00303001	-.00301722
.40	1.50	-.05495339	-.00302320	-.00301813
.80	2.00	-.05665612	-.00302553	-.00301995
1.00	2.50	-.05750740	-.00302783	-.00302087
1.00	3.00	-.05750740	-.00303011	-.00302087
2.00	3.00	-.06176291	-.00303024	-.00302542

Table II.3. Errors in the calculation of $\int_0^1 x^3\,dx$.

4POINTS TRAPEZOIDAL RULE : .02777778
MIDPOINT RULE : -.00781250

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00782511	-.00124960	-.00122425
.06	.50	-.00788816	-.00123690	-.00122553
.10	.70	-.00793856	-.00124208	-.00122655
.10	1.00	-.00793856	-.00124975	-.00122655
.20	1.00	-.00806446	-.00124992	-.00122912
.20	2.00	-.00806446	-.00127544	-.00122912
.20	3.00	-.00806446	-.00130088	-.00122912
.40	1.50	-.00831580	-.00126301	-.00123424
.80	2.00	-.00881659	-.00127642	-.00124447
1.00	2.50	-.00906606	-.00128948	-.00124959
1.00	3.00	-.00906606	-.00130219	-.00124959
2.00	3.00	-.01030415	-.00130382	-.00127511

8POINTS TRAPEZOIDAL RULE : .00510204
MIDPOINT RULE : -.00195313

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00195635	-.00014405	-.00014249
.06	.50	-.00197250	-.00014327	-.00014257
.10	.70	-.00198542	-.00014359	-.00014263
.10	1.00	-.00198542	-.00014406	-.00014263
.20	1.00	-.00201770	-.00014407	-.00014279
.20	2.00	-.00201770	-.00014565	-.00014279
.20	3.00	-.00201770	-.00014722	-.00014279
.40	1.50	-.00208224	-.00014488	-.00014311
.80	2.00	-.00221118	-.00014570	-.00014374
1.00	2.50	-.00227560	-.00014651	-.00014405
1.00	3.00	-.00227560	-.00014730	-.00014405
2.00	3.00	-.00259707	-.00014739	-.00014563

24POINTS TRAPEZOIDAL RULE : .00047259
MIDPOINT RULE : -.00021701

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00021738	-.00000506	-.00000504
.06	.50	-.00021918	-.00000505	-.00000504
.10	.70	-.00022063	-.00000505	-.00000504
.10	1.00	-.00022063	-.00000506	-.00000504
.20	1.00	-.00022424	-.00000506	-.00000504
.20	2.00	-.00022424	-.00000508	-.00000504
.20	3.00	-.00022424	-.00000509	-.00000504
.40	1.50	-.00023147	-.00000507	-.00000504
.80	2.00	-.00024592	-.00000508	-.00000505
1.00	2.50	-.00025315	-.00000509	-.00000506
1.00	3.00	-.00025315	-.00000509	-.00000506
2.00	3.00	-.00028926	-.00000510	-.00000507

Table II.4. Errors in the calculation of $\int_0^1 \sin x \, dx$

4POINTS TRAPEZOIDAL RULE : -.00426436
MIDPOINT RULE : .00119932

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00117531	.00018011	.00017622
.06	.50	.00105534	.00017798	.00017641
.10	.70	.00095941	.00017865	.00017657
.10	1.00	.00095941	.00017984	.00017657
.20	1.00	.00071981	.00017954	.00017697
.20	2.00	.00071981	.00018350	.00017697
.20	3.00	.00071981	.00018745	.00017697
.40	1.50	.00024151	.00018092	.00017776
.80	2.00	-.00071154	.00018170	.00017935
1.00	2.50	-.00118628	.00018308	.00018014
1.00	3.00	-.00118628	.00018506	.00018014
2.00	3.00	-.00354243	.00018207	.00018410

8POINTS TRAPEZOIDAL RULE : -.00078206
MIDPOINT RULE : .00029942

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00029343	.00002048	.00002024
.06	.50	.00026348	.00002035	.00002025
.10	.70	.00023953	.00002039	.00002026
.10	1.00	.00023953	.00002046	.00002026
.20	1.00	.00017967	.00002045	.00002029
.20	2.00	.00017967	.00002069	.00002029
.20	3.00	.00017967	.00002093	.00002029
.40	1.50	.00005999	.00002053	.00002034
.80	2.00	-.00017915	.00002059	.00002043
1.00	2.50	-.00029860	.00002067	.00002048
1.00	3.00	-.00029860	.00002080	.00002048
2.00	3.00	-.00089476	.00002062	.00002072

24POINTS TRAPEZOIDAL RULE : -.00007242
MIDPOINT RULE : .00003326

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00003259	.00000071	.00000071
.06	.50	.00002926	.00000071	.00000071
.10	.70	.00002660	.00000071	.00000071
.10	1.00	.00002660	.00000071	.00000071
.20	1.00	.00001995	.00000071	.00000071
.20	2.00	.00001995	.00000071	.00000071
.20	3.00	.00001995	.00000072	.00000071
.40	1.50	.00000665	.00000071	.00000071
.80	2.00	-.00001995	.00000071	.00000071
1.00	2.50	-.00003325	.00000071	.00000071
1.00	3.00	-.00003325	.00000072	.00000071
2.00	3.00	-.00009972	.00000071	.00000072

Table II.5. Errors in the calculation of $\int_0^1 (1+x)^{-1}dx$

4POINTS TRAPEZOIDAL RULE : .00685282
MIDPOINT RULE : -.00192729

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00196329	-.00041060	-.00040464
.06	.50	-.00214321	-.00040784	-.00040494
.10	.70	-.00228707	-.00040922	-.00040518
.10	1.00	-.00228707	-.00041101	-.00040518
.20	1.00	-.00264641	-.00041146	-.00040578
.20	2.00	-.00264641	-.00041741	-.00040578
.20	3.00	-.00264641	-.00042335	-.00040578
.40	1.50	-.00336374	-.00041534	-.00040697
.80	2.00	-.00479304	-.00042012	-.00040936
1.00	2.50	-.00550503	-.00042399	-.00041056
1.00	3.00	-.00550503	-.00042695	-.00041056
2.00	3.00	-.00903862	-.00043146	-.00041651

8POINTS TRAPEZOIDAL RULE : .00127229
MIDPOINT RULE : -.00048663

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00049565	-.00005068	-.00005030
.06	.50	-.00054074	-.00005051	-.00005032
.10	.70	-.00057680	-.00005059	-.00005034
.10	1.00	-.00057680	-.00005071	-.00005034
.20	1.00	-.00066695	-.00005073	-.00005038
.20	2.00	-.00066695	-.00005112	-.00005038
.20	3.00	-.00066695	-.00005150	-.00005038
.40	1.50	-.00084716	-.00005098	-.00005045
.80	2.00	-.00120725	-.00005127	-.00005061
1.00	2.50	-.00138712	-.00005151	-.00005068
1.00	3.00	-.00138712	-.00005170	-.00005068
2.00	3.00	-.00228481	-.00005196	-.00005106

24POINTS TRAPEZOIDAL RULE : .00011812
MIDPOINT RULE : -.00005423

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	-.00005524	-.00000186	-.00000185
.06	.50	-.00006025	-.00000185	-.00000185
.10	.70	-.00006426	-.00000186	-.00000185
.10	1.00	-.00006426	-.00000186	-.00000185
.20	1.00	-.00007429	-.00000186	-.00000185
.20	2.00	-.00007429	-.00000186	-.00000185
.20	3.00	-.00007429	-.00000187	-.00000185
.40	1.50	-.00009434	-.00000186	-.00000185
.80	2.00	-.00013444	-.00000186	-.00000186
1.00	2.50	-.00015449	-.00000187	-.00000186
1.00	3.00	-.00015449	-.00000187	-.00000186
2.00	3.00	-.00025471	-.00000187	-.00000186

Table II.6. Errors in the calculation of $\int_0^1 \log(1+x)dx$

4POINTS TRAPEZOIDAL RULE : -.00460060
MIDPOINT RULE : .00129395

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00127376	.00024207	.00023802
.06	.50	.00117287	.00023989	.00023822
.10	.70	.00109221	.00024061	.00023839
.10	1.00	.00109221	.00024184	.00023839
.20	1.00	.00089072	.00024159	.00023880
.20	2.00	.00089072	.00024570	.00023880
.20	3.00	.00089072	.00024980	.00023880
.40	1.50	.00048849	.00024314	.00023962
.80	2.00	-.00031297	.00024419	.00024127
1.00	2.50	-.00071220	.00024574	.00024210
1.00	3.00	-.00071220	.00024779	.00024210
2.00	3.00	-.00269359	.00024528	.00024621

8POINTS TRAPEZOIDAL RULE : -.00084933
MIDPOINT RULE : .00032500

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00031997	.00002897	.00002871
.06	.50	.00029480	.00002883	.00002872
.10	.70	.00027467	.00002887	.00002873
.10	1.00	.00027467	.00002895	.00002873
.20	1.00	.00022435	.00002894	.00002876
.20	2.00	.00022435	.00002920	.00002876
.20	3.00	.00022435	.00002946	.00002876
.40	1.50	.00012377	.00002904	.00002881
.80	2.00	-.00007722	.00002911	.00002891
1.00	2.50	-.00017762	.00002921	.00002897
1.00	3.00	-.00017762	.00002934	.00002897
2.00	3.00	-.00067868	.00002920	.00002923

24POINTS TRAPEZOIDAL RULE : -.00007876
MIDPOINT RULE : .00003616

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00003560	.00000104	.00000104
.06	.50	.00003281	.00000104	.00000104
.10	.70	.00003057	.00000104	.00000104
.10	1.00	.00003057	.00000104	.00000104
.20	1.00	.00002498	.00000104	.00000104
.20	2.00	.00002498	.00000104	.00000104
.20	3.00	.00002498	.00000105	.00000104
.40	1.50	.00001381	.00000104	.00000104
.80	2.00	-.00000855	.00000104	.00000104
1.00	2.50	-.00001972	.00000104	.00000104
1.00	3.00	-.00001972	.00000105	.00000104
2.00	3.00	-.00007558	.00000104	.00000104

Table II.7. Errors in the calculation of $\int_0^1 (1+x^2)^{-1}dx$

4POINTS TRAPEZOIDAL RULE : -.00462893
MIDPOINT RULE : .00130197

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00126099	.00031003	.00030619
.06	.50	.00105621	.00030781	.00030638
.10	.70	.00089248	.00030839	.00030654
.10	1.00	.00089248	.00030957	.00030654
.20	1.00	.00048351	.00030906	.00030694
.20	2.00	.00048351	.00031299	.00030694
.20	3.00	.00048351	.00031690	.00030694
.40	1.50	-.00033291	.00031000	.00030772
.80	2.00	-.00195964	.00030992	.00030930
1.00	2.50	-.00276998	.00031086	.00031009
1.00	3.00	-.00276998	.00031282	.00031009
2.00	3.00	-.00679167	.00030771	.00031401

8POINTS TRAPEZOIDAL RULE : -.00085034
MIDPOINT RULE : .00032552

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00031529	.00003587	.00003562
.06	.50	.00026414	.00003573	.00003563
.10	.70	.00022323	.00003577	.00003564
.10	1.00	.00022323	.00003584	.00003564
.20	1.00	.00012097	.00003582	.00003567
.20	2.00	.00012097	.00003607	.00003567
.20	3.00	.00012097	.00003632	.00003567
.40	1.50	-.00008346	.00003588	.00003572
.80	2.00	-.00049192	.00003589	.00003582
1.00	2.50	-.00069596	.00003596	.00003587
1.00	3.00	-.00069596	.00003609	.00003587
2.00	3.00	-.00171426	.00003580	.00003613

24POINTS TRAPEZOIDAL RULE : -.00007876
MIDPOINT RULE : .00003617

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00003503	.00000126	.00000126
.06	.50	.00002935	.00000126	.00000126
.10	.70	.00002481	.00000126	.00000126
.10	1.00	.00002481	.00000126	.00000126
.20	1.00	.00001344	.00000126	.00000126
.20	2.00	.00001344	.00000126	.00000126
.20	3.00	.00001344	.00000127	.00000126
.40	1.50	-.00000928	.00000126	.00000126
.80	2.00	-.00005473	.00000126	.00000126
1.00	2.50	-.00007744	.00000126	.00000126
1.00	3.00	-.00007744	.00000127	.00000126
2.00	3.00	-.00019102	.00000126	.00000127

Table II.8. Errors in the calculation of $\int_0^1 (1+x^2)^{-\frac{1}{2}}dx$.

4POINTS TRAPEZOIDAL RULE : -.00327793
MIDPOINT RULE : .00092193

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00087598	.00017346	.00017061
.06	.50	.00064631	.00017170	.00017076
.10	.70	.00046268	.00017206	.00017087
.10	1.00	.00046268	.00017294	.00017087
.20	1.00	.00000402	.00017236	.00017117
.20	2.00	.00000402	.00017530	.00017117
.20	3.00	.00000402	.00017822	.00017117
.40	1.50	-.00091161	.00017268	.00017175
.80	2.00	-.00273602	.00017185	.00017293
1.00	2.50	-.00364482	.00017217	.00017352
1.00	3.00	-.00364482	.00017363	.00017352
2.00	3.00	-.00815520	.00016790	.00017644

8POINTS TRAPEZOIDAL RULE : -.00060143
MIDPOINT RULE : .00023026

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00021878	.00001988	.00001970
.06	.50	.00016139	.00001977	.00001971
.10	.70	.00011548	.00001979	.00001971
.10	1.00	.00011548	.00001985	.00001971
.20	1.00	.00000074	.00001981	.00001973
.20	2.00	.00000074	.00002000	.00001973
.20	3.00	.00000074	.00002018	.00001973
.40	1.50	-.00022863	.00001984	.00001977
.80	2.00	-.00068693	.00001980	.00001984
1.00	2.50	-.00091587	.00001983	.00001988
1.00	3.00	-.00091587	.00001992	.00001988
2.00	3.00	-.00205844	.00001959	.00002006

24POINTS TRAPEZOIDAL RULE : -.00005570
MIDPOINT RULE : .00002558

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00002430	.00000069	.00000069
.06	.50	.00001793	.00000069	.00000069
.10	.70	.00001282	.00000069	.00000069
.10	1.00	.00001282	.00000069	.00000069
.20	1.00	.00000007	.00000069	.00000069
.20	2.00	.00000007	.00000070	.00000069
.20	3.00	.00000007	.00000070	.00000069
.40	1.50	-.00002543	.00000069	.00000069
.80	2.00	-.00007642	.00000069	.00000069
1.00	2.50	-.00010192	.00000069	.00000070
1.00	3.00	-.00010192	.00000070	.00000070
2.00	3.00	-.00022937	.00000069	.00000070

Table II.9. Errors in the calculation of $\int_0^1 |x-\cdot 5|^{\frac{1}{2}} dx$.

4POINTS TRAPEZOIDAL RULE : .03646327
MIDPOINT RULE : .01155839

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.01153324	.01664354	.01666266
.06	.50	.01140752	.01665301	.01666170
.10	.70	.01130701	.01664903	.01666092
.10	1.00	.01130701	.01664325	.01666092
.20	1.00	.01105593	.01664293	.01665899
.20	2.00	.01105593	.01662370	.01665899
.20	3.00	.01105593	.01660452	.01665899
.40	1.50	.01055473	.01663267	.01665513
.80	2.00	.00955606	.01662178	.01664742
1.00	2.50	.00905858	.01661155	.01664357
1.00	3.00	.00905858	.01660197	.01664357
2.00	3.00	.00658963	.01659879	.01662434

8POINTS TRAPEZOIDAL RULE : .00897805
MIDPOINT RULE : .00446236

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00445616	.00560741	.00560839
.06	.50	.00442519	.00560789	.00560834
.10	.70	.00440041	.00560769	.00560830
.10	1.00	.00440041	.00560739	.00560830
.20	1.00	.00433848	.00560737	.00560820
.20	2.00	.00433848	.00560638	.00560820
.20	3.00	.00433848	.00560539	.00560820
.40	1.50	.00421467	.00560684	.00560800
.80	2.00	.00396728	.00560628	.00560761
1.00	2.50	.00384371	.00560575	.00560741
1.00	3.00	.00384371	.00560525	.00560741
2.00	3.00	.00322698	.00560507	.00560642

24POINTS TRAPEZOIDAL RULE : .00132677
MIDPOINT RULE : .00093345

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00093276	.00104893	.00104894
.06	.50	.00092935	.00104894	.00104894
.10	.70	.00092661	.00104893	.00104894
.10	1.00	.00092661	.00104893	.00104894
.20	1.00	.00091978	.00104893	.00104894
.20	2.00	.00091978	.00104892	.00104894
.20	3.00	.00091978	.00104891	.00104894
.40	1.50	.00090612	.00104893	.00104894
.80	2.00	.00087879	.00104892	.00104893
1.00	2.50	.00086512	.00104891	.00104893
1.00	3.00	.00086512	.00104891	.00104893
2.00	3.00	.00079682	.00104891	.00104892

Table II.10. Errors in the calculation of $\int_0 x^{\frac{1}{2}}dx$.

4POINTS TRAPEZOIDAL RULE : -.03538438

MIDPOINT RULE : .00631073

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00627568	.00337285	.00336089
.06	.50	.00610050	.00336657	.00336150
.10	.70	.00596044	.00336882	.00336198
.10	1.00	.00596044	.00337246	.00336198
.20	1.00	.00561059	.00337202	.00336320
.20	2.00	.00561059	.00338410	.00336320
.20	3.00	.00561059	.00339615	.00336320
.40	1.50	.00491219	.00337719	.00336562
.80	2.00	.00352061	.00338149	.00337047
1.00	2.50	.00282741	.00338665	.00337289
1.00	3.00	.00282741	.00339267	.00337289
2.00	3.00	-.00061292	.00338832	.00338498

8POINTS TRAPEZOIDAL RULE : -.01037468

MIDPOINT RULE : .00236551

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00235679	.00113526	.00113412
.06	.50	.00231324	.00113467	.00113418
.10	.70	.00227841	.00113489	.00113422
.10	1.00	.00227841	.00113524	.00113422
.20	1.00	.00219133	.00113521	.00113434
.20	2.00	.00219133	.00113637	.00113434
.20	3.00	.00219133	.00113752	.00113434
.40	1.50	.00201727	.00113574	.00113457
.80	2.00	.00166947	.00113622	.00113503
1.00	2.50	.00149573	.00113675	.00113526
1.00	3.00	.00149573	.00113732	.00113526
2.00	3.00	.00062866	.00113708	.00113642

24POINTS TRAPEZOIDAL RULE : -.00180590

MIDPOINT RULE : .00048170

COL1	COL2	OQF1	OQF2	GMR
.01	1.00	.00048073	.00021232	.00021229
.06	.50	.00047591	.00021230	.00021229
.10	.70	.00047205	.00021231	.00021229
.10	1.00	.00047205	.00021232	.00021229
.20	1.00	.00046240	.00021232	.00021230
.20	2.00	.00046240	.00021234	.00021230
.20	3.00	.00046240	.00021237	.00021230
.40	1.50	.00044309	.00021233	.00021230
.80	2.00	.00040449	.00021234	.00021231
1.00	2.50	.00038520	.00021235	.00021232
1.00	3.00	.00038520	.00021237	.00021232
2.00	3.00	.00028873	.00021236	.00021234

10. The Sequence $\left\{\alpha_j\right\}_{j=0}^{N}$

So far we have been concerned with the properties of the optimal formula over H_N when the sequence $\left\{\alpha_j\right\}_{j=0}^{N}$ defining the metric in H_N was given. For the practical use of the formula however this sequence must be chosen according to the information that is available about the functions in H_N.

As an example suppose that the functions $f \in H_1$ satisfy the conditions

$$\int_{t_1}^{t_2} f^2(x)dx \leq M_0 ,$$

$$\int_{t_1}^{t_2} f'^2(x)dx \leq M_1 .$$

Then with this information we can improve the bound on $|E^*(f)|$ for we can write

$$|E^*(f)|^2 \leq ||E^*||^2||f||^2$$

$$= \int_{t_1}^{t_2} g^*(x)dx \int_{t_1}^{t_2} \alpha_0{}^2 f^2(x)+f'^2(x)dx,$$

$$\leq \int_{t_1}^{t_2} g^*(x)dx \,.\, (\alpha_0{}^2 M_0+M_1),$$

$$= \frac{2}{r^2} \sum_{j=0}^{n}{}'' (\tfrac{1}{2}h_j - \frac{1}{r}\tanh\tfrac{1}{2}rh_j)(r^2M_0+M_1), \qquad .1$$

(using $r = \alpha_0$.)

$$= 2 \sum_{j=0}^{n}{}'' \frac{(\frac{1}{2}rh_j - \tanh \frac{1}{2}rh_j)}{r^3} . (r^2 M_0 + M_1).$$

Let us denote $\psi_j(r) = r^{-3}(\frac{1}{2}rh_j - \tanh \frac{1}{2}rh_j)$.

Then ψ_j has the following properties;

(1) $\lim_{r\to 0} \psi_j(r) = \psi_j(0) = h_j{}^3/24,$

(2) $\lim_{r\to 0} \psi_j{}'(r) = \psi_j{}'(0) = 0$ and

(3) $\lim_{r\to 0} \psi_j''(r) = \psi_j''(0) = -\dfrac{h_j{}^5}{120}$.

If we denote

$$B(r) = 2 \sum_{j=0}^{n}{}'' r^{-3}(\tfrac{1}{2}rh_j - \tanh \tfrac{1}{2}rh_j)(r^2 M_0 + M_1)$$

we can see that

$$B(0) = 2 \sum_{j=0}^{n}{}'' \frac{M_1 h_j{}^3}{24} \quad \text{and}$$

$$B'(0) = \lim_{r\to 0} 2 \sum_{j=0}^{n}{}''(\psi_j'(r)(r^2 M_0 + M_1) + 2rM_0 \psi_j(r))$$

$$= M_1 \psi_j'(0) = 0.$$

Further

$$B''(0) = \lim_{r\to 0} 2 \sum_{j=0}^{n}{}''(\psi_j''(r)(r^2 M_0 + M_1) + 4rM_0 \psi_j'(r) + 2M_0 \psi_j(r))$$

$$= 2 \sum_{j=0}^{n}{}'' M_1 \psi_j''(0) + 2M_0 \psi_j(0)$$

.2

$$= 2 \sum_{j=0}^{n}{}'' - \frac{M_1 h_j^5}{120} + \frac{M_0 h_j^3}{12}$$

$$= \frac{1}{6} \sum_{j=0}^{n}{}'' h_j^3 (M_0 - \frac{M_1}{10} h_j^2).$$

If $B''(0) \geqslant 0$ then we should set $\alpha_0 = 0$ since this minimizes $B(r)$. However when this sum is negative we can choose $r_0 > 0$ such that the estimate

$$B(r_0) < B(0) = \frac{M_1}{12} \sum_{j=0}^{n}{}'' h_j^3.$$

If for example we use the optimal mesh (i.e. $h_j = \frac{t_2 - t_1}{n}$, $j=0,\ldots,n$) then whenever

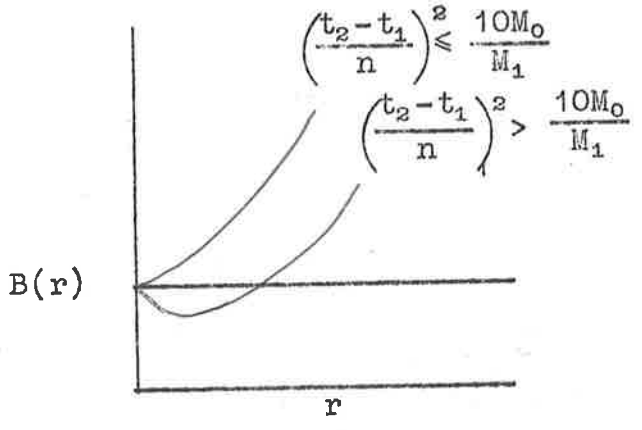
$$\left(\frac{t_2 - t_1}{n}\right)^2 > \frac{10M_0}{M_1},$$

the sum

$$B''(0) = \frac{1}{6} \sum_{j=0}^{n}{}'' \left(\frac{t_2 - t_1}{n}\right)^3 \left(M_0 - \frac{M_1}{10} \left(\frac{t_2 - t_1}{n}\right)^2\right)$$

$$< 0$$

and such an r_0 exists. Clearly then this best choice r_0 will be the solution of the equation $B'(r) = 0$.



For the case N=2 the situation is much less clear. If we suppose that, as well as M_0 and M_1, there exists M_2 such that

$$\int_{t_1}^{t_2} f''^2(x)dx \leqslant M_2$$

then there could well exist (for a certain range of M_0, M_1, M_2), $\alpha_0, \alpha_1 \neq 0$ generalizing the result obtained for N=1. However we did not find this generalization. The manipulations involved clearly make this a difficult task. As an alternative approach the errors of the formulae were examined in the hope that they might shed some light on the question of how to choose α_0 and α_1, but once again the values of α_0 and α_1 leading to the smallest errors could not be linked with any of the properties of the integrand (e.g. the values of M_0, M_1 and M_2). While it is clear that in some cases α_0 and α_1 should be set to zero, and the Midpoint Rule or the Krylov formula should be used, (e.g. Tables II.2, II.3) in other cases (e.g. Table II.7) non-zero values of α_0 and α_1 lead to the smallest error of the OQF1 and OQF2. Indeed in Table II.8 the OQF1 with $\alpha_0{}^2 = 0.2$ does considerably better than OQF2 and in turn the OQF2 with $\alpha_0{}^2 = 2$, $\alpha_1{}^2 = 3$ does better than the G.M.R. Of course we should distinguish between a formula that gives the smallest error for a particular function and a formula that gives the smallest

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error bound for a class of functions. We only use the experimental evidence as a possible guide to choosing the latter. Seemingly the only valid conclusion we can draw is that in the absence of any knowledge about how to choose α_0, α_1 and α_2 we should use the Krylov formula. However there <u>do</u> exist α_0, α_1 and α_2 which are non zero and which lead to results which are better than those obtained by the Krylov formula.

11. Concluding Remarks

We may summarize the contents of this thesis as follows.

We have shown that any exponential spline is defined completely by the jumps R_{jk} in its derivatives. We have established the one-to-one relation between the class G^N_{N-1}, of splines in H_N and the class S^N_p of error functionals and then shown that the spline realizing the error with smallest norm can be found by minimizing $\|g\|$ independently on each subinterval (lemma 2).

For N=1 and 2 we have explicitly derived the weights and mesh which define the quadrature formula that has least estimate of error $|E(f)|$ with respect to the norm $\|f\|$ for functions in H_N. For N=2 we have obtained as intermediate results the optimal formulae when

(a) the mesh is prescribed, and

(b) only the two end intervals h_0 and h_n of the mesh are prescribed.

Further we have shown that the optimal formula for N=2 does not use derivative values. It turns out that the conditions defining the derivative weights to be zero give the optimal mesh (c.f. Gaussian quadrature derived using Hermite formula). We have derived two expressions (lemmas 3 and 4) for $\|E^*\|$: the first was used to determine the optimal mesh and the second to derive the convergence properties of the formulae. The second expression is also useful for the practical computation of $\|E^*\|$.

We have introduced the Generalized Midpoint Rule and shown that, when α_0 vanishes the optimal formula is the G.M.R. We have shown also that as the mesh size decreases the optimal formula tends rapidly to the G.M.R. Thus we have characterized all the remaining formulae that are of interest for $N \leqslant 2$.

The optimal closed formula has been derived.

We have shown that all the function weights to the formula optimal on any mesh are positive (and so the optimal formulae are well suited to automatic computation from the point of view of round-off error). In addition we have shown that the optimal mesh can be easily determined numerically by standard iterative procedures. Finally, for $N=1$ we have indicated the way that we may choose α_0, if we have quantitative estimates of the smoothness of f, so that the bound on $|E^*(f)|$ is minimized.

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