EXISTENCE AND UNIQUENESS OF BEST APPROXIMANTS, WITH NUMERICAL APPLICATIONS

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ABSTRACT

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Part I of the thesis deals with existence and uniqueness theorems. Strengthening a result due to J.Blatter, it is proved in chapter 3 that a normed linear space is complete if every closed, bounded, and convex set is proximinal. It is also shown, that in a semi-reflexive, locally convex, real linear metric space, every closed, bounded and convex set is proximinal. An example is constructed which proves that not every reflexive space is sequentially convex. In chapter 4, sequential and local uniform convexity are shown to be independent properties. It is proved that a sequentially convex space can be equivalently renormed with a locally uniformly convex norm. Various spaces are shown to be incapable of uniformly convex renorming. In chapter 5, a number of convexity properties and a class of convergence processes are generalized to metric spaces. It is shown that Clarkson's renorming technique can be extended to metrics and that each closed subset of a metric space can be made proximinal by introducing an equivalent metric. Chapter 6 provides a link between the abstract material of previous chapters and the numerical applications of part II. A unified theory is developed which comprises both discrete and continuous Chebyshev approximation.

Part II of the thesis contains numerical applications to the approximation of functions, data analysis, mathematical modelling, and optimization. Chapter 7 deals with a modified exchange algorithm for Chebyshev approximation. In chapter 8, closed formulae for linear Chebyshev approximants are derived. A computer approximation is obtained which is subject to restrictions on the number of non-zero bits in its binary representation. In chapter 9, an algorithm is developed which determines the L_1 solution set and selects a strictly best solution. Chapter 10 deals with the problem of balancing the input and output streams of mineral processing plants. A comparison is made of various existing methods and some new algorithms are suggested. In chapter 11, an integer programming algorithm is developed which allows the user to search for sub-optimal and alternative optimal solutions. Codings of the algorithms in chapters 7, 9, 10, and 11 are listed in the appendix of programs. A separate pocket at the end of the thesis contains two papers published in advance.

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CONTENTS

Chapter 0

Introduction

This thesis is divided into two main parts. Part I is largely theoretical and deals with abstract existence and uniqueness theorems. Part II contains various numerical applications to functional approximation, data analysis, mathematical modelling, and optimization. The theoretical part centres on the following problem of approximation theory: let $(E, ||\cdot||)$ be a normed linear space and M a subset of E. For each $y \varepsilon E$ we define the distance of y from M by

$$d(y,M) = \inf_{x \varepsilon M} ||y-x|| \quad .$$

If there is an element $x \varepsilon M$ so that $d(y,M) = ||y-x||$, then x is said to be a proximum in M of y. M is called proximinal if every $y \varepsilon E$ has a proximum $x \varepsilon M$. The set of proxima is defined by the metric projection $P_M : E \to 2^M$, with

$$P_M(y) = \{x \varepsilon M : ||y-x|| = d(y,M)\}.$$

General conditions for the existence and uniqueness of proxima are of interest in many areas of pure and applied mathematics. For the special case that M is a subspace of E, there is now a more or less complete theory. (For a good account of this theory, see the comprehensive book by I. Singer [22].) In recent years, research has therefore concentrated on the problem of non-linear approximation. It soon became apparent that many results of the linear theory remain valid if M is assumed to be a convex set, but not necessarily a subspace, and if certain additional conditions are satisfied. Thus we have the following generalization of a well known result about closed subspaces.

Theorem 0.1 Let M be a closed convex subset of a uniformly convex Banach space $\mathbf{B}$. Then M is a Chebyshev set, i.e. for each $y \varepsilon B \sim M$ there is exactly one proximum in M.

An introduction to the elements of linear and convex approximation is given in chapter 1 of this thesis. Chapter 2 deals with Clarkson's method of equivalent renorming. In his seminal paper of 1936, Clarkson [2] showed that each separable Banach space can be given a strictly convex norm which is equivalent to the original norm. Clarkson also showed that this result cannot be extended to uniformly convex norms. His proof consists of constructing a non-differentiable function of bounded variation from $[0,1]$ into L_1 (theorem 2.4). Since differentiability is a necessary condition for the existence of an equivalent, strictly convex norm, the space L_1 is not strictly or uniformly convex renormable. Using similar constructions, Clarkson drew the same conclusion for certain other spaces. More generally, we show in Chapter 4 that non-reflexive spaces cannot be given an equivalent norm which is uniformly or sequentially convex (theorem and corollary 4.5). Chapter 3 deals with convexity properties which lie between strict and uniform convexity, such as local uniform convexity and sequential convexity. The former is due to Lovaglia [6], the latter was introduced by Ky Fan and Glicksberg [6], who pointed out that in theorem 0.1, uniform convexity can be replaced by sequential convexity but left the exact logical relationship between sequential and locally uniform convexity unresolved. An important contribution was then made by R.R. Phelps [17] and R.C. James who proved the following characterization theorem.

<u>Theorem 0.2</u> A Banach space B is reflexive if and only if every closed convex subset of B is proximinal.

J. Blatter [30] proved that a normed linear space is complete if every closed convex subset is proximinal. Since a reflexive space is always complete, this follows immediately from theorem 0.2. However, similar arguments can be used to establish a slightly stronger result: a normed linear space is complete if every closed, bounded and convex subset is proximinal (see theorem 3.5). It also follows that a sequentially convex Banach space is reflexive and strictly convex (Corollary 3.9). At the end of chapter 3 we construct a counterexample (example 3.1) which proves that, conversely, not every reflexive space is sequentially convex. Starting from theorem 0.2, we then conclude in chapter 4 that sequential convexity and local uniform convexity are independent properties. In 1978, M.A.Smith [20] proved, that sequential convexity does not imply local uniform convexity. His counter-example consists of a norm which is strictly and sequentially convex, but not locally uniformly convex. In chapter 4 we construct a norm which achieves the same result, without being strictly convex (example 4.1). In the opposite direction we use a theorem by Kadetz (theorem 4.3) and the results of chapter 3 to complete the proof that sequential and local uniform convexity are independent properties. We also show in this chapter that a sequentially convex space can be given an equivalent norm which is uniformly convex.

The following fundamental existence theorem of approximation theory also applies to metric spaces.

<u>Theorem 0.3</u> If M is a compact subset of a metric space, then M is proximinal.

In order to generalize other existence and uniqueness theorems to metric spaces without a linear structure, it will be necessary to modify various convexity properties of normed space theory. Some results of this type appear in an article by Ahuja, Narang and Trehan [13]. Taking this paper as a starting point, we shall discuss certain weak convexity properties and investigate a problem suggested by I.Singer (see [22, p.378]): "It would be interesting to study in metric spaces the problem of best approximation by elements of sets G belonging to certain special classes of sets, for instance convex sets $G \subset E$ in the sense of K.Menger, i.e. having the property that for any distinct $x, z \in E$ there exists a $y \in E$ with $x \neq y \neq z$ such that $d(x,z) = d(x,y) + d(y,z)$."

We shall refer to Menger's convexity as semi-convexity and show that, if M is an approximatively compact semi-convex set in a strictly convex metric space, then M is a Chebyshev set (theorem 5.1). We shall also modify the concept of τ-compactness, which is due to F.Deutsch [27] and L.P.Vlasov [26], and prove a suitable generalization of theorem 5.1. The fact that a compact or complete semi-convex set in a metric space is convex in the usual sense, can already be found in Menger's paper (see [23, p.83 ff.]). It is therefore impossible to replace approximative compactness by compactness or completeness. Accordingly, theorems 5.3 and 5.4 deal with convex subsets.

We conclude Chapter 5 by showing how the geometric properties of a metric space can be improved by introducing an equivalent metric. Using the universality of the space of continuous functions we can apply Clarkson's ideas to certain metric spaces in order to guarantee uniqueness of best approximations. As for existence, it will be demonstrated that each closed subset can be made proximinal by introducing an equivalent, "almost" isometric metric.

This result has no analogue in a normed space.

Chapter 6 provides a link between the abstract material of part I and the numerical applications of subsequent chapters. The emphasis lies on best approximination in the L_1 and L_∞ norms. It is shown that the minimax solution of a linear system can be regarded as a best continuous approximation on a compact metric space. A unified theory is developed which comprises both continuous and discrete approximation (theorems 6.5 - 6.8). The treatment of certain discrete L_1 results draws on material in the book by J.R.Rice [58, vol.I]. In particular, the proofs of lemmas 6.10 and 6.11 follow the line of reasoning used by Rice to establish the corresponding interval results. The alternation property of L_p approximants is shown to extend to generalized polynomials (lemma 6.16, theorem 6.17).

Chapter 7 contains a modified exchange algorithm for best Chebyshev approximation. The basic idea is to obtain an initial reference for subsequent exchange iterations by considering certain features of the error vector of the L_2 approximant. A FORTRAN version of this algorithm, subroutine MINMAX, is included in the appendix of programs. MINMAX is about three times faster than the linear programming algorithm by Barrodale and Phillips.

Chapter 8 deals with some aspects of segmented Chebyshev approximation. Although the best polynomial approximation to a given continuous function is known to exist, uniquely in fact, it remains an open question whether such a polynomial can be obtained by a general finite-step method. Such a method is feasible if the approximant is linear and if the continuous function satisfies certain additional conditions. It is shown that these sufficient conditions can be slightly weakened so as to satisfy only convexity and differentiability. The method is then applied to a problem of computer approximation, which imposes an upper bound on the number of non-zero bits in the binary representation of the coefficient of x, in order to minimize the execution time for linear approximants. The remainder of Chapter 8 is concerned with segmented linear approximation to functions of two variables. While the usual arguments for the existence of polynomial approximants carry over from the single variable case, the uniqueness theory breaks down. However, it was shown by Collatz [38], that a linear best approximant is unique if the approximated function has continuous partial derivatives at all interior points of a closed, strictly convex set of the plane. It is shown that, if the approximated function satisfies certain convexity and differentiability conditions, then it is possible to generalize the single variable case and derive closed expressions for the coefficients and maximum error of a best linear approximant.

Chapter 9 is concerned with the problem of non-unique linear approximants in the L_1 norm. Approximation packages generally supply only one L_1 solution and ignore alternative optima. At most, an exit code indicates that alternative optima may exist. As is detailed in chapter 6, the solutions form a two-dimensional convex set. In chapter 9, an algorithm is developed which determines this solution set and then proceeds to select from it a unique "best" of infinitely many best solutions. This is done by minimizing the L_2 norm of the error vector, with the parameters constrained to belong to the L_1 solution set. A FORTRAN coding of this algorithm is included in the appendix of programs (see the subroutines SOLVE and STRICT). A similar criterion, due to J.R.Rice, of choosing a "best" of all best Chebyshev approximants, is described in chapter 6 (see the remarks following theorem 6.5). Chapter 9 also includes a refinement of the usual linear programming technique for determining a best linear L_1 approximation. It consists of forcing the line through two interpolating points during the first two iterations. The interpolating points are chosen so that their L_2 errors r_j, r_k are numerically minimal, with $\mathrm{sgn}(r_j r_k) \leq 0$.

Chapter 10 deals with the problem of balancing the input and output streams of a mineral processing plant. A comparison is made of various existing computational techniques, emphasizing microcomputer implementation. A new algorithm is developed and coded in BASIC (see the program MINBAL in the appendix). The inconsistent systems arising from the material balance problem are traditionally solved by least squares methods. An adaptive package, incorporating other norms, is suggested and these norms are applied to a test problem.

An algorithm for alternative optimal and sub-optimal solutions in integer programming is developed in chapter 11. It is based on some elementary number theory and deals with the following problem: determine non-negative integers $x_1, \ldots, x_n$ such that $f(\underline{x}) = c_1 x_1 + \ldots + c_n x_n = \min!$, subject to linear constraints of the form $\underline{A}\,\underline{x} \leq \underline{b}$. There may also be secondary constraints of the type $\|\underline{x}\| = \min!$ Initially, it is assumed that the constrained minimum c of f is known. If the c_i are non-negative, then $\underline{0} \leq \underline{x} = \underline{D}\,\underline{t} + \underline{k} \leq \underline{s}$, where $\underline{D}$ is triangular, the t_i are arbitrary parameters, $\underline{k}$ is constant, and $s_i = c/c_i$. Upper and lower bounds for $\underline{t}$ define a superset of the feasible parameter set. Infeasible solutions are eliminated by a simple test for $\underline{A}\,\underline{x} \leq \underline{b}$ and $\underline{x} \geqslant \underline{0}$. An adaptive version of the algorithm is outlined which may be used as an alternative to standard integer programming packages.

I. EXISTENCE AND UNIQUENESS THEOREMS

Chapter 1

Strict and Uniform Convexity

Let E be a normed linear space with real or complex scalars, let M be a subset of E and $y \varepsilon E$. If

$$\| y-x \| = d(y,M),$$

then x is called a proximum, best approximant, or element of best approximation, to y in M. The set of all proxima to y in M will be denoted by $P_M(y)$. If $P_M(y)$ contains at least (at most) one proximum, M will be referred to as a proximinal (semi-Chebyshev) set. If $P_M(y)$ is a singleton set for every $y \varepsilon E$, M is said to be a Chebyshev set. A subset K of E will be called convex if $x,y \varepsilon K$ implies $\alpha x + \beta y \varepsilon K$ for all $\alpha, \beta \geq 0$ such that $\alpha + \beta = 1$.

Theorem 1.1 If M is a convex set in a normed space, then the set $P_M(y)$ is convex.

Proof First note that the intersection of convex sets is convex and that $P_M(y) = M \cap S$, where $S = \{x : \| x-y \| \leqq d(x,M)\}$. Moreover, if $x_1, x_2 \varepsilon S$ and $0 \leqq \alpha \leqq 1$, then $\|x_1 - y\|$, $\|x_2 - y\| \leqq d(y,M)$ and $\| \alpha x_1 + (1-\alpha) x_2 - y \| = \| \alpha(x_1 - y) + (1-\alpha) \times (x_2 - y) \| \leqq \alpha \| x_1 - y \| + (1-\alpha) \|x_2 - y\| \leqq d(y,M)$, i.e. S is also convex. It follows that $P_M(y)$ is convex. //

We next show that if M is a finite-dimensional subspace of a normed space E, then $P_M(y)$ is non-empty. Let $x \varepsilon M$ and $\| x \| > 2 \| y \|$. Then $\| x-y \| \geq \| x \| - \| y \| > \| y \| \geq$

$d(y,M)$. It therefore suffices to consider the function $\phi(x) = \|x-y\|$ on the set $B = \{x\varepsilon M : \|x\| \leq 2\|y\|\}$. This function is continuous, since $|\phi(x_1)-\phi(x_2)| \leq \phi(x_1-x_2) \leq \|x_1 - x_2\|$. B is a closed and bounded subset of a finite dimensional space and therefore compact, which implies that $\phi(x)$ assumes its minimum $d(y,M)$ for some $x_o \varepsilon B$. We therefore have the following result.

<u>Theorem 1.2</u> If M is finite-dimensional, then M is proximinal.

<u>Example 1.1</u> Consider the space $(R^2, \|\cdot\|_1)$ and let $M = \{(x_1,x_2):x_1 = x_2\}$. Then with $y = (1,0)$, $\inf_{x\varepsilon M} \|y-x\|_1$ $= \inf_{x_1\varepsilon R} (|x_1 - 1| + |x_1|) = 1$ and

$$P_M(y) = \{(x_1,x_2) : 0 \leq x_1 \leq 1\}. \qquad //$$

The example demonstrates that a proximum is not necessarily unique. In order to guarantee uniqueness, we impose a restriction on the norm of E:

<u>Definition 1.1</u> Let x,y be points in the normed linear space E. We say that E, or more precisely the norm of E, is <u>strictly convex</u> (or rotund) if the unit sphere $S = \{x\varepsilon E: \|x\| = 1\}$ contains no line segment, i.e.

$\|x\| = \|y\| = \|x+y\|/2 = 1$ implies that $x=y$.

Equivalently, $\|x+y\| = \|x\| + \|y\|$ implies $x=\alpha y$, $\alpha>0$.

<u>Example 1.2</u> The space $E = C[0,1]$ is not strictly convex. To see this, let $0 < c \leq 1$ and define

$$f_c(t) = \begin{cases} t/c, & 0 \leq t \leq c \\ 1, & c \leq t \leq 1 . \end{cases}$$

Then $\|f_c\|_\infty = 1$. If $0 < c < d \leq 1$ and

$$g = \lambda f_c + (1-\lambda)f_d, \quad 0 \leq \lambda \leq 1,$$

then $\|g\|_\infty \leq 1$, and since $g(t_o) = 1$ for $d \leq t_o \leq 1$, we actually have $\|g\|_\infty = 1$ for $0 \leq \lambda \leq 1$. Thus the unit sphere of C contains the segment $[f_c, f_d]$ and every point on this segment is a point of minimum distance 1 from 0. //

<u>Theorem 1.3</u> If M is a finite-dimensional subspace of a strictly convex normed linear space E, then M is a Chebyshev subspace.

<u>Proof</u> We only have to prove uniqueness. If $x_1, x_2 \varepsilon M$ such that $x_1 \neq x_2$ and if

$$\|y-x_1\| = \|y-x_2\| = d(y,M),$$

then

$$\|y-x_1 + y - x_2\| < 2d(y,M),$$

since E is strictly convex. Hence

$$\|y - (x_1 + x_2)/2\| < d(y,M),$$

contradicting the definition of x_1 and x_2. //

The last two theorems cannot be extended to infinite-dimensional spaces as the following example demonstrates.

<u>Example 1.3</u> (see Cheney [21,p.21]). Let $s = (s_1, s_2, \ldots) \varepsilon c_o$, the space of sequences which converge to zero, and define a norm on c_o by $\|s\| = \max |s_i|$. Then

$M = \{s \in c_o : \sum_1^\infty 2^{-i} s_i = 0\}$ is an infinite-dimensional subspace of c_o. Let $t = (t_1, t_2, \ldots) \in c_o \sim M$ and put $\sum 2^{-i} t_i = \delta$. Then $\delta \neq 0$ and the sequences

$$u^{(1)} = (-2/1)(\delta,0,0,0,\ldots)+t$$

$$u^{(2)} = (-4/3)(\delta,\delta,0,0,\ldots)+t$$

$$u^{(3)} = (-8/7)(\delta,\delta,\delta,0,\ldots)+t, \ldots$$

all lie in M. Moreover,

$$\|u^{(n)} - t\| = 2^n|\delta|/(2^n - 1) \to |\delta|.$$

For any $v \in P_M(t)$, $\|v-t\| \leq |\delta|$. If N is now chosen so that $|v_i - t_i| < |\delta|/2$ for all $i \geq N$, then

$$|\sum 2^{-i} t_i| = |\sum 2^{-i}(t_i - v_i)| \leq \sum 2^{-i}|t_i - v_i|$$

$$\leq |\delta| \sum_1^{N-1} 2^{-i} + (|\delta|/2) \sum_{i \geq N} 2^{-i} < |\delta|,$$

which is a contradiction. Hence $P_M(t) = \phi$. //

It is interesting to note where the proof of the theorem 1.2 breaks down if M is infinite-dimensional. Consider the subspace

$$M = \{s \in \ell_2 : s = (0, s_2, s_3, \ldots)\}.$$

If $B = M \cap \{s : \|s\|_2 = 1\}$, then B is a closed and bounded subset of M. But it is easy to see that B is not compact, by noting that the sequence $s_1 = (0,1,0,\ldots)$, $s_2 = (0,0,1,0,\ldots), \ldots$ has no convergent subsequence since $\|s_i - s_j\| = \sqrt{2}$ for $i \neq j$.

In order to extend theorem 1.3 to infinite-dimensional subspaces we require the completeness of E and a stronger form of convexity.

Definition 1.2 (Clarkson [2]). Let E be a normed linear space. Then E is called uniformly convex if for all $\varepsilon (0 < \varepsilon \leqq 2)$ there is a $\delta(\varepsilon) > 0$ so that the conditions

$$\|x\| = \|y\| = 1 \text{ and } \|x + y\|/2 > 1-\delta \qquad (x, y \varepsilon E)$$

imply $$\|x - y\| < \varepsilon.$$

Theorem 1.4 Let B be a uniformly convex Banach space. If M is a closed convex subset of B (in particular, a closed subspace) then M is a Chebyshev set.

Proof Let $y \varepsilon B \sim M$ and assume w.ℓ.o.g. that $y=0$. Put $\inf_{x \varepsilon M} \|x\| = \alpha$. Since M is closed, $\alpha > 0$ and there is a sequence (x_n) in M such that $\|x_n\| \to \alpha$. Setting $u_n = x_n/\alpha$, we have $\|u_n\| \to 1$. For a given $\varepsilon > 0$ we now choose $\delta(\varepsilon) > 0$ according to definition 1.2. Next let $\|u_n\| - 1 < \delta$ for $n \geq N$, say, and define $v_n = u_n/\|u_n\|$. Then $\|v_n\| = \|v_m\| = 1$. Since M is convex, $\|u_n + u_m\| \geq 2$. We therefore have $\|v_n + v_m\|/2$

$$= \|u_n + u_m - (1 - \|u_n\|^{-1})u_n - (1 - \|u_m\|^{-1})u_m\|/2 \geq$$

$$\geq \|u_n + u_m\|/2 - (\|u_n\| - 1)/2 - (\|u_m\| - 1)/2 > 1 - \delta.$$

It now follows from the uniform convexity of B that $\|v_n - v_m\| < \varepsilon$, i.e. (v_n) is a Cauchy sequence. Since B is a Banach space, there exists a $v \varepsilon B$ such that $v_n \to v$. Moreover,

$$\|u_n - v\| \leqq \|u_n - v_n\| + \|v_n - v\|$$

$\leqq \|u_n\|(1 - \|u_n\|^{-1}) + \|v_n - v\|$,

i.e. $u_n = x_n/\alpha \to v$ and $x_n \to \alpha v$.

But $\alpha v \in M$, since M is closed. The uniqueness part now follows from the fact that a uniformly convex space is strictly convex (see the next theorem).

<u>Theorem 1.5</u> If E is a uniformly convex normed linear space, then E is strictly convex. The converse holds if E is finite-dimensional.

<u>Proof</u> If E is uniformly convex and $\|x\| = \|y\| = \|x + y\|/2 = 1$, then $\|x - y\| < \varepsilon$ for any $\varepsilon > 0$. It follows that $x = y$.

Conversely, suppose E is finite-dimensional and strictly convex. For a given $\varepsilon > 0$ define the set

$$S = \{(x,y) \in E \times E : \|x\| = \|y\| = 1 \;\&\; \|x - y\| \geq \varepsilon\}.$$

Clearly, S is compact. Define a function f by

$$f(x,y) = 1 - \|x + y\|/2.$$

Then f is continuous. Moreover $f(x,y) > 0$, since E is strictly convex. Hence there is a $\delta > 0$ so that $\inf_{x,y \in S} f(x,y) = \delta$. For $\|x\| = \|y\| = 1$, it therefore follows from $\|x - y\| \geq \varepsilon$ that $1 - \|x + y\|/2 \geq \delta$, i.e. $\|x + y\|/2 > 1 - \delta$ implies $\|x - y\| < \varepsilon$. //

The next theorem is due to Clarkson [2].

<u>Theorem 1.6</u> A Hilbert space is unformly convex.

<u>Proof</u> Put $\|x\| = \|y\| = 1$ in the parallelogram identity.

Then

$$||x + y||^2 + ||x - y||^2 = 2||x||^2 + 2||y||^2.$$

It follows that if $||x + y|| \to 2$, then

$$||x - y||^2 = 4 - ||x + y||^2 = 4(1 - ||x + y||^2/4) \to 0. \quad //$$

Clarkson showed in the same paper that the spaces L_p and ℓ_p $(1 < p < \infty)$ are also uniformly convex. His proof is based on the following result.

<u>Lemma</u> For the spaces L_p and ℓ_p, with $p \geq 2$, we have

(i) $||x + y||^p + ||x - y||^p \leq 2^{p-1}(||x||^p + ||y||^p)$

(ii) $2(||x||^p + ||y||^p)^{q-1} \leq ||x + y||^q + ||x - y||^q$,

where $q = p/(p-1)$. For $1 < p < 2$, these inequalities hold in the reverse sense.

For a proof of the lemma, see Hewitt and Stromberg [3], p.225. To prove uniform convexity for $p \geq 2$, put $||x|| = ||y|| = 1$ in (i). Then $||x + y||^p + ||x - y||^p \leq 2^p$ and $||x - y||^p \leq 2^p(1 - ||x + y||^p/2^p) \to 0$ as $||x + y||/2 \to 1$. For $1 < p < 2$, reverse the sense of inequality (ii). We therefore have

<u>Theorem 1.7</u> (Clarkson). The spaces L_p and ℓ_p $(1 < p < \infty)$ are uniformly convex.

Theorem 1.7 is not true for $p=1$ or ∞. The spaces concerned also lack the weaker property of strict convexity. To prove this for $L_1[0,1]$, say, put $f=2x$, $g=2-2x$. Then $||f|| = ||g|| = ||f + g||/2$, but $f \neq g$. By choosing $f=x$, $g=1$ we can show that $L_\infty[0,1]$ is not strictly convex. The same result is established for ℓ_1 by considering the

sequences $s = (1/2, 0, 1/4, 0, 1/8, 0, \ldots)$, $t = (0, 1/2, 0, 1/4, 0, \ldots)$ and for ℓ_∞ by choosing $s = (1, 1/2, 1/4, \ldots)$ and $t = (1, 1, 1, \ldots)$.

Chapter 2

Clarkson's Method of Equivalent Renorming

In his paper on uniformly convex spaces, Clarkson [2] considered the following problem: given a Banach space $(B, \|\cdot\|)$, is there an equivalent norm $\|\cdot\|'$ which satisfies a certain convexity property such as strict convexity. (Recall that two norms $\|\cdot\|, \|\cdot\|'$ are <u>equivalent</u> if there exist positive constants k, K such that $k\|x\| \leqq \|x\|' \leqq K\|x\|$ for all $x \varepsilon B$.) Clarkson found that any separable Banach space can be given an equivalent strictly convex norm.

<u>Theorem 2.1</u> (Clarkson). If $(B, \|\cdot\|)$ is a separable Banach space, then there exists a strictly convex norm $\|\cdot\|'$ which is equivalent to $\|\cdot\|$.

The sequence space $(\ell_1, \|\cdot\|_1)$, the space of integrable functions $(L_1[0,1], \|\cdot\|_1)$ and the space of continuous functions $(C[0,1], \|\cdot\|_\infty)$ are separable and can be renormed in this way. We first prove the theorem for $C[0,1]$ and then apply a result due to Banach and Mazur, which will be stated here without proof.

<u>Theorem 2.2</u> (Banach and Mazur). If $(E, \|\cdot\|_E)$ is a separable normed linear space, then E is isometric to a closed linear manifold of $C[0,1]$.

<u>Proof of theorem 2.1</u> Let (x_n) be a sequence which is dense in $[0,1]$ and define a sequence (F_n) of bounded linear

functionals by $F_n(f) = f(x_n)$ for all $f \in C[0,1]$. It is easy to see that if $F_n(f) = 0$ for $n = 1,2,3,\ldots,$ then $f = 0$. Now let

$$\|f\|_C = (\|f\|_\infty^2 + \sum_{n=1}^{\infty} 2^{-2n}|F_n(f)|^2)^{\frac{1}{2}}.$$

To see that $\|\cdot\|_C$ satisfies the triangle inequality, note that

$$\|f+g\|_C = (\|f+g\|_\infty^2 + \sum 2^{-2n}|F_n(f) + F_n(g)|^2)^{\frac{1}{2}} \leqq$$

$$(\|f\|_\infty^2 + 2\|f\|_\infty \|g\|_\infty + \|g\|_\infty^2 +$$

$$+ \sum 2^{-2n}|F_n(f)|^2 + 2\sum 2^{-2n}|F_n(f)||F_n(g)| + \sum 2^{-2n}|F_n(g)|^2)^{\frac{1}{2}} \leqq$$

$$[\|f\|_\infty^2 + \sum 2^{-2n}|F_n(f)|^2 + \|g\|_\infty^2 + \sum 2^{-2n}|F_n(g)|^2 +$$

$$+ 2(\|f\|_\infty^2 + \sum 2^{-2n}|F_n(f)|^2)^{\frac{1}{2}}(\|g\|_\infty^2 + \sum 2^{-2n}|F_n(g)|^2)^{\frac{1}{2}}]^{\frac{1}{2}} =$$

$$(\|f\|_\infty^2 + \sum 2^{-2n}|F_n(f)|^2)^{\frac{1}{2}} + (\|g\|_\infty^2 + \sum 2^{-2n}|F_n(g)|^2)^{\frac{1}{2}}$$

$$= \|f\|_C + \|g\|_C. \tag{2.1}$$

Clearly, the remaining axioms of a norm are also satisfied. Since

$$\|f\|_\infty \leqq \|f\|_C \leqq (\|f\|_\infty^2 + \|f\|_\infty^2 \sum 2^{-2n})^{\frac{1}{2}} = (2/\sqrt{3})\|f\|_\infty,$$

the norms $\|\cdot\|_\infty$ and $\|\cdot\|_C$ are equivalent. We see from (2.1) that

$$\|f+g\|_C = \|f\|_C + \|g\|_C \tag{2.2}$$

implies

$$\|f+g\|_\infty = \|f\|_\infty + \|g\|_\infty.$$

Thus if $f,g\neq 0$ are functions in $C[0,1]$ which satisfy equation (2.2), we can write

$$[(\|f\|_\infty + \|g\|_\infty)^2 + \sum 2^{-2n}|F_n(f) + F_n(g)|^2]^{\frac{1}{2}} =$$

$$(\|f\|_\infty^2 + \sum 2^{-2n}|F_n(f)|^2)^{\frac{1}{2}} + (\|g\|_\infty^2 + \sum 2^{-2n}|F_n(g)|^2)^{\frac{1}{2}}.$$

It follows from the equality condition of the Cauchy-Schwarz inequality that there is a positive number k so that $kF_n(f) = F_n(g)$, i.e. $kf = g$. This concludes the proof that $\|\cdot\|_C$ is strictly convex. By theorem 2.2, there exists an isometry $T:E \to C[0,1]$, with $\|x\|_E = \|T(x)\|_\infty$ for all $x \varepsilon E$. If we now define a new norm on E by $\|x\|_E' = \|T(x)\|_C$, then $\|\cdot\|_E$ and $\|\cdot\|_E'$ are equivalent. If

$$\|x\|_E' = \|y\|_E' = \|x + y\|_E'/2 = 1,$$

then

$$\|T(x)\|_C = \|T(y)\|_C = \|T(x + y)\|_C/2 = 1,$$

and since $\|\cdot\|_C$ is strictly convex, it follows that $T(x) = T(y)$. Using the fact that an isometry is injective, we deduce that $x = y$, i.e. $\|\cdot\|_E'$ is strictly convex. //

Theorem 2.1 was strengthened by Kadetz [5], who proved that a separable Banach space can be given an equivalent norm which is locally uniformly convex. (For a definition of local uniform convexity, see chapter 3). A number of negative results in Clarkson's paper demonstrate that the renorming technique cannot be extended to uniform convexity. The argument is based on the following theorem which will be stated without proof.

Theorem 2.3 (Clarkson). Let F be a function of bounded variation from a Euclidean space to a Banach space which can be given an equivalent strictly convex norm. Then F is differentiable almost everywhere.

Consider the function $F:[0,1] \to L_1[0,1]$:

$$t \mapsto \phi_t(s) = \begin{cases} 1, & 0 \leq s \leq t \\ 0, & t < s \leq 1. \end{cases}$$

Let $\delta F/\delta t = (F(t+\delta t) - F(t))/\delta t, \quad \delta t \neq 0$. Then

$$\|\delta F/\delta t\|_{L_1} = \|(\phi_{t+\delta t} - \phi_t)/\delta t\|_{L_1} = 1,$$

i.e. F is of bounded variation. On the other hand, F is nowhere differentiable on $[0,1]$. We therefore have

Theorem 2.4 The space $L_1[0,1]$ cannot be renormed so as to be uniformly convex.

Using similar arguments, Clarkson drew the same conclusion for the spaces L_∞ (bounded, measurable functions), C, ℓ_∞ (bounded sequences) and c (convergent sequences). We shall see in the next section that theorem 2.4 holds, in fact, for all non-reflexive spaces. We finally conclude from this discussion that the converse of theorem 1.5 cannot be extended to infinite dimensional spaces:

Example 2.1 Let (x_n) be a sequence which is dense in $[0,1]$ and define a sequence F_n by $F_n(f) = f(x_n)$ for all $f \in C[0,1]$ as in the proof of theorem 2.1. Then

$$\|f\|_C = \left(\|f\|_\infty^2 + \sum_{n=1}^{\infty} 2^{-2n}|F_n(f)|^2\right)^{\frac{1}{2}}$$

is a norm which is strictly, but not uniformly convex. //

Chapter 3

Further Convexity Properties

The convexity properties discussed in this section are stronger than strict convexity and weaker than uniform convexity. The first definition goes back to Lovaglia [9]:

Definition 3.1 A normed linear space is called locally uniformly convex if $x \varepsilon E$, $\|x\| = 1$ and $\varepsilon > 0$ implies there exists $\delta(\varepsilon, x) > 0$ such that $\|x-y\| < \varepsilon$ if $\|y\| = 1$ and $\|x+y\|/2 > 1-\delta$.

Theorem 3.1 Uniform convexity implies local uniform convexity which in turn implies strict convexity. In a finite-dimensional space all three are equivalent.

Proof The first implication follows immediately from the definition. Now suppose $\|a\| = \|b\| = \|a+b\|/2 = 1$ and $a \neq b$. Take $\varepsilon = \|a-b\|$. Since the space is locally uniformly convex there exists a $\delta(\varepsilon, a) > 0$ so that if $\|y\| = 1$, $\|a+y\|/2 > 1-\delta$, then $\|a-y\| < \varepsilon$. But $\|a+b\|/2 = 1 > 1-\delta$ and $\|b\| = 1$. Therefore $\|a-b\| < \varepsilon$, contradiction. It follows that the space is strictly convex. The equivalence of all three properties in the finite-dimensional case follows from theorem 1.5. //

We shall later see that local uniform convexity is not sufficient to ensure proximinality of closed convex sets. But Lovaglia found a relationship between differentiability of the norm and local uniform convexity. Thus, if the dual space B* is locally uniformly convex, then the norm in the Banach space B is strongly differentiable, i.e.

$$\lim_{h \to 0} (\|x_o + h x\| - \|x_o\|)/h$$

exists uniformly on $\|x\| \leq 1$. Moreover, if B is locally uniformly convex and linear functionals attain their maximum on the unit sphere in B, then the norm in B^* is strongly differentiable.

Another important convexity property is due to Fan and Glicksberg [6]:

<u>Definition 3.2</u> Let K be a convex set. If (x_n) is a sequence in K such that

$$\lim_n \|x_n\| = \inf_{x \in K} \|x\|,$$

then it is called a <u>minimizing sequence</u> for K. A normed linear space is said to be <u>sequentially convex</u> if every minimizing sequence is a Cauchy sequence.

The relationship between sequential convexity and locally uniform convexity was not fully clarified in [6]. We shall see in Chapter 4 that the two properties are in fact independent. Since, a fortiori, sequential convexity does not imply uniform convexity, it follows that the next result represents a strengthening of theorem 1.4.

<u>Theorem 3.2</u> (Fan and Glicksberg). If M is a closed convex subset of a Banach space B and if B is sequentially convex, then M is a Chebyshev set.

<u>Proof</u> As in the proof of theorem 1.4 we put $\inf_{x \in M} \|x\| = \alpha$. Then $\alpha > 0$ and there exists a minimizing sequence (x_n) in M.

Since B is sequentially convex, (x_n) is a Cauchy sequence. But B is complete and M is closed. Hence $x_n \to x \varepsilon M$. To prove uniqueness, suppose $\|x\| = \|y\| = \alpha$ for $x, y \varepsilon M$. Then $(x,y,x,y,\ldots)$ is a minimizing sequence and therefore a Cauchy sequence, i.e. $x = y$. //

Further to the sufficient conditions of theorems 1.4 and 3.2 we next state necessary and sufficient conditions for the proximinality of all closed, convex subsets of a Banach space.

<u>Lemma 3.3</u> Let E be a normed linear space, H a hyperplane given by $f(x) = \alpha$, where $f \varepsilon E^*$, i.e. f is a continuous linear functional on E, and let $y \varepsilon E$. Then

$$d(y,H) = |f(y) - \alpha| / \|f\|.$$

<u>Proof</u> Since $\|y-x\| \geq |f(y-x)|/\|f\| = |f(y)-\alpha|/\|f\|$, $d(y,H) \geq |f(y) - \alpha| / \|f\|$. Now let $0 < \varepsilon < \|f\|$. By the definition of $\|f\|$ there exists $z \varepsilon E$ such that $|f(z)| > (\|f\| - \varepsilon)\|z\|$. Multiplying this inequality by $|f(y) - \alpha|/|f(z)|$, we obtain $|f(y) - \alpha| > (\|f\|-\varepsilon)\|z\| \times$ $\times |f(y) - \alpha|/|f(z)|$. Now put $x = y - ((f(y) - \alpha)/f(z))z$. Then $x \varepsilon H$ and the inequality becomes $\|y - x\| < |f(y) - \alpha| / (\|f\|-\varepsilon)$. Since $\varepsilon>0$ is arbitrary small, we also have $d(y,H) \leqq |f(y)-\alpha|/\|f\|$.

<u>Theorem 3.4</u> A Banach space B is reflexive if and only if each closed convex subset of B is proximinal.

<u>Proof</u> $\Leftarrow$ First assume that B is not reflexive. Then B has a non-reflexive, closed subspace M. By a well-known

theorem of James [10], a Banach space is reflexive if and only if each continuous linear functional attains its supremum on the unit sphere of every closed linear subspace. Let

$$S = \{x\varepsilon B : \|x\| = 1\} \text{ and}$$

$$S_M^* = \{f\varepsilon M^* : \sup_{S\cap M} |f(x)| = 1\}.$$

Then there exists $F\varepsilon S_M^*$ such that $F^{-1}(1)$ does not meet $S \cap M$. Clearly $F^{-1}(1)$ is a closed convex subset of B. We show that $F^{-1}(1)$ is not proximinal. By lemma 3.3, the distance d from the origin to the hyperplane $F^{-1}(1)$ is given by

$$d = |F(0) - 1|/\|F\| = 1.$$

But this distance is not achieved by any element of $F^{-1}(1)$ since $F^{-1}(1)$ does not intersect the set $S \cap M$. It follows that $F^{-1}(1)$ is not proximinal.

$\Longrightarrow$ We use the well-known result that reflexivity is equivalent to weak compactness of the unit ball $U = \{x\varepsilon B : \|x\| \leq 1\}$, see Day [1, p.69]. Let M be a closed convex set and $y\varepsilon B \sim M$. Define a sequence (B_n) of balls with centre y and radius $d(y,M) + n^{-1}$. Then $(B_n \cap M)$ is a decreasing sequence of non-empty, weakly compact, convex subsets of M. By a theorem of Smulian (see Dunford and Schwartz [18, p.433]) there is therefore an element $z\,\varepsilon \cap(B_n \cap M)$. It is easy to see that $z\,\varepsilon\, M$ and $\|z-y\| = d(y,M)$. //

J.Blatter [30] proved that if X is a normed linear space in which every closed convex subset is proximinal, then X is complete. Since a reflexive space is always complete, Blatter's result immediately follows from theorem 3.4. We can, however, use his line of reasoning to obtain a stronger result.

<u>Theorem 3.5</u> If X is a normed linear space in which every closed, bounded and convex subset is proximinal, then X is complete.

<u>Proof</u> We prove the contrapositive. Suppose X is not complete and let $\hat{X}$ be the completion of X. Then $(\hat{X})^* = X^*$ (see Koethe [28, p.261]). If $\hat{y} \in \hat{X} \sim X$ and $\|\hat{y}\| = d$, then $\hat{x} = \hat{y}/d \in \hat{X} \sim X$ and $\|\hat{x}\| = 1$. By the Hahn-Banach theorem there is an $f \in X^*$ such that $\|f\| = 1$ and $f(\hat{x}) = \|\hat{x}\| = 1$. Let (z_n) be a sequence in X such that $z_n \to \hat{x}$. Then $f(z_n) \to f(\hat{x}) = 1$. Putting $f(z_n) = \delta_n$, it is easy to see that $x_n = (1+1/n)z_n/\delta_n \to \hat{x}$ and $f(x_n) = 1+1/n$.

Let $M_1 = H(x_1, x_2, \ldots)$, the convex hull of the sequence (x_n). Then $\bar{M}_1$ is a closed, bounded and convex set. We show that $\bar{M}_1$ is not proximinal. Note that, if $x \in M_1$, then $x = \sum \theta_i x_i$, $\theta_i \geq 0$, $\sum \theta_i = 1$, and

$$f(x) = f(\sum \theta_i x_i) = \sum \theta_i \; f(x_i) = \sum \theta_i (1+1/i) > 1.$$

Moreover, if $x \in \bar{M}_1$, then $f(x) \geq 1$ by the continuity of f. Next note that

$$1 \leq |f(x)| \leq \|f\| \; \|x\| = \|x\| \quad \text{for all} \quad x \in M_1$$

and that

$$\lim \|x_n\| = \|\hat{x}\| = 1.$$

Hence $d(0, M_1) = \inf_{x \in \bar{M}_1} \|x\| = 1.$

If we can show that $f(x) > 1$ for all $x \varepsilon \bar{M}_1$, then

$$1 < |f(x)| \leq ||x||,$$

i.e. $\bar{M}_1$ is not proximinal. Suppose, to the contrary, there exists some $x_1 \varepsilon \bar{M}_1$ such that $f(x_1) = 1$. Define $M_k = H(x_k, x_{k+1}, \ldots)$. By choosing K sufficiently large we can ensure that $x_1 \notin \bar{M}_K$. Now put $P = H(x_1, \ldots, x_{K-1})$ and $Q = M_K$. If (y_n) is any sequence in M_1 such that $y_n \to x_1$, then

$$y_n = \alpha_n p_n + \beta_n q_n$$

for some $\alpha_n, \beta_n \geq 0$, $\alpha_n + \beta_n = 1$, $p_n \varepsilon P$, $q_n \varepsilon Q$.
If $p \varepsilon P$, then

$f(p) = f(\sum\theta_i x_i) = \sum\theta_i f(x_i) = \sum\theta_i(1 + 1/i) \geq 1 + 1/(K-1)$

for $\theta_i \geq 0$, $\sum\theta_i = 1$. Similarly, if $q \varepsilon Q$, then

$f(q) = f(\sum\theta_i' x_i) > 1$. Hence

$$f(y_n) = \alpha_n f(p_n) + \beta_n f(q_n) > \alpha_n(1 + 1/(K-1)) + \beta_n$$
$$= 1 + \alpha_n/(K-1).$$

But $f(y_n) \to f(x_1) = 1$. It follows that $\alpha_n \to 0$ and $\beta_n \to 1$. Moreover, $\ell im(\alpha_n p_n) = 0$ since P is a bounded set. Hence

$\ell im(\alpha_n p_n + \beta_n q_n) = \ell im\, q_n = x_1$, where $q_n \varepsilon Q = M_K$,

i.e. $x_1 \varepsilon \bar{M}_K$, which contradicts the definition of K. //

The 'only if' part of the proof of theorem 3.4 is essentially due to M.M.Day [19] and was first published in 1941. The 'if' part is outlined in a paper by R.R.Phelps [17] who attributes it to R.C.James. We can exploit the concept of weak compactness in a more general setting.

Definition 3.3 A linear topological space E is said to be locally convex if for each $a \in E$ and for each neighbourhood $N(a)$ of a, there is a convex neighbourhood $M(a)$ such that $a \in M \subset N$. The dual E^* and bidual E^{**} of E are defined as usual. If $E = E^{**}$ then E is called semi-reflexive. (A semi-reflexive Banach space is reflexive).

The 'only if' part of theorem 3.4 depends on Smulian's characterization of weak compactness in Banach spaces, which does not carry over to general locally convex spaces. However, one half of Smulian's result can be generalized for our purposes. We require two theorems from convexity theory.

Definition 3.4 Two convex sets A and B are said to be strongly separated by a hyperplane $f(x) = \alpha$ if for some $\varepsilon > 0$ and for all $a \in A$, $b \in B$

$$f(a) \leqq \alpha - \varepsilon < \alpha + \varepsilon \leqq f(b).$$

Theorem 3.6 Two convex sets A and B in a locally convex space X can be strongly separated by a closed hyperplane if and only if $0 \notin \overline{B-A}$.

For a proof see Holmes [29, p.64]. The proof of the next theorem is an adaptation of arguments used in [29, p.146].

Theorem 3.7 If a convex subset M of a real locally convex linear space X is w-compact, then every decreasing sequence of non-empty closed convex subsets of M has a non-empty intersection.

Proof Let M be w-compact. Take any decreasing sequence of non-empty closed convex subsets K_n of M. Select $x_n \in K_n$ for $n=1,2,\ldots$ and suppose, choosing a subsequence if necessary, that $x_n \rightharpoonup x_o \in M$. (The half-arrow denotes weak convergence.) We shall show that for any $f \in X^*$

$$\ell = \underline{\lim}\, f(x_n) \leqq f(x_o) \leqq \overline{\lim}\, f(x_n) = L. \qquad (3.1)$$

Let $f(x_o) > L + \varepsilon$ for some $\varepsilon > 0$. Then there are only finitely many x_n such that $|f(x_n) - f(x_o)| < \varepsilon$, contradicting $x_n \rightharpoonup x_o$. Hence $f(x_o) \leqq L$ and similarly $f(x_o) \geq \ell$. Now suppose $x_o \notin \bigcap_{n=1}^{\infty} K_n$. Then there exists N such that $x_o \notin K_N$. Using the previous theorem with $\mathbf{B} = \{x_o\}$ and $\mathbf{A} = K_N$, we see that there is some $f \in X^*$ such that $f(x_n) < f(x_o)$ for all $n \geq N$, i.e. $\overline{\lim}\, f(x_n) < f(x_o)$, contradicting (3.1). Hence $x_o \in \bigcap_{n=1}^{\infty} K_n$. //

We now use the fact that every bounded subset M of a locally convex semi-reflexive space E is relatively w-compact. (The converse is also true, see Koethe [28, p.299].) If we also assume that M is closed and convex, it follows from the last theorem that a decreasing sequence of non-empty closed convex subsets B_n of M has a non-empty intersection. Now let $y \in E \sim M$ and put

$$B_n = \{x : d(x,y) \leqq d(y,M) + 1/n\}.$$

Then there exists some $x_o \in \bigcap_{n=1}^{\infty}(B_n \cap M)$ and $d(x_o,y) = d(x_o,M)$. We therefore have

Theorem 3.8 If E is a semi-reflexive, locally convex, real linear metric space, then every closed bounded and convex subset M of E is proximinal.

We can easily extend theorem 3.4 to include a uniqueness criterion. This result appears in Singer [22] and Cudia [8].

<u>Theorem 3.9</u> A Banach space B is reflexive and strictly convex if and only if each closed convex subset M of B is a Chebyshev set.

<u>Proof</u> If the space B in theorem 3.4 is also strictly convex, then the proximum must be unique. Conversely, suppose B is not strictly convex. Then the boundary of the unit sphere contains a line segment with at least two best approximations to the origin. //

<u>Corollary 3.9</u> If a Banach space is sequentially convex, then it is reflexive and strictly convex.

We now give a counterexample to demonstrate that a reflexive space is not necessarily sequentially convex. The norm used appears in a different context in the paper by M.A.Smith [20].

<u>Example 3.1</u> Let $x = (x_j) \in \ell_2$ and define

$$\|x\|_S = \max\{|x_1|, (\sum_{j=2}^{\infty} x_j^2)^{\frac{1}{2}}\} .$$

It is easy to see that $\|\cdot\|_S$ is a norm on ℓ_2.

It follows from

$$(1/\sqrt{2})\|x\|_2 \leq \|x\|_S \leq \|x\|_2$$

that $\|\cdot\|_S$ is equivalent to the usual ℓ_2 norm. We define a linear map

$$T : \ell_2 \to \ell_2 : (x_1, x_2, \ldots) \mapsto (x_1/1, x_2/2, \ldots)$$

and a new norm

$$\|x\|_W = (\|x\|_S^2 + \|Tx\|_2^2)^{\frac{1}{2}} .$$

We then have

$$\|x\|_S \leqq \|x\|_W = \|x\|_S \ (1 + \|Tx\|_2^2 / \|x\|_2^2)^{\frac{1}{2}}$$

$$\leqq \|x\|_S(1 + 2\|Tx\|_S^2/\|x\|_S^2) \leqq \|x\|_S(1 + 2\|T\|_S^2) ,$$

i.e. $\|\cdot\|_W$ and $\|\cdot\|_2$ are equivalent norms.

Now let

$$x = (1/\sqrt{2},\ 0,\ 0,\dots), \qquad y = (2/\sqrt{2},\ 0,\ 0,\ \dots)$$

and

$$K = \{x : \|x\|_W \leqq 1\}.$$

Then

$$\|x\|_S = 1/\sqrt{2}, \qquad Tx = (1/\sqrt{2},\ 0,\ 0,\ \dots) ,$$

$$\|Tx\|_2 = 1/\sqrt{2} \quad \text{and} \quad \|x\|_W = 1.$$

From $\|y\|_W = 2$ and $\|x-y\|_W = 1$ we have

$$d(y,K) = 1,$$

where d is calculated according to the norm $\|\cdot\|_W$.

Next define a sequence $(x^{(n)})$ by

$$x^{(n)} = (1/\sqrt{2} - 1/n, 0, 0, \dots, 1/\sqrt{2} \underset{(n)}{-} 1/n, 0, 0, \dots), \ n \geq 2 .$$

Then

$$Tx^{(n)} = (1/\sqrt{2} - 1/n, 0, 0, \dots, (1/\sqrt{2} \underset{(n)}{-} 1/n)/n, 0, 0, \dots),$$

$\|x^{(n)}\|_S = 1/\sqrt{2} - 1/n$ and $\|x^{(n)}\|_W =$

$$= [2(1/\sqrt{2} - 1/n)^2 + (1/\sqrt{2} - 1/n)^2 /n^2]^{\frac{1}{2}}$$

$$= [1-4/(n\sqrt{2}) + 5/(2n^2) - 2/(n^3\sqrt{2}) + 1/n^4]^{\frac{1}{2}} < 1,$$

i.e. $x^{(n)} \varepsilon K$. Moreover,

$$x^{(n)} - y = (-1\sqrt{2} - 1/n, 0, 0, \dots, 1/\sqrt{2} \underset{(n)}{-} 1/n, 0, 0, \dots)$$

$T(x^{(n)} - y) = (-1/\sqrt{2} - 1/n, 0, 0, \ldots, (1/\sqrt{2} - 1/n)/n, 0, 0, \ldots)$,

$\|x^{(n)} - y\|_S = 1/\sqrt{2} + 1/n$ and $\|x^{(n)} - y\|_W =$

$= [2(1/\sqrt{2} + 1/n)^2 + (1/\sqrt{2} - 1/n)^2/n^2]^{\frac{1}{2}}$

$= [1 + 4/(n\sqrt{2}) + 5/(2n^2) - 2/(n^3\sqrt{2}) + 1/n^4]^{\frac{1}{2}} \to 1.$

It follows that $(x^{(n)})$ is a minimizing sequence.

But $x^{(n)} - x^{(n+1)}$

$$= (1/(n+1) - 1/n, 0, 0, \ldots, \underset{(n)}{1/\sqrt{2} - 1/n}, \underset{(n+1)}{-1/\sqrt{2} + 1/(n+1)}, 0, 0, \ldots)$$

and $T(x^{(n)} - x^{(n+1)})$

$$= (1/(n+1) - 1/n, 0, 0, \ldots, (1/\sqrt{2} - 1/n)/n, (-1/\sqrt{2} + 1/(n+1))/(n+1), 0, 0, \ldots).$$

It follows that $\|x^{(n)} - x^{(n+1)}\|_S$

$= [(1/\sqrt{2} - 1/n)^2 + (1/\sqrt{2} - 1/(n+1))^2]^{\frac{1}{2}}$ and

$\|x^{(n)} - x^{(n+1)}\|_W = [(1/\sqrt{2} - 1/n)^2 + (1/\sqrt{2} - 1/(n+1))^2 +$

$+ (1/(n+1) - 1/n)^2 + (1/n^2)(1/\sqrt{2} - 1/n)^2 +$

$+ (1/(n+1)^2)(1/(n+1) - 1/\sqrt{2})^2]^{\frac{1}{2}}$,

i.e. $(x^{(n)})$ is not a Cauchy sequence. The result now follows in view of theorem 4.2 //

Chapter 4

The Relationship Between Sequential Convexity and Local Uniform Convexity

In order to disprove the conjecture that local uniform convexity implies sequential convexity we first establish some properties of equivalent norms (theorems 4.1 and 4.2) and then apply a theorem by Kadetz [5], which will be stated without proof.

Theorem 4.1 Let B be a Banach space and $\|\cdot\|$, $\|\cdot\|'$ equivalent norms on B, with

$$k\|x\| \leq \|x\|' \leq K\|x\| \quad \text{for all } x \in B.$$

If the corresponding operator norms on B^* and B^{**} are $\|\cdot\|_*$, $\|\cdot\|'_*$ and $\|\cdot\|_{**}$, $\|\cdot\|'_{**}$ respectively, then

(i) $(1/K)\|f\|_* \leq \|f\|'_* \leq (1/k)\|f\|_*$ for all $f \in B^*$,

(ii) $k\|g\|_{**} \leq \|g\|'_{**} \leq K\|g\|_{**}$ for all $g \in B^{**}$.

Proof For $f \in B^*$, $\|f\|'_* = \sup_{\|x\|' \leq 1} |f(x)| \leq \sup_{k\|x\| \leq 1} |f(x)|$

$= \frac{1}{k} \sup_{\|x\| \leq 1} |f(x)| = \frac{1}{k} \|f\|_*$.

Moreover, $\|f\|'_* \geq \sup_{K\|x\| \leq 1} |f(x)| = \frac{1}{K} \|f\|_*$, which proves (i).

Repeating the argument for the second dual gives (ii). //

Theorem 4.2 Let B be a Banach space and $\|\cdot\|$, $\|\cdot\|'$ equivalent norms on B. Then $(B, \|\cdot\|)$, $(B, \|\cdot\|')$ are either both reflexive or both non-reflexive.

Proof This follows from the definition of reflexivity and the previous theorem.

Theorem 4.3 (Kadetz). If $(B, \|\cdot\|)$ is a separable Banach space, then there exists a locally uniformly convex norm $\|\cdot\|'$, which is equivalent to $\|\cdot\|$.

It now follows that if local uniform convexity implied sequential convexity we could make the separable space ℓ_1 sequentially convex by equivalent renorming. But Corollary 3.9 would then imply that ℓ_1 is reflexive, which disproves the conjecture.

We can also prove that, conversely, sequential convexity does not imply local uniform convexity. A supposed counter-example due to Anderson, which is cited in the survey paper by Cudia [8, p.83] was shown to be fallacious by M.A.Smith (private communication, 1976). In 1978 Smith [20] succeeded in constructing a norm which is not locally uniformly convex and has the following properties: (i) strict convexity, (ii) reflexity, (iii) convergence property (H). Property (H) is well-known to hold in any Hilbert space:

Definition 4.1 A normed linear space E has property (H) (also called the Radon-Riesz property) if $x, x^{(n)} \in E$, $\|x^{(n)}\| \to \|x\|$ and $x^{(n)} \rightharpoonup x$ implies $x^{(n)} \to x$. ($\rightharpoonup$ denotes weak convergence in E.)

Fan and Glicksberg proved [6, p.560] that a Banach space is sequentially convex if and only if it is reflexive and has property (H). Smith's example therefore demonstrates that sequential convexity does not imply local uniform convexity. We shall now derive the same result in a different way, using a norm which is not strictly convex.

<u>Example 4.1</u> Let $x = (x_1, x_2, \ldots) \in \ell_2$ and define

$$\|x\|_F = |x_1| + \left(\sum_{j=2}^{\infty} x_j^2\right)^{\frac{1}{2}}.$$

It is easy to see that $\|\cdot\|_F$ is a norm on ℓ_2. We prove that $\|\cdot\|_F$ has the following properties

(i) $\|\cdot\|_F$ and $\|\cdot\|_2$ are equivalent,

(ii) $\|\cdot\|_F$ is not strictly convex,

(iii) $\|\cdot\|_F$ is sequentially convex.

(i) Follows from $\|x\|_2 \leq \|x\|_F \leq 2\|x\|_2$.

(ii) Let $x = (1,0,0,\ldots)$, $y = (0, 1/\sqrt{2}, 1/\sqrt{2}^2, 1/\sqrt{2}^3, \ldots)$.

Then $\|x\|_F = \|y\|_F = 1$ and $\|x+y\|_F = 2$.

(iii) We first show that $\|\cdot\|_F$ has property (H). Let $x, x^{(n)} \in \ell_2$, with

$$\|x^{(n)}\|_F \to \|x\|_F \quad \text{and} \quad x^{(n)} \rightharpoonup x .$$

If $x = 0$, then $x^{(n)} \to 0$. For $x \neq 0$ assume w.ℓ.o.g. that $\|x^{(n)}\|_F = \|x\|_F = 1$. Then

$$|x_1^{(n)}| + \left[\sum_{j=2}^{\infty} (x_j^{(n)})^2\right]^{\frac{1}{2}} = 1 = |x_1| + \left(\sum_{j=2}^{\infty} x_j^2\right)^{\frac{1}{2}} \qquad (4.1)$$

Let $y^{(n)} = (x_2^{(n)}, x_3^{(n)}, \ldots)$ and $y = (x_2, x_3, \ldots)$.

Since $x^{(n)} \rightharpoonup x$, we have $x_1^{(n)} \to x_1$. We can now deduce from (4.1) that $\|y^{(n)}\|_2 \to \|y\|_2$.

Since also $y^{(n)} \rightharpoonup y$, we obtain

$$\|y^{(n)} - y\|_2 \to 0 \quad \text{and}$$

$$\|x^{(n)} - x\|_F = |x_1^{(n)} - x_1| + \|y^{(n)} - y\|_2 \to 0,$$

i.e. $\|\cdot\|_F$ has property (H). Moreover, the space $(\ell_2, \|\cdot\|_F)$ is reflexive. Hence it is sequentially convex as required. //

While the example shows that a sequentially convex space need not be strictly or locally uniformly convex, it can nevertheless be renormed with a locally uniformly convex norm. This follows from corollary 3.9 and a result by Lindenstrauss, Asplund, Troyanski et al.

<u>Theorem 4.4</u> Each reflexive normed linear space can be renormed with an isometric norm which is both locally uniformly convex and strongly differentiable.

<u>Proof</u> See Day [1, p.72].

In view of theorems 3.2, 3.4 and 3.9 we can deduce from theorem 4.2 another important result about the renorming of Banach spaces.

<u>Theorem 4.5</u> A non-reflexive Banach space cannot be renormed with a uniformly convex or a sequentially convex norm.

The converse of theorem 4.5 is false, i.e. there are reflexive spaces which are not uniformly convex renormable. An example, due to M.M.Day can be found in Koethe [28, p.361]. It remains an open question whether every reflexive Banach space can be given a strictly convex norm.

We are now in a position to replace Clarkson's proofs of various renorming results (see the remarks following theorem 2.4) by a simple corollary to the last theorem.

<u>Corollary 4.5</u> The spaces L_1, L_∞, C, ℓ_∞ and c cannot be renormed with uniformly convex norms.

It is clear that we can add other spaces such as ℓ_1, c_0 and BV, the space of functions of bounded variation, to Clarkson's original list.

The results of this chapter can be summarized by saying that only certain weaker convexity properties, e.g. strict and local uniform convexity, can be obtained by Clarkson's method. While equivalent renorming can improve uniqueness properties and certain local properties of a space, it is impossible to affect global proximinality in this way.

Chapter 5

Convexity and Best Approximation in Metric Spaces

We now discuss the problem of best approximation by elements of a subset M of a metric space X. In trying to generalize the theory of metric spaces we first note that the convexity properties of a normed linear space will have to be modified to allow for the lack of linear structure. Non-linear spaces are not just of theoretical interest as the following examples demonstrate: the space of all non-decreasing functions on $[a,b]$, the space of functions f on $[a,b]$ with $f(a) = c \neq 0$ and the space of functions f with $\int_a^b f = c \neq 0$. Definitions of this type appear in a paper by Ahuja, Narang and Trehan [13]. These authors generalize the notions of strict and uniform convexity and show that certain approximation results, such as theorem 1.4, remain true for metric spaces. Ahuja et al. make the assumption that M is <u>convex</u>, i.e. for any two points $x,y \in M$ any point between x and y is also in M, and that the space X is <u>strongly convex</u> which means that if $x,y \in X$, then there is a unique $z \in X$ such that $d(x,z) = d(z,y) = d(x,y)/2$. (See also Rolfsen [14].) We shall see that these convexity properties can sometimes be replaced by weaker conditions.

<u>Definition 5.1</u> A set M will be called <u>semi-convex</u> if for all $x,y \in M$ there exists at least one <u>intermediate point</u> $z \in M$ such that

$$d(x,z) + d(z,y) = d(x,y).$$

A metric space is called <u>strictly convex</u>, if $x \neq y$, $d(x,x_0) \leq r$

and $d(y,x_o) \leq r$ implies $d(z,x_o) < r$ whenever z is an intermediate point of x and y.

Definition 5.2 Let (X,d) be a metric space and M a semi-convex subset of X. If (x_n) is a sequence in M such that

$$\lim d(x_n,x_o) = \inf_{x \varepsilon M} d(x,x_o)$$

for some point $x_o \varepsilon X \sim M$, then (x_n) is called a minimizing sequence. (X,d) is called sequentially convex, if every minimizing sequence is a Cauchy sequence.

Definition 5.3 (see Efimov and Stechkin [24]). A set M is said to be approximatively compact if every minimizing sequence in M has a sub-sequence convergent in M.

Theorem 5.1 Let M be an approximatively compact semi-convex subset of a strictly convex metric space (X,d). Then M is a Chebyshev set.

Proof The proximinality of M was proved by Efimov and Stechkin [24] and does not depend on the semi-convexity of M: first note from

$$|d(x,y_1) - d(x,y_2)| \leq d(y_1,y_2), \qquad (x,y_1,y_2 \varepsilon X),$$

that for any given x, the functional $f(y) = d(x,y)$ is uniformly continuous in y. For any $x_o \varepsilon X \sim M$ there exists a sequence $(d(x_o,y_n))$ with $y_n \varepsilon M$, such that $\lim d(x_o,y_n) = d(x_o, M)$. Since M is approximatively compact, there is a subsequence (y_{n_k}) of (y_n) which converges to some $y \varepsilon M$. The uniform continuity of $d(x,y)$ now gives

$$d(x_o,y) = d(x_o, \lim y_{n_k}) = \lim d(x_o,y_{n_k}) = d(x_o,M).$$

It follows that M is proximinal.

Now let $y,y' \varepsilon M$, with $d(x_o,y) = d(x_o,y') = d(x_o,M)$, and let $z \varepsilon M$ be an intermediate point of y,y'. Since (X,d) is strictly convex we have $d(x_o,z) < d(x_o,M)$, which contradicts the definition of $d(x_o,M)$. Hence $y = y'$ and M is a Chebyshev set. //

<u>Example 5.1</u> Let $A = \{x \varepsilon Q : x \varepsilon (-1,1)\}$, $X = R \sim A$, and $M = [-1,1] \sim A$. Then M is approximatively compact and semi-convex, but not convex. This shows that the above result is stronger than Ahuja's theorem 2 [13, p.95], in which M is assumed to be convex. //

If in definition 5.3 convergence is replaced by weak convergence, we obtain a generalization of approximative compactness which was first proposed by W.Breckner [11]. Corresponding to three types of weak compactness, we obtain in this way three weak types of approximative compactness, which enable us to deduce that the following sets are proximinal

1. Closed convex subsets of reflexive Banach spaces.
2. Weak* closed subsets of the dual space.
3. Weakly closed sets of operators on a Hilbert space.

L.P.Vlasov [26] introduced the concept of τ-compactness which includes the various forms of compactness mentioned above. Similar ideas are contained in an article by F.Deutsch [27], who obtains a very general approximation theorem which adds the following subsets of $C[a,b]$ to the above list:

4. Spline functions with free knots.
5. Exponential sums.
6. Rational functions.

We now adapt the definition of approximative τ-compactness for metric spaces and prove a corresponding generalization of theorem 5.1. Recall that $(A,\leqq)$ is called a directed set if for all $\alpha,\beta \in A$ there is some $\gamma \in A$ so that $\alpha \leqq \gamma$ and $\beta \leqq \gamma$, where the relation '$\leqq$' is reflexive, transitive, and antisymmetric.

Definition 5.4 Let M be an arbitrary set. If $\alpha \in A$ defines an element $x_\alpha \in M$, then the (x_α) form a net in M. A subset B of A is said to be cofinal if for all $\alpha \in A$ there is some $\beta \in B$ such that $\beta \geq \alpha$. The corresponding net (x_β) will be called a cofinal subnet of (x_α).

Now let (X,d) be a metric space. We define a class of convergence processes called τ-convergence in the following way. Each τ-convergent net (x_α) in X is associated with a unique element $x \in X$ so that for all $y \in X$.

(i) $d(x_\alpha,x) \overset{\tau}{\to} 0 \;\Rightarrow\; d(x_\alpha,y) \overset{\tau}{\to} d(x,y)$,

(ii) $d(x_\alpha,x) \overset{\tau}{\to} 0 \;\Rightarrow\; d(x,y) \leqq \overline{\lim}\, d(x_\alpha,y)$.

The following are examples of τ-convergence.

Example 5.2

1. Convergence in a metric space : $d(x_\alpha,x) \to 0$.

2. Weak convergence : $f(x_\alpha) \to f(x)$ for each $f \in X^*$.

3. Weak* convergence in X^* : $f_\alpha(x) \to f(x)$ for each $x \in X$.

4. Pointwise convergence in $C(X)$ on a dense subset X_o of the compact Hausdorff space X : $f_\alpha(x) \to f(x)$ for each $x \in X_o$.

If M is a subset of X, then M is called <u>approximatively</u> <u>τ-compact</u>, if for all $x \in X \sim M$ and any minimizing net (x_α) such that $d(x_\alpha, x) \to d(x, M)$, there is a cofinal subnet of (x_α), which τ-converges to some point in M. A set F is <u>τ-closed</u> if it contains the limit of each τ-convergent net. The metric projection $P_M : X \to 2^M$ will be called <u>upper</u> <u>τ-metric</u> <u>semi-continuous</u> at x_o if for any (x_α) with $d(x_\alpha, x_o) \to 0$ and for any τ-open set $U \supset P_M(x_o)$, there is some β such that $U \supset P_M(x_\alpha)$ for all $\alpha \geq \beta$.

<u>Theorem 5.2</u> Let M be an approximatively τ-compact, semi-convex subset of a strictly convex metric space X. Then M is a Chebyshev set and the metric projection P_M is upper τ-metric semi-continuous.

<u>Proof</u> Let $x_o \in X \sim M$ and (y_α) be a net in M so that $d(y_\alpha, x_o) \to d(x_o, M)$. Then there exists a cofinal subnet (y_β) which τ-converges to some $y \in M$. Hence

$$d(y_\beta, x_o) \xrightarrow{\tau} d(y, x_o)$$

and
$$d(y, x_o) \leq \overline{\lim}\, d(y_\beta, x_o) = d(x_o, M),$$

i.e. $y \in P_M(x_o)$ and M is proximinal. The uniqueness of y follows as in the proof of theorem 1.4.

Now suppose P_M is not upper semi-continuous. Then there exists a net (x_α) with $d(x_\alpha, x_o) \to 0$ and a τ-open set $U \supset P_M(x_o)$, so that for any β there is some $\alpha \geq \beta$ with $P_M(x_\alpha) \sim U \neq \phi$. If one element p_α is selected from each set $P_M(x_\alpha) \sim U$, then

$$d(x_o, M) \leqq d(x_o, p_\alpha) \leqq d(x_o, x_\alpha) + d(x_\alpha, p_\alpha)$$

$$= d(x_o, x_\alpha) + d(x_\alpha, M) \to d(x_o, M),$$

i.e. (p_α) is a minimizing net. Next let (p_β) be a cofinal subnet of (p_α), with $p_\beta \xrightarrow{\tau} p_o \varepsilon M$.
Then

$$d(p_o, x_o) \leqq \overline{\lim}\ d(p_\beta, x_o) = d(x_o, M),$$

i.e. $p_o \varepsilon P_M(x_o) \subset U$. Since p_β is an element of the τ-closed set $X \sim U$, we have $p_o \varepsilon X \sim U$. This contradiction shows that P_M is upper τ-metric semi-continuous. //

Since compactness implies approximative compactness we can extend theorem 0.3 to include a uniqueness condition. We also state a metric space version of theorem 3.2. It can be proved that a compact or complete semi-convex set is convex in the usual sense. The two theorems are therefore stated for convex sets.

<u>Theorem 5.3</u> Let M be a compact, convex set in a strictly convex metric space. Then M is a Chebyshev set.

<u>Theorem 5.4</u> If M is a closed convex subset of a complete sequentially convex metric space (X,d), then M is a Chebyshev set.

Proof Let $x_o \varepsilon X \sim M$ and $\alpha = d(x_o, M)$. Then $\alpha > 0$ and there is a minimizing sequence (y_n) in M. Existence and uniqueness of the proximum now follow as in the proof of theorem 3.2. //

We next show how the approximation properties of a metric space can be improved by introducing an equivalent metric. The following theorem will be needed (see Kantorowitch and Akilow [16, p.235]):

Theorem 5.5 Every separable metric space (X,d) is isometric to a subset of the space $C[0,1]$.

Proof Let $M = \{x_1, x_2, \ldots\}$ be dense in X. Define a mapping

$$U : X \to \ell_\infty : x \mapsto y = (y_1, y_2, \ldots)$$

by

$$y_j = d(x, x_j) - d(x_1 . x_j)$$

for $j = 1,2,3,\ldots$. Since

$$|y_j| = |d(x,x_j) - d(x_1, x_j)| \leqq d(x, x_1)$$

we have $y \varepsilon \ell_\infty$. Now let $U(x) = y$ and $U(x') = y'$. It is easy to see that $\|y - y'\|_\infty$

$$= \sup |y_j - y'_j| = \sup |d(x, x_j) - d(x', x_j)| \leqq d(x, x'). \quad (5.1)$$

It now follows from the definition of M that there exists $x_n \varepsilon M$ so that $d(x, x_n) \leqq \varepsilon/2$, with $0 < \varepsilon < d(x, x')$. But $d(x', x_n) \geq d(x', x) - d(x_n, x) \geq d(x', x) - \varepsilon/2 > 0$.

Hence

$$|y_n - y'_n| = d(x,x') - d(x_n,x) = |d(x_n,x') - d(x_n,x)|$$

$$\geq d(x',x_n) - \varepsilon/2 \geq d(x',x) - \varepsilon,$$

i.e. $\|y - y'\|_\infty \geq d(x,x') - \varepsilon$.

Since $\varepsilon > 0$ is arbitrary, we have

$$\|y - y'\|_\infty > d(x,x').$$

Using (5.1) we see that $\|y - y'\|_\infty = d(x,x')$, which shows that X is isometric to a subset of ℓ_∞. The linear hull of this subset is clearly separable and the result now follows from theorem 2.2. //

We are now in a position to generalize Clarkson's method to semi-convex metric spaces.

<u>Theorem 5.6</u> Let (X,d) be a separable, semi-convex metric space. Then there is a strictly convex metric d' which is equivalent to d.

<u>Proof</u> By theorem 5.5 there is an isometry $T : X \to C[0,1]$, with $d(x_1,x_2) = \|T(x_1) - T(x_2)\|_\infty$.

Now let $d'(x_1,x_2) = \|T(x_1) - T(x_2)\|_C$, where $\|\cdot\|_C$ is defined as in the proof of theorem 2.1. Then $\|\cdot\|_C$ is strictly convex and we have

$$\|x\|_\infty \leqq \|x\|_C \leqq (2/\sqrt{3})\|x\|_\infty.$$

Let $\varepsilon > 0$ be given. If $d(x_1,x_2) < \varepsilon\sqrt{3}/2$, then

$$d'(x_1,x_2) \leqq (2/\sqrt{3})d(x_1,x_2) < \varepsilon.$$

Conversely, if $d'(x_1,x_2) < \varepsilon\sqrt{3}/2$, then

$$d(x_1,x_2) \leqq d'(x_1,x_2) < \varepsilon \sqrt{3}/2 < \varepsilon,$$

i.e. d and d' are equivalent metrics.

We finally show that d' is strictly convex. Let $d'(x,x_o), d'(y,x_o) \leqq r$ and $d'(z,x_o) = r$, where z is an intermediate point of x,y. It follows from the definition of d' and the strict convexity of $\|\cdot\|_C$ that $T(x) = T(y)$. But T is injective. Hence $x = y$ and d' is strictly convex. //

Equivalent metrization can be used to make a given closed set proximinal. We require the following

<u>Lemma 5.6</u> (see Singer [22,p.391]). Let (X,d) be a metric space and M a subset of X. Then

$$|d(x,M) - d(y,M)| \leqq d(x,y)$$

for all $x,y \in X$.

<u>Proof</u> Let $x,y \in X$ and $\varepsilon > 0$. Then there exists an element $m \in M$ such that $d(y,m) \leqq d(y,M) + \varepsilon$.

Hence $d(x,M) \leqq d(x,m) \leqq d(x,y) + d(y,m)$

$$\leqq d(x,y) + d(y,M) + \varepsilon.$$

Since $\varepsilon > 0$ is arbitrary,

$$d(x,M) - d(y,M) \leqq d(x,y). \quad //$$

We now define a new metric $d_{(n)}$ by

$$d_{(n)}(x,y) = \max \{d(x,y), (1+1/n)|d(x,M) - d(y,M)|\}.$$

It is easy to see that d and $d_{(n)}$ are equivalent. First note that $d_{(n)}(x,y) \geq d(x,y)$. If

$$d(x,y) \geq (1+1/n)|d(x,M) - d(y,M)|$$

then $d_{(n)}(x,y) = d(x,y)$. But if

$$d(x,y) < (1+1/n)|d(x,M) - d(y,M)|$$

then

$$d_{(n)}(x,y) = (1+1/n)|d(x,M) - d(y,M)| \leqq (1+1/n)d(x,y)$$

by the lemma. Hence

$$d(x,y) \leqq d_{(n)}(x,y) \leqq (1+1/n)\ d(x,y),$$

i.e. d and $d_{(n)}$ are equivalent.

Now let M be a closed proper subset of X and $y \in X \sim M$. Then for any $x \in M$,

$$d_{(n)}(x,y) = \max\ \{d(x,y),\ (1+1/n)d(y,M)\} \geq$$

$$\geq (1+1/n)d(y,M) > 0.$$

If we now choose a point $m \in M$ such that

$$d(m,y) < (1+1/n)d(y,M),$$

then

$$d_{(n)}(m,y) = (1+1/n)d(y,M) = \max\{d(y,M),(1+1/n)d(y,M)\}$$

$$= \inf_{x \in M} \max\ \{d(x,y),\ (1+1/n)d(y,M)\}$$

$$= \inf_{x \in M} d_{(n)}(y,x),$$

i.e. M is proximinal. We therefore have the following

<u>Theorem 5.7</u> Let (X,d) be a metric space and M a closed

proper subset of X. Then M is proximinal with respect to the metric

$$d_{(n)}(x,y) = \max \{d(x,y),\ (1+1/n)|d(x,M) - d(y,M)|\},$$

which is equivalent to d, with

$$d(x,y) \leqq d_{(n)}(x,y) \leqq (1+1/n)d(x,y)$$

for all $x,y \in X$.

<u>Example 5.2</u> Let $X = \ell_1$, $y = (0,0,0,\ldots)$ and $M = \{x = (0, x_2, x_3, \ldots) \in \ell_1 : \sum_{n=2}^{\infty} n\, x_n /(n+1) = 1\}$. Then M is a closed convex subset of ℓ_1. Let d be the metric defined by the ℓ_1 norm. Then $d(x,0) > 1$ for all $x \in M$. Since $m_n = (0,0,\ldots,(n+1)/n,0,0,\ldots) \in M$ and
(n)

$d(m_n,0) = 1 + 1/n$, we see that $d(y,M) = 1$, i.e. M is not proximinal with respect to d. On the other hand, if $x \in M$ then

$$\begin{aligned} d_{(n)}(x,0) &= \max \{d(x,0),\ (1+1/n)d(y,M)\} \\ &= \max \{d(x,0),\ 1+1/n\}. \end{aligned}$$

If p is chosen so that $p > n$, then $d(m_p,0) = 1+1/p < 1 + 1/n$ and $d_{(n)}(m_p,0) = 1 + 1/n = d_{(n)}(y,M)$. Hence M is proximinal with respect to $d_{(n)}$. //

The example demonstrates that the proxima obtained in this way are not generally unique. Since a proximinal set is always closed we can use theorem 5.7 to characterize the closed sets in a metrizable topological space. Using the metric $d_{(1)}$, this was done by V.L.Klee [25], who also showed that if M is proximinal with respect to all equivalent metrics, then M is compact.

Chapter 6

Best Approximation in the L_p norms

The purpose of this chapter is to provide a link between the abstract material of part I of this thesis and the numerical applications of part II. We shall concentrate on L_1 and L_∞ approximation, with occasional references to the L_2 norm. Historically, the three norms date back to the early 1800s. The earliest reference to discrete L_1 and L_∞ can be found in Laplace's "Mécanique Céleste", which was published in 1799. Laplace's ideas gained a certain notoriety for arithmetic unwieldiness and were soon eclipsed by the least squares technique of Gauss and Legendre. Although the period from about 1850 to 1950 saw considerable advances in L_1 and L_∞ theory through the work of Chebyshev, Weierstrass, de la Vallée-Poussin, Banach, Jackson and others, the practical importance of these results remained somewhat limited until the arrival of electronic computers in the early 1950s. Computers created an urgent need for efficient methods of functional approximation, an area in which the L_∞ norm offers distinct advantages over other norms. At the same time, the spectacular increase in computing power revived research into a number of algorithms which had hitherto been regarded as computationally too expensive. Laplace's ideas on the solution of inconsistent linear systems as well as the algorithms of Remes belong to this category.

In subsequent chapters, frequent use will be made of an important alternation property, which characterizes polynomials of best L_∞ approximation. This property was discovered by Chebyshev in the 1850s. For a proof see Cheney [21,p.75]. We first require the following definition.

<u>Definition 6.1</u> A set of functions $\{g_1,\ldots,g_n\}$ satisfies the <u>Haar</u> <u>condition</u> if every set of vectors of the form

$$g(x_i) = (g_1(x_i),\ldots,g_n(x_i)), \quad i = 1(1)n,$$

is linearly independent for any distinct x_i, i.e. if the determinant

$$\begin{vmatrix} g_1(x_1) & \cdots & g_n(x_1) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ g_1(x_n) & \cdots & g_n(x_n) \end{vmatrix}$$

does not vanish for distinct $x_1,\ldots,x_n$. //

It is easy to show that the Haar condition holds if and only if every generalized polynomial

$$g(x) = \sum_{i=1}^{n} c_i g_i(x) \not\equiv 0$$

has at most $n-1$ distinct zeros.

<u>Theorem 6.1</u> Let $g_1,\ldots,g_n \in C[a,b]$ and $f \in C(X)$, where X is a closed subset of $[a,b]$. If $\{g_1,\ldots,g_n\}$ satisfies the Haar condition, then the generalized polynomial

$$g(x) = \sum_{i=1}^{n} c_i g_i(x)$$

is a best uniform approximant to f on X if and only if there are $n+1$ points $x_1, \ldots, x_{n+1} \in X$, with $x_1 < \ldots < x_{n+1}$, such that

$$|g(x_i) - f(x_i)| = \|g - f\|_\infty$$

and $g(x_i) - f(x_i)$ alternates in sign for $i=1,\ldots,n+1$.

In the language of chapter 1, the linear space $M = \langle g_1,\ldots,g_n \rangle$ is a finite-dimensional subspace of $C[a,b]$. It is clear from theorem 1.2 that M is proximinal. Although the L_∞ norm is not strictly convex, the polynomial approximant in theorem 6.1 is in fact unique. The function subspaces which have this uniqueness property are characterized by theorem 6.2, which is due to A.Haar [59]. The proof given below follows Achieser [12,p.67 ff.], who considers "n linearly independent real functions of the point P of a bounded closed set in ordinary space of any number of dimensions". This terminology suggests that the author refers to finite-dimensional domains, but the proof easily carries over to compact Hausdorff spaces and in particular to compact metric spaces.

<u>Theorem 6.2</u> Let $M = \langle f_1,\ldots,f_n \rangle$ be an n-dimensional subspace of $C(X)$, where X is a compact metric space. Then M is a Chebyshev subspace if and only if the set $\{f_1,\ldots,f_n\}$ satisfies the Haar condition.

<u>Proof</u> $\Rightarrow$ Suppose the Haar condition is not satisfied. Then there exist n distinct points $x_1,\ldots,x_n$ in X so that

$$\begin{vmatrix} f_1(x_1) & \dots & f_n(x_1) \\ \vdots & & \vdots \\ f_1(x_n) & \dots & f_n(x_n) \end{vmatrix} = 0 \ ,$$

and we can find scalars $a_1, \dots, a_n$ (not all zero), with $a_1 f_k(x_1) + \dots + a_n f_k(x_n) = 0$, $k=1,\dots,n$. It follows that

$$a_1 f(x_1) + \dots + a_n f(x_n) = 0 \qquad (6.1)$$

for any function f in M.

Now let

$$F(x) = b_1 f_1(x) + \dots + b_n f_n(x)$$

be a function in M with $\|F\|_\infty < 1$ and $F(x_i) = 0$. If $g \in C(X)$ with $|g(x)| \leq 1$ on X and $g(x_i) = \operatorname{sgn} a_i$ for $a_i \neq 0$ $(i=1,\dots,n)$, then the function

$$h(x) = g(x)[1 - |F(x)|]$$

satisfies

$$|h(x)| \leq 1 \quad \text{and} \quad h(x_i) = \operatorname{sgn} a_i$$

for $a_i \neq 0$ $(i=1,\dots,n)$. If for some $f \in M$, $\|h-f\|_\infty < 1$, then $\operatorname{sgn} f(x_i) = \operatorname{sgn} a_i$ for $a_i \neq 0$ $(i=1,\dots,n)$, contradicting equation (6.1). It follows that $\|h-f\|_\infty \geq 1$ for all f in M.

Conversely, let $|\varepsilon| \leq 1$. Then

$$\begin{aligned} |h(x) - \varepsilon F(x)| &\leq |h(x)| + \varepsilon |F(x)| \\ &= |g(x)| [1 - |F(x)|] + |\varepsilon F(x)| \\ &\leq 1 - |F(x)| + |\varepsilon||F(x)| \leq 1. \end{aligned}$$

Hence εF is a best approximant to h for all $|\varepsilon| \leq 1$, i.e. $P_M(h)$ is an infinite set and M is not semi-Chebyshev. //

To prove sufficiency, a number of lemmas are required. In each case the Haar condition is assumed.

Lemma 6.3 Let

$$\begin{vmatrix} f_i(x_i) & f_{i+1}(x_i) & \dots & f_k(x_i) \\ \vdots & & & \vdots \\ f_i(x_k) & f_{i+1}(x_k) & \dots & f_k(x_k) \end{vmatrix} \neq 0 \quad (1 \leq i < k < n). \tag{6.2}$$

Then for any q, $k < q \leq n$, there exist points $x_{k+1}, x_{k+2}, \dots, x_q$, such that

$$\begin{vmatrix} f_i(x_i) & f_{i+1}(x_i) & \dots & f_q(x_i) \\ \vdots & & & \vdots \\ f_i(x_q) & f_{i+1}(x_q) & \dots & f_q(x_q) \end{vmatrix} \neq 0.$$

Proof It follows from (6.2) and the Haar condition that the non-trivial generalized polynomial

$$f(x) = \begin{vmatrix} f_i(x_i) & \dots & f_k(x_i) & f_{k+1}(x_i) \\ \vdots & & \vdots & \vdots \\ f_i(x_k) & \dots & f_k(x_k) & f_{k+1}(x_k) \\ f_i(x) & \dots & f_k(x) & f_{k+1}(x) \end{vmatrix}$$

has at most $n-1$ zeros. Hence there is a point x_{k+1} such that $f(x_{k+1}) \neq 0$. //

Lemma 6.4 If $x_1, \dots, x_k$ $(k<n)$ are distinct points, then the matrix

$$\begin{pmatrix} f_1(x_1) & \dots & f_n(x_1) \\ \vdots & & \vdots \\ f_1(x_k) & \dots & f_n(x_k) \end{pmatrix}$$

has at least one non-zero minor of order k.

<u>Proof</u> We first prove the result for $k=1$. If $f_i(x_1) = 0$ for $i=1,\dots,n$, choose y_2 such that $f_2(y_2) \neq 0$ and use lemma 6.3 to determine $y_3,\dots,y_n$ such that

$$\begin{vmatrix} f_2(y_2) & \dots & f_n(y_2) \\ \vdots & & \vdots \\ f_2(y_n) & \dots & f_n(y_n) \end{vmatrix} \neq 0 .$$

Then

$$\begin{vmatrix} f_1(x) & f_2(x) & \dots & f_n(x) \\ f_1(y_2) & f_2(y_2) & \dots & f_n(y_2) \\ \vdots & & & \vdots \\ f_1(y_n) & f_2(y_n) & \dots & f_n(y_n) \end{vmatrix}$$

has n distinct zeros $x_1, y_2,\dots,y_n$ which contradicts the Haar condition. Hence $f_i(x_1) \neq 0$ for some i, $1 \leqq i \leqq n$.

Next suppose the lemma is true for $k=1,\dots,m-1$.

W.ℓ.o.g. we assume

$$\begin{vmatrix} f_2(x_2) & \dots & f_m(x_2) \\ \vdots & & \vdots \\ f_2(x_m) & \dots & f_m(x_m) \end{vmatrix} \neq 0 .$$

By the previous lemma we can find points $y_{m+1},\dots,y_n$ such that

$$\begin{vmatrix} f_2(x_2) & \dots & f_n(x_2) \\ \vdots & & \vdots \\ f_2(y_n) & \dots & f_n(y_n) \end{vmatrix} \neq 0 .$$

If the assertion was false, then

$$\begin{vmatrix} f_1(x) & \cdots & f_n(x) \\ f_1(x_2) & \cdots & f_n(x_2) \\ \vdots & & \vdots \\ f_1(y_n) & \cdots & f_n(y_n) \end{vmatrix}$$

would be a non-trivial polynomial with n zeros $x_1,\ldots,x_m, y_{m+1},\ldots,y_n$, which contradicts the Haar condition. //

<u>Lemma 6.5</u> Let $F(x) = \alpha_1 f_1(x) + \ldots + \alpha_n f_n(x)$ be a function in M and $f \in C(X)$.

If $|f(x) - F(x)| = \|f(x) - F(x)\|_\infty$ (6.3)

for fewer than n values of x, then $F \notin P_M(f)$.

<u>Proof</u> Suppose $x_1,\ldots,x_m$ $(m < n)$ are distinct points in X for which (6.3) holds. Then by lemma 6.4 we can solve the underdetermined system

$$\beta_1 f_n(x_k) + \ldots + \beta_n f_n(x_k) = f(x_k) - F(x_k)$$

$(k=1,\ldots,m)$ for $\beta_1,\ldots,\beta_n$.

Let

$$G(x) = \beta_1 f_1(x) + \ldots + \beta_n f_n(x)$$

and

$$r(x) = f(x) - F(x).$$

For each $x_k (k=1,\ldots,m)$, choose a closed neighbourhood N_k such that

$$\mu_k(F) = \min_{x \in N_k} |r(x)| > 0 \quad \text{and} \quad \min_{x \in N_k} |G(x)| \geq \|f-F\|_\infty/2.$$

Next suppose that $M_k = \max_{x\varepsilon N_k}|G(x)|$, $M = \max_{x\varepsilon N^*}|G(x)|$,

and $L^*(F) = \max_{x\varepsilon N^*}|r(x)|$, where $N^* = X \sim N_1 \sim \dots \sim N_M$.

Clearly,

$$\mu = \mu(F) = \max_{x\varepsilon X}|r(x)| - \max_{x\varepsilon N^*}|r(x)| > 0 \ .$$

Now choose ε such that

$$0 < \varepsilon < \min\ (\mu/M,\ \mu_1/M_1,\dots,\mu_m/M_m).$$

Put

$$\gamma_i = \alpha_i + \varepsilon\beta_i \quad (i=1,\dots,n)$$

and

$$H(x) = \gamma_1 f_1(x) + \dots + \gamma_n f_n(x).$$

Then

$$|f(x) - H(x)| = |f(x) - F(x) - \varepsilon\ G(x)| = |r(x) - \varepsilon G(x)|.$$

Hence

$$\begin{aligned}|f(x) - H(x)| &\leqq |r(x)|(1 - \varepsilon|G(x)/r(x)|)\\ &\leqq ||f-F||_\infty\ (1 - \varepsilon/2)\end{aligned}$$

whenever $x \varepsilon N_k$ $(k=1,\dots,m)$, and

$$\begin{aligned}|f(x) - H(x)| &\leqq |r(x)| + \varepsilon|G(x)| \leqq L^*(F) + \varepsilon M\\ &< ||f-F||_\infty\end{aligned}$$

whenever $x\ \varepsilon N^*$. We therefore have

$$||f-H||_\infty = \max_{x\varepsilon X}|f(x) - H(x)| < ||f-F||_\infty. \quad //$$

We can now prove the sufficiency of the Haar condition.

<u>Proof</u> $\Leftarrow$ Suppose $F(x) = \alpha_1 f_1(x) + \dots + \alpha_n f_n(x)$ and $G(x) = \beta_1 f_1(x) + \dots + \beta_n f_n(x)\ \varepsilon\ P_M(f)$. Since

$$|\tfrac{1}{2}(F+G) - f| \leqq \tfrac{1}{2}|F - f| + \tfrac{1}{2}|G - f|,$$

we also have $\frac{1}{2}(F+G) \varepsilon P_M(f)$. By lemma 6.5, the equation

$$|f(x) - [F(x) + G(x)]/2| = L$$

has at least n zeros $x_1,\ldots,x_n \varepsilon X$, where

$$L = \|(F+G)/2 - f\|_\infty = \|F - f\|_\infty = \|G - f\|_\infty.$$

But for $|f(x_i) - [F(x_i) + G(x_i)]/2|$ to equal L, it is necessary that

$$f(x_i) - F(x_i) = f(x_i) - G(x_i) = \pm L.$$

It follows that the non-trivial polynomial $(\alpha_1 - \beta_1) f_1(x) + \ldots + (\alpha_n - \beta_n) f_n(x)$ has n distinct zeros, which proves the sufficiency of the Haar condition. //

Although theorem 6.2 is a result about functions defined on a compact Hausdorff space, its practical importance is restricted to the single variable case, because functions of several variables do not in general satisfy the Haar condition. This can be established by the following simple argument (see A.Haar [59,p.311]). Suppose the function

$$g(x) = \sum_{i=1}^{n} \lambda_i g_i(x) \not\equiv 0$$

satisfies the Haar condition on the unit square $X = [0,1]^2$. Then there exist at most $n-1$ distinct points $x_j \varepsilon X$ such that $\sum \lambda_i g_i(x_j) = 0$. It follows that, if $\sum_{i=1}^{n} \lambda_i g_i(x_j) = 0, j = 1(1)n$, holds for n distinct points, then $\lambda_i = 0$, i.e.

$$\begin{vmatrix} g_1(x_1) & \cdots & g_n(x_1) \\ \vdots & & \vdots \\ g_1(x_n) & \cdots & g_n(x_n) \end{vmatrix} \neq 0.$$

If we now interchange x_1 and x_2, say, keeping all x_j distinct in the process, then the above determinant changes its sign and therefore must equal zero for some position of x_1 and x_2, contradicting the Haar condition.

A characterization of the set X was first given by Mairhuber [60] in 1956. Similar results hold for $C(X)$ when X is a compact Hausdorff space and for $C_o(X)$ when X is a locally compact Hausdorff space (see Phelps [17] and Lutts [65]).

<u>Theorem 6.4</u> (Mairhuber) Let $g_1,\ldots,g_n \in C(X)$, where X is a compact subset of R^k, containing at least n points $(n \geq 2)$. Then the set $\{g_1,\ldots,g_n\}$ satisfies the Haar condition if and only if X is homeomorphic to a closed subset of the circumference of a circle.

The alternation property of theorem 6.1 also characterizes discrete best approximants. Discrete and continuous Chebyshev approximation are usually treated as separate topics, each with its own existence, uniqueness, and characterization theorems. (See for example chapters 2 and 3 in Cheney [21] or Watson [66].) However, it is possible to develop a unified theory in which discrete approximation is regarded as a special case of continuous approximation. We give a brief outline of such a theory.

Let $X = \{x_1,\dots,x_m\} = \{1,\dots,m\}$. Define a function $f : X \to R$ by

$$f(x_i) = a_i. \qquad i=1(1)m.$$

If X is given the discrete topology, then each singleton set $\{x_i\}$ is open, i.e. f is continuous. This topology is induced by the discrete metric d defined by

$$d(x,y) = \begin{cases} 0 & \text{if} \quad x = y \\ 1 & \text{if} \quad x \neq y. \end{cases}$$

It is clear that (X, d) is a compact metric space and $C(X) = R^m$.

Let $f, f_1,\dots,f_n \in C(X)$. We can write

$$f = (a_1,\dots,a_m)^T , \quad f_i = (a_1^i,\dots,a_m^i)^T ,$$

i.e. $\quad f(k) = a_k, \qquad f_i(k) = a_k^i$

for $k=1,\dots,m$. The Haar condition demands that for any n distinct points $x_i = k_i$ in X, where $i=1,\dots,n$ and $1 \leq k_i \leq m$, the vectors

$$(f_1(x_i),\dots,f_n(x_i)) = (a_{k_i}^1,\dots,a_{k_i}^n)$$

are linearly independent. Denote the $m \times n$ matrix $(f_1,\dots,f_n)$ by A. The Haar condition can then be expressed by saying that every $n \times n$ submatrix of A is non-singular. We retain the equivalent definition that any generalized polynomial

$$\sum_{i=1}^{n} \alpha_i f_i \not\equiv 0$$

has at most $n-1$ zeros in X. Clearly, $\{f_1,\dots,f_n\}$ always satisfies the Haar condition if $m < n$.

The problem of determining $\alpha = (\alpha_1, \ldots, \alpha_n)^T$ so that

$$\|A\alpha - b\|_\infty = \min! \ ,$$

where A is a given mxn matrix, can now be interpreted as a problem of continuous approximation. If we identify A with $(f_1, \ldots, f_n)$ and b with f, we require

$$\|\sum_{i=1}^{n} \alpha_i f_i - f\|_\infty = \min \ !$$

<u>Example 6.1</u> Find the minimax solution of the system

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \\ 8 \end{pmatrix}$$

we have $m=3$, $n=2$, $X = \{1,2,3\}$. The matrix A satisfies the Haar condition and

$$\|\alpha_1(1,1,2)^T + \alpha_2(-1,1,1)^T - (2,4,8)^T\|_\infty$$

is a minimum for the unique solution $(\alpha_1, \alpha_2) = (10/3, 1)$. Note that

$$g(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x)$$

has only one zero in X. We find

$$f(1) = \alpha_1 - \alpha_2 = 0 \quad \text{for } \alpha_1 = \alpha_2.$$

But $\quad f(2) = \alpha_1 + \alpha_2 \neq 0$

and $\quad f(3) = 2\alpha_1 + \alpha_2 \neq 0.$ //

<u>Example 6.2</u> An example in Watson [66,p.33] is intended to show that a linear system can have a (strongly) unique solution when the Haar condition is not satisfied. However, the system

$$\begin{pmatrix}1\\0\end{pmatrix} \alpha = \begin{pmatrix}0\\0\end{pmatrix}$$

is equivalent to $1.\alpha = 0$, i.e. the Haar condition is satisfied and the solution is unique.

Example 6.3 Solve $\alpha_1 + 3\alpha_2 = 6$ in the minimax sense. This is an underdetermined system, with $m=1$, $n=2$, $X=\{1,2\}$. The Haar condition is satisfied, and we have $\|\alpha_1 + 3\alpha_2 - 6\|_\infty = 0$ for $(\alpha_1,\alpha_2) = (\alpha_1, 2-\alpha_1/3)$ and any α_1. The unique element of M is

$$\alpha_1 f_1 + \alpha_2 f_2 = \alpha_1 . 1 + (2-\alpha_1/3).3 = 6 = f \in M,$$

i.e. the approximated function coincides with the approximant. //

Note that the word "solution" can denote the vector α or the generalized polynomial $\sum \alpha_i f_i$. By theorem 6.2, the latter is unique if and only if A satisfies the Haar condition. For uniqueness of the former, the Haar condition is necessary but, as example 6.3 demonstrates, not sufficient. To clarify the situation, we distinguish between consistent and inconsistent systems. $A\alpha = b$ is consistent if and only if b lies in the linear span of the columns f_i of A, i.e. if and only if $f \in M$. A consistent system has a unique solution α if and only if the columns of A are linearly independent. For an inconsistent system, the minimax solution α is unique if and only if A satisfies the Haar condition.

We now show that the characterization theorem for the minimax solution of $A\alpha = b$ can be deduced from the corresponding continuous result. In the literature, these theorems are usually treated independently of each other, with separate proofs for the continuous and discrete case (see for example Cheney [21,pp.35 and 73]).

<u>Theorem 6.5</u> (Continuous Characterization Theorem)

Let $f, f_1, \ldots, f_n \in C(X)$, where X is a compact metric space. $\|\sum_{i=1}^{n} \alpha_i f_i - f\|_\infty$ is a minimum if and only if

$$\underline{0} \in H\{r(x)(f_1(x), \ldots, f_n(x)) : |r(x)| = \|r\|_\infty\}$$

where $r(x) = \sum_{i=1}^{n} \alpha_i f_i(x) - f(x)$ and H denotes the convex hull of a set.

To obtain the discrete version, let

$$M = \{x \in K : |r(x)| = \|r\|_\infty\} ,$$

where $X = \{1, \ldots, m\}$. If $x=j$, $1 \leq j \leq m$, then

$$(f_1(x), \ldots, f_n(x)) = (a_j^1, \ldots, a_j^n) = A^j ,$$

the jth row of A, i.e. the necessary and sufficient condition becomes

$$\underline{0} \in H\{r(j)A^j : j \in M\}.$$

Let $\sigma_j = \operatorname{sgn} r(j)$. Then there exist numbers $\theta_j \geq 0$ such that $\sum_{j \in M} \theta_j = 1$ and

$$\underline{0} = \sum_{j \in M} \theta_j r(j) A^j = \sum_{j \in M} \theta_j \sigma_j r(j) \sigma_j A^j.$$

Put $\sum_{j\varepsilon M} \theta_j \sigma_j\, r(j) = k$. Then

$$\underline{0} = \sum_{j\varepsilon M} \phi_j \sigma_j A^j,$$

where $\phi_j = \theta_j \sigma_j\, r(j)/k \geq 0$ and $\sum_{j\varepsilon M} \phi_j = 1$.

Hence $\underline{0} \;\varepsilon\; H\{\sigma_j A^j : j \;\varepsilon\; M\}$ and we obtain

<u>Theorem 6.6</u> (Discrete Characterization Theorem)

Let $\alpha = (\alpha_1,\ldots,\alpha_n)^T$. $||A\alpha - b||_\infty$ is a minimum if and only if

$$\underline{0} \;\varepsilon\; H\{\sigma_j A^j : j \;\varepsilon\; M\},$$

where $M = \{j : |r_j(\alpha)| = ||A\alpha - b||_\infty\}$ and A^j is the jth row of A.

The next result is usually stated as a theorem about inconsistent systems of equations (see Cheney [21,p.36]).

<u>Theorem 6.7</u> Let $g(x) = \sum_{i=1}^{n} c_i g_i(x)$ be a best Chebyshev approximation to f on a compact metric space X. Then there exists a finite subset X_o of X, containing at most n+1 points such that g is a best Chebyshev approximation to f on X_o. If, in addition, $\{g_1,\ldots,g_n\}$ satisfies the Haar condition, then X_o contains exactly n+1 points.

<u>Proof</u> By theorem 6.5, $\underline{0} \;\varepsilon\; H(S)$, where $S = \{r(x)(g_1(x),\ldots,g_n(x)) : |r(x)| = ||r||_\infty\}$. It now follows from Carathéodory's theorem (see Cheney [21,p.17]) that we can find (at most) n+1 points, $x_1,\ldots,x_k \;\varepsilon\; X$

$(k \leq n+1)$, so that $\underline{0} = \sum_{i=1}^{k} \theta_i r(x_i)(g_1(x_i),\ldots,g_n(x_i))$ for some $\theta_i \geq 0$ and $\sum\theta_i = 1$. Hence

$\underline{0} \in H\{r(x_i)(g_1(x_i),\ldots,g_n(x_i)) : |r(x_i)| = \|r\|_\infty,\ i=1(1)k\}$.

The result now follows, using theorem 6.5 in the opposite direction. If $\{g_1,\ldots,g_n\}$ satisfies the Haar condition, we require $k \geq n+1$, i.e. $k=n+1$. //

It is clear from our previous discussion that theorem 6.7 covers inconsistent systems of equations. Thus if $\alpha = (\alpha_1,\ldots,\alpha_n)^T$ is a minimax solution of the over-determined $m\times n$ system $A\alpha = b$, then α is a minimax solution of a subsystem comprising at most $n+1$ equations. The subsystem has exactly $n+1$ equations if A satisfies the Haar condition. We finally obtain a discrete version of the alternation property (theorem 6.1), which also applies to $A\alpha = b$. In view of theorem 6.7 we shall assume that X contains $n+1$ points.

<u>Theorem 6.8</u> Let $f, g_1,\ldots,g_n \in C(X)$, where $X = \{x_0,\ldots,x_n\}$ is a set of $n+1$ points in $[a,b]$. If $\{g_1,\ldots,g_n\}$ satisfies the Haar condition, then

$$g(x) = \sum_{i=1}^{n} c_i g_i(x)$$

is a best uniform approximant to f if and only if there is an ordering $x_{k_1} < \ldots < x_{k_{n+1}}$ of the points of X so that

$$|g(x_{k_i}) - f(x_{k_i})| = \|g-f\|_\infty$$

and $g(x_{k_i}) - f(x_{k_i})$ alternates in sign for $i=1,\ldots,n+1$.

<u>Proof</u> Let $g = (b_1,\ldots,b_{n+1})^T$, $g(x_{k_i}) = b_i$, $i=1\ldots,n+1$. Let $G(x) = a_o + a_1 x + \ldots + a_n x^n$ be the interpolating polynomial of degree n for the points (x_{k_i}, b_i), $i=1,\ldots,n+1$. Then $g = G$ on X and g is a best approximant to f on X if and only if G is. The result now follows from theorem 6.1. //

The algorithm of chapter 7 is based on the fact that the error components of the best L_∞ approximant agree in sign with those of the L_2 approximation. More precisely, we have the result stated below. First recall that a norm $\|\cdot\|$ on R^n is called <u>monotone</u> if

$$|x_i| \leqq |y_i| \ (i=1,\ldots,n) \quad \text{implies} \quad \|x\| \leqq \|y\|.$$

All L_p norms $(1 \leqq p \leqq \infty)$ are monotone.

<u>Theorem 6.9</u> The points of a hyperplane H in R^n which minimize two monotone norms have components of equal sign.

<u>Proof</u> See Cheney [21,p.40].

The following method of selecting a unique best of all best (or "strict") Chebyshev approximations is due to J.R.Rice [42]. Disregarding the $n+1$ components r_i of equal maximal magnitude $\|r\|_\infty$, the maximum error of the remaining components is minimized. If necessary, the process is repeated.

<u>Example 6.4</u> The minimax solution of the system

$$x_2 = 0$$

$$x_2 = 1$$

$$x_1 + x_2 = 0$$

are given by $(x_1,x_2) = (\lambda,\frac{1}{2})$, $\lambda \varepsilon [-1,0]$, i.e. $r_1 = 1/2$, $r_2 = -1/2$, $r_3 = \lambda + 1/2$. Since $|r_3|$ is minimal for $\lambda = -1/2$, $(x_1,x_2) = (-1/2,1/2)$ is the required strict solution. //

It was proved by J.Déscloux [60] that the strict approximation is the limit of the best L_p approximation as $p \to \infty$ (Pólya's algorithm). A limitation of Rice's definition is that it only applies to finite point sets. Chapter 9 contains a definition of strict L_1 approximation which can be extended to intervals. In this context, some results of discrete L_1 approximation are required. The treatment below draws on material in the book by J.R.Rice [58, vol.I]; the proofs of lemmas 6.10 and 6.11 follow the line of reasoning used by Rice to establish the corresponding interval results.

Consider the following problem. The data points $(x_i, f(x_i))$, $i=1(1)m$, are to be approximated in the L_1 norm by a function of the form

$$L(A,x) = \sum_{i=1}^{n} a_i\phi_i(x),$$

where A denotes the unknown parameters $(a_1,...,a_n)$.

I.e. we wish to minimize the function

$$\Delta_1(f,x) = \sum_{i=1}^{m} |f(x_i) - L(A,x_i)|,$$

which is equivalent to selecting a point $(a_1,\ldots,a_n,d)$ from the set

$$K = \{(A,d) \in R^{n+1} : \Delta_1(f,A) \leqq d\},$$

so that d is minimal. It is easy to see that K is convex : if (A_1,d_1), $(A_2,d_2) \in K$ and $\lambda,\mu \geq 0$, with $\lambda + \mu = 1$, then

$$\Delta_1(f,\lambda A_1 + \mu A_2) = \sum_{i=1}^{m} |f(x_i) - L(\lambda A_1 + \mu A_2,x_i)|$$

$$= \sum_{i=1}^{m} |(\lambda + \mu)f(x_i) - \lambda L(A_1,x_i) - \mu L(A_2,x_i)|$$

$$\leqq \lambda \sum_{i=1}^{m} |f(x_i) - L(A_1,x_i)| + \mu \sum_{i=1}^{m} |f(x_i) - \mu(A_2,x_i)|$$

$$\leqq \lambda d_1 + \mu d_2, \text{i.e. } \lambda(A_1,d_1) + \mu(A_2,d_2) \in K.$$

We now define a plane H in R^{n+1} by

$$H(g(x_i), a) = \{(A,d) : \sum_{i=1}^{m} L(A,x_i)g(x_i) = a - d\},$$

where a is the distance of H from the origin. Then

$$n = (\sum_{i=1}^{m} \phi_1(x_i)g(x_i),\ldots, \sum_{i=1}^{m} \phi_n(x_i)g(x_i),1)$$

is a vector perpendicular to H, since

$$(a_1,\ldots,a_n,d).n = \sum_{i=1}^{m} L(A,x_i)g(x_i) + d = a,$$

where "." denotes the inner product in R^{n+1} and $(a_1,\ldots,a_n,d)$ is any point in H. H is called a <u>plane of support</u> of K at the boundary point (A_o,d_o) of K, if

$(A_o, d_o) \varepsilon H$ and H divides R^{n+1} into two halfspaces H^+ and H^-, with $K \subset H^+$ and

$$H^+ = \{(A,d) : \sum_{i=1}^{m} L(A,x_i)g(x_i) \geq a-d\}.$$

<u>Lemma 6.10</u> Let (A_o, d_o) be any point on the boundary of K, i.e.

$$\sum_{i=1}^{m} |L(A_o,x_i) - f(x_i)| = d_o.$$

Then $H(s(x_i), a_f)$ is a plane of support of K at (A_o, d_o), where

$$s(x_i) = \operatorname{sgn}[f(x_i) - L(A_o,x_i)] \tag{6.6}$$

$$\text{and} \quad a_f = \sum_{i=1}^{m} f(x_i)s(x_i).$$

<u>Proof</u> Since $d_o = \sum_{i=1}^{m} |f(x_i) - L(A_o,x_i)|$

$= \sum_{i=1}^{m} [f(x_i) - L(A_o,x_i)]s(x_i)$, we have

$$L(A_o,x_i)s(x_i) = a_f - d_o,$$

i.e. $(A_o, d_o) \varepsilon H(s(x_i), a_f)$. To show that $K \subset H^+(s(x_i), a_f)$, note that, if $(A,d) \varepsilon K$, then

$$d \geq \Delta_1(f,A) = \sum_{i=1}^{m} |L(A,x_i) - f(x_i)|$$

$$= \sum_{i=1}^{m} [f(x_i) - L(A,x_i)]\operatorname{sgn}[f(x_i) - L(A,x_i)]$$

$$\geq \sum_{i=1}^{m} [f(x_i) - L(A,x_i)]s(x_i)$$

$$= a_f - \sum_{i=1}^{m} L(A,x_i)s(x_i).$$

Hence

$$\sum_{i=1}^{m} L(A,x_i)s(x_i) \geq a_f - d,$$

i.e. $(A,d) \varepsilon H^+ (s(x_i), a_f)$. //

In the following discussion, the assumption is made that for all x_i there exists an L, such that $L(A,x_i) \neq 0$. We define the sets

$X = \{x_1,\ldots,x_m\}$,

$X_o = \{x_i \varepsilon X : \phi_j(x_i) = 0,\ j=1(1)n\}$,

$X_1 = X \sim X_o$,

$Z(A) = \{x_i \ \varepsilon\ X : f(x_i) - L(A,x_i) = 0\}$,

$Z_o(A) = \{x_i \ \varepsilon\ X_1 : f(x_i) - L(A,x_i) = 0\}$.

The number of elements in any subset S of X will be denoted by $\nu(S)$.

Lemma 6.11

$$\Delta_1(f,A^*) \leqq \Delta_1(f,A^* + tA), \quad \text{for all} \quad t, \tag{6.7}$$

if and only if

$$\left| \sum_X L(A,x_i)\operatorname{sgn}[f(x_i) - L(A^*,x_i)]\right| \leqq \sum_{Z_o(A^*)} | L(A,x_i)|. \tag{6.8}$$

Inequality (6.7) is strict for all $t \neq 0$, if inequality (6.8) is.

Proof $\Leftarrow$ Let $s(x_i) = \operatorname{sgn}[f(x_i) - L(A^*,x_i)]$ and $s_t(x_i) = \operatorname{sgn}[f(x_i) - L(A^*,x_i) - tL(A,x_i)]$. Then

$\Delta_1(f,A^* + tA) - \Delta_1(f,A^*)$

$$= \sum_X [f(x_i) - L(A^*,x_i) - tL(A,x_i)]\, s_t(x_i)$$

$$- \sum_X [f(x_i) - L(A^*,x_i)]\, s(x_i)$$

$$= \sum_{Z_o(A^*)} |tL(A,x_i)| - \sum_{X_1 \sim Z_o(A^*)} [tL(A,x_i)]\, s(x_i)$$

$$+ \sum_{X_1 \sim Z_o(A^*)} |f(x_i) - L(A^*,x_i) - tL(A,x_i)|$$

$$- \sum_{X_1 \sim Z_o(A^*)} [f(x_i) - L(A^*,x_i) - tL(A,x_i)]\, s(x_i) \quad (6.9)$$

The first difference on the R.H.S. of (6.9) is non-negative because of (6.8), the second difference is non-negative by definition of $s(x_i)$, which proves inequality (6.7).

$\Longrightarrow$ Suppose (6.8) is false. Then

$$\left| \sum_X L(A,x_i)\operatorname{sgn}[f(x_i) - L(A^*,x_i)] \right| > \sum_{Z_o(A^*)} |L(A,x_i)|. \quad (6.10)$$

Let $E_\varepsilon = \{x_i \varepsilon X_1 : |f(x_i) - L(A^*,x_i)|\} \leq \varepsilon$. Taking $\varepsilon = tK$, we obtain $\Delta_1(f,A^* + tA) - \Delta_1(f,A^*)$

$$= - \sum_X [tL(A,x_i)]\, s(x_i) + \sum_{Z_o(A^*)} |tL(A,x_i)|$$

$$+ \sum_{E_\varepsilon \sim Z_o(A^*)} [f(x_i) - L(A^*,x_i) - tL(A,x_i)]\, [s_t(x_i) - s(x_i)], \quad (6.11)$$

where $K = \max_X |L(A,x_i)|$.

If $x_i \varepsilon E_\varepsilon \sim Z_o(A^*)$, then

$|f(x_i) - L(A^*,x_i) - tL(A,x_i)| \leq 3\varepsilon/2 = 3tK/2$,

i.e. the absolute value of the third $\sum$-term on the R.H.S. of (6.11) is bounded by $(3/2)tK\nu(E_\varepsilon \sim Z_o(A^*))$.

Hence $\Delta_1(f, A^* + tA) - \Delta_1(f, A^*)$

$$= |t| \sum_{Z_o(A^*)} |L(A, x_i)| - t \sum_X L(A, x_i)s(x_i) + o(t) \qquad (6.12)$$

If t and $\sum_X L(A, x_i)s(x_i)$ have the same sign, it follows from (6.10) that the R.H.S. of (6.12) is negative for some small t, contradicting (6.7). //

<u>Theorem 6.12</u> $L(A^*, x)$ is a best L_1 approximation to $f(x)$ on $X = \{x_1, \ldots, x_m\}$ if and only if

$$\left|\sum_X L(A, x_i)\,\mathrm{sgn}[f(x_i) - L(A^*, x_i)]\right| \le \sum_{Z(A^*)} |L(A, x_i)|$$

for all A. (6.13)

$L(A^*, x)$ is unique if inequality (6.13) is strict.

Theorem 6.12 follows immediately from the preceding lemma. We are now in a position to prove the main result of this section.

<u>Remark</u> Let K be a convex set. Recall that a point k in K is said to be an <u>extreme point</u> of K if it cannot be expressed as a convex combination of two other points in K.

<u>Theorem 6.13</u> Let $\{\phi_1(x), \ldots, \phi_n(x)\}$ satisfy the Haar condition. Then the set $P_M(f)$ of best L_1 approximants from $M = \langle\phi_1, \ldots, \phi_n\rangle$ to f on $X = \{x_1, \ldots, x_m\}$ is a closed convex set. The extreme points of $P_M(f)$ are the best L_1 approximants to f for which $\nu(Z(A^*)) \ge n$.

<u>Proof</u> Let $L(A_1, x), L(A_2, x) \in P_M(f)$, $\alpha + \beta = 1$ and $\alpha, \beta \ge 0$.

Then $\sum_X |f(x_i) - L(\alpha A_1 + \beta A_2, x_i)| \le$

$$\alpha \sum_X |f(x_i) - L(A_1, x_i)| + \beta \sum_X |f(x_i) - L(A_2, x_i)|,$$

which shows that $P_M(f)$ is convex. If $\lim A_k = A_o$, then by the continuity of $L(A_k, x)$ and of the L_1 norm,

$$\lim_k \sum_X |f(x_i) - L(A_k, x_i)| = \sum_X |f(x_i) - L(A_o, x_i)|,$$

which shows that $P_M(f)$ if closed. To prove the second part of the theorem, suppose $\nu(Z(A^*)) = k < n$. By the Haar condition, there exists an approximant L such that $L(A_o, x_i) = 0$ for $x_i \varepsilon\ Z(A^*)$. Let

$$M = \max_X |L(A_o, x_i)| \text{ and}$$

$$\varepsilon = \min_{X \sim Z(A^*)} (|f(x_i) - L(A^*, x_i)|).$$

If $|t| < \varepsilon/(2M)$, then

$$\operatorname{sgn}[f(x) - L(A^* + tA_o, x)] = \operatorname{sgn}[f(x) - L(A^*, x)]. \quad (6.14)$$

It now follows from theorem 6.12 that, if $L(A^*, x)\ \varepsilon\ P_M(f)$, then (6.13) is satisfied. Using (6.14), we replace $\operatorname{sgn}[f(x) - L(A^*, x)]$ in (6.13) by $\operatorname{sgn}[f(x) - L(A^* + tA_o, x)]$ and deduce that $L(A^* + tA_o, x)\ \varepsilon\ P_M(f)$. We similarly show that $L(A^* - tA_o, x)\ \varepsilon\ P_M(f)$. Since

$$L(A^*, x) = \tfrac{1}{2}L(A^* + tA_o, x) + \tfrac{1}{2}L(A^* - tA_o, x),$$

$L(A^*, x)$ is not an extreme point of $P_M(f)$. //

We restate theorem 6.13 in a form which will be used in chapter 9.

Corollary 6.13 The set $P_M(f)$ of theorem 6.13 is the convex hull of best approximations which interpolate f in at least n points of X.

In particular, the parameters a and b of a best linear L_1 approximation $ax+b$ to m data points (x_i, y_i), $i=1(1)m$, form a two-dimensional set whose extreme points interpolate the data in at least two points.

As might be expected from the convexity properties of the L_1 norm, best L_1 approximants are not necessarily unique, but uniqueness can be guaranteed by imposing additional conditions either on the norm or the approximating functions. Uniqueness via the first method is the subject of chapter 9. It is not known whether the second method is feasible in the discrete case. As for interval approximation, the hypothesis which guarantees uniqueness of best L_∞ approximants also works for L_1 approximants. This result was proved by D.Jackson [61] in 1921, three years after the publication by Haar of the corresponding L_∞ result. The proof given below follows E.W.Cheney [62].

Lemma 6.14 Let $r, g \in C[a,b]$. If r has a finite number of zeros in $[a,b]$ and

$$\int_a^b g(x) \operatorname{sgn} r(x)\,dx \neq 0,$$

then there exists a real number λ such that

$$\int_a^b |r(x) - \lambda\, g(x)|\,dx < \int_a^b |r(x)|\,dx.$$

Proof Let $x_1, \ldots, x_k \in (a,b)$ be zeros of r. Choose $\varepsilon > 0$ sufficiently small so that

$$I = [a+\varepsilon, x_1 - \varepsilon] \cup \ldots \cup [x_k + \varepsilon, b - \varepsilon]$$

consists of $k+1$ disjoint closed intervals. Let $J = [a,b] \sim I$ and assume w.l.o.g. that $\int_a^b g \operatorname{sgn} r > 0$. For $\varepsilon > 0$ sufficiently small,

$$\int_I g \operatorname{sgn} r \, dx > \int_J |g| \, dx. \tag{6.15}$$

Since I is closed and contains no zeros of r,

$$\delta = \min_{x \in I} |r(x)| > 0.$$

If $M = \max_{a \leq x \leq b} |g(x)|$ and $0 < \lambda < \delta/M$, then

$$|\lambda g(x)| < \delta \leqq |r(x)| \quad \text{for all} \quad x \in I.$$

Now let $x \in I$. If $r(x) > 0$, then $\lambda|g(x)| < r(x)$,

i.e. $0 < r(x) - \lambda g(x)$.

If $r(x) < 0$, then $\lambda|g(x)| < -r(x)$,

i.e. $r(x) - \lambda g(x) < 0$.

Hence $\operatorname{sgn}[r(x) - \lambda g(x)] = \operatorname{sgn} r(x)$ for all $x \in I$.

It follows that

$$\int_a^b |r - \lambda g| dx$$

$$= \int_I (r - \lambda g) \operatorname{sgn} r \, dx + \int_J |r - \lambda g| dx$$

$$= \int_I |r| dx - \lambda \int_I g \operatorname{sgn} r \, dx + \int_J |r - \lambda g| dx$$

$$= \int_a^b |r| dx - \lambda \int_I g \operatorname{sgn} r \, dx - \int_J |r| dx + \int_J |r - \lambda g| dx$$

$$= \int_J (|r - \lambda g| - |r|) dx + \int_a^b |r| dx - \lambda \int_I g \operatorname{sgn} r \, dx$$

$$\leq \lambda \int_J |g|\,dx + \int_a^b |r|\,dx - \lambda \int_I g \operatorname{sgn} r\,dx$$

$$< \int_a^b |r|\,dx, \quad \text{by (6.15).} \quad //$$

Theorem 6.15 Let $M = \langle f_1, \ldots, f_n \rangle$ be an n-dimensional subspace of $C[a,b]$. If M satisfies the Haar condition, then it is a Chebyshev subspace.

Proof In view of theorem 1.2, we only have to prove that M is semi-Chebyshev. Suppose g_1, g_2 are two best approximants to $f \in C[a,b]$. Since $P_M(f)$ is convex, $g_o = (g_1 + g_2)/2$ is also a best approximant.

Hence

$$\int (|f - g_o| - |f - g_1|/2 - |f - g_2|/2)\,dx = 0.$$

Since the integrand is non-positive and continuous on $[a,b]$ it must equal the zero function,

i.e. $|f - g_o| = |f - g_1|/2 + |f - g_2|/2.$

If $f - g_o$ has m zeros, with $m \geq n$, then $f - g_1$, $f - g_2$ and $g_1 - g_2$ have the same m zeros. Hence $g_1 = g_2$ by the Haar condition.

Now suppose $r = f - g_o$ has at most $n-1$ zeros. These will be a subset of the $n+1$ points $a = x_o < x_1 < \ldots < x_n = b$. Take any $g = \sum \alpha_i f_i \in M$ and let $\int_{x_{i-1}}^{x_i} g\,dx = \phi_i(g)$. Then for suitably chosen $\sigma_i = 0$ or ± 1,

$$\int_a^b g \operatorname{sgn} r\,dx = \sum_{i=1}^n \sigma_i \int_{x_{i-1}}^{x_i} g\,dx = \sum_{i=1}^n \sigma_i \phi_i(g) = 0.$$

For if this expression did not vanish, the lemma would give

$$\int |r - \lambda g|\,dx < \int |r|\,dx,$$

contradicting the definition of r. In particular,

$\sum_{i=1}^{n} \sigma_i \phi_i (f_j) = 0$, i.e. the matrix $(\phi_i(f_j))$ and its transpose are singular. Hence there exist scalars $\beta_1, \ldots, \beta_n$ (not all zero) so that

$$\sum_{i=1}^{n} \beta_i \phi_j (f_i) = 0,$$

i.e. for the non-zero function $h = \sum_{i=1}^{n} \beta_i f_i$, we have

$$0 = \phi_i (h) = \int_{x_{i-1}}^{x_i} h\,dx .$$

Hence h has n roots, contradicting the Haar condition. //

The algorithm in chapter 7 is based on the fact that a best L_2 approximant satisfies the alternating sign property, if not the equal error property, of theorem 6.1. This result seems to be due to E.Stiefel [63]. A generalization to L_p polynomial approximation can be found in the book by Werner [39]. In the version given below, the result is extended to generalized polynomial approximants satisfying the Haar condition.

<u>Lemma 6.16</u> Let $f, g_i \in C[a,b]$, $i=1(1)n$.

Suppose $L(A,x) = \sum_{i=1}^{n} a_i g_i(x)$ and $\{g_1,\ldots,g_n\}$ satisfies the Haar condition on $[a,b]$. Set

$$\Delta_p(A) = \left[\int_a^b |f(x) - L(A,x)|^p dx\right]^{1/p} \quad (1 < p < \infty) \tag{6.16}$$

and assume that f is not a generalized polynomial. Then $\Delta_p(A)$ is continuously differentiable and the best L_p approximant $L(A^*,x)$ to f is given by the system

$$\frac{\partial \Delta_p(A)}{\partial a_i} =$$

$$[\Delta_p(A)]^{1-p} \int_a^b |f-L(A,x)|^{p-1} \operatorname{sgn}\,[L(A,x) - f(x)] \,.$$

$$\cdot g_i(x)\,dx = 0 \tag{6.17}$$

<u>Proof</u> $\dfrac{\partial}{\partial a_i} |f-L(A,x)|^p$

$$= \frac{\partial}{\partial a_i} [f-L(A,x)]^p \operatorname{sgn}\,[f-L(A,x)]^p$$

$$= \begin{cases} p|f-L(A,x)|^{p-1}\operatorname{sgn}\,[f-L(A,x)].(-g_i) & \text{if } f \neq L(A,x) \\ 0, & \text{if } f = L(A,x). \end{cases}$$

But $p|f-L(A,x)|^{p-1} \operatorname{sgn}\,[f-L(A,x)] \to 0$ as $f \to L(A,x)$, i.e. $|f-L(A,x)|^p$ is continuously differentiable. Differentiating under the integral sign, we find that $\Delta_p(A)$ is also continuously differentiable. Equation (6.17) now follows as a necessary condition. By the convexity of the set

$$K = \{(A,d) \in R^{n+1} : \Delta_p(A) \leq d\},$$

the parameter A^* defined by (6.17) must be a minimum. Since the set $\{g_1,\dots,g_n\}$ satisfies the Haar condition it is linearly independent, which ensures the existence of a solution for the system (6.17). //

<u>Theorem 6.17</u> The error function $f-L(A^*,x)$ of the best L_p approximant $L(A^*,x)$ defined in lemma 6.6 changes sign at least n times.

<u>Proof</u> Let $\check{b} \varepsilon R^n$ be an arbitrary unit vector. Since $\Delta_p(A^*)$ is minimal,

$$\frac{\partial \Delta_p(A)}{\partial \check{b}} = 0 \qquad \text{for } A = A^*.$$

Hence

$$[\Delta_p(A^*)]^{1-p} \int_a^b |f-L(A^*,x)|^{p-1} \operatorname{sgn} [L(A^*,x)-f] \,.$$
$$. L(\check{b},x)dx = 0 \,. \tag{6.18}$$

Since $\Delta_p(A^*) \neq 0$ by hypothesis,

$$\int_a^b |f-L(A^*,x)|^{p-1} \operatorname{sgn}[L(A^*,x)-f] \; L(\check{b},x)dx = 0. \tag{6.19}$$

Now suppose that $f-L(A^*,x)$ changes sign m times, with $m < n$. Then we can find a generalized polynomial $L(\check{b},x) = \sum_{i=1}^{n} \check{b}_i g_i(x)$ which changes sign at the same points in $[a,b]$ as $f-L(A^*,x)$. Hence the function

$$[L(A^*,x) - f] \sum_{i=1}^{n} \check{b}_i g_i(x)$$

does not change sign in $[a,b]$, contradicting (6.19). It follows that $f-L(A^*,x)$ changes sign at least n times. //

II. NUMERICAL APPLICATIONS

Chapter 7

A Modified Exchange Algorithm for Best Chebyshev Approximation

Given n data points (x_i, y_i), $i = 1(1)n$, a line $y = ax + b$ is to be determined so that the norm of $\underline{r} = (r_1, \ldots, r_n)$ is a minimum, where

$$r_i = ax_i + b - y_i.$$

An L_1, L_2 or L_∞ line is obtained according as the norm is defined by

$$\|\underline{r}\|_1 = \sum|r_i|, \quad \|\underline{r}\|_2 = (\sum r_i^2)^{\frac{1}{2}} \quad \text{or} \quad \|\underline{r}\| = \max|r_i|.$$

These methods are maximum likelihood for the double exponential, the Gaussian and the uniform distribution, respectively. The L_∞ norm can be used if the data are thought not to contain any outliers. The L_1 norm, on the other hand, is the least sensitive to outliers and gives good results if some of the data points are suspect. In order to ensure the uniqueness of L_2 and L_∞ approximations we assume that the x_i are distinct. In certain applications especially to the social sciences, little or nothing is known about the underlying error distribution, and the customary compromise of choosing the L_2 norm can lead to inappropriate results. There is, therefore, a need for adaptive regression packages, which allow the user to experiment with different norms and all possible solutions. Such a package could, for example, include a facility for "robust" economic forecasting, by computing a band of L_p approximations and deducing upper and lower bounds for each forecast. These bounds are given by the parameters YMAX and YMIN of subroutine EXTRAP in the appendix of programs. The output parameters ICODE and JCODE indicate the norm used to obtain YMAX and YMIN, respectively. If the outlying points are wildly inaccurate, the L_1 approximation should provide the most accurate forecasts. If, on the other hand, the outliers herald a new trend, then the L_∞ approximation can be expected to yield better results. Similar adaptive packages could be designed for the solution of inconsistent linear systems. A possible application for such a package is outlined in chapter 10.

There are also computational advantages in this unified approach, since the amount of arithmetic involved in obtaining the L_1 and L_∞ lines can be substantially reduced by using the L_2 line as an initial estimate. We briefly describe the L_∞ theory.

It is well known (see theorem 6.17) that a best polynomial $L_p (p>1)$ approximation satisfies the alternating sign property. Thus in the linear case these are points P_k, P_ℓ, P_m such that

$$\operatorname{sgn}(r_k r_\ell) = \operatorname{sgn}(r_\ell r_m) = -1. \qquad (7.1)$$

If these points are chosen so that the absolute errors are as large as possible, one or two exchange iterations will normally suffice to obtain the L_∞ line. As in example 7.1 below, the L_2 line frequently leads immediately to the required solution and the exchange method need not be applied.

With P_k, P_ℓ, P_m defined as above, we determine the equal error line through the points $(x_k, y_k + e)$, $(x_\ell, y_\ell - e)$, $(x_m, y_m + e)$. The resulting system

$$ax_k + b - (y_k + e) = 0$$

$$ax_\ell + b - (y_\ell - e) = 0$$

$$ax_m + b - (y_m + e) = 0$$

has a non-trivial solution if

$$e = [(x_k-x_\ell)(y_\ell-y_m)+(x_m-x_\ell)(y_k-y_\ell)]/[2(x_k-x_m)]. \qquad (7.2)$$

The required equal error line has the equation

$$(y-y_k-e)(x_m-x_k) = (y_m-y_k)(x-x_k). \qquad (7.3)$$

If $\max|r_i| = e$, the equal error line is also the required L_∞ line. Otherwise there exists an integer M, $1 \le M \le n$, such that $\max|r_i| = r_M$. x_M now replaces one of the x_k, x_ℓ, x_m in such a way that the resulting triple satisfies the alternating sign property (7.1). The process can be shown to terminate in a finite number of steps when $\max|r_i| = e$.

<u>Example 7.1</u> The L_2 line for the 31 data points in Table 7.1 is given by

$$y = 0.370\,565x + 0.054\,435.$$

We note from the table that r_9, r_{24}, r_{30} is an alternating error triple with maximum absolute values. We therefore choose the initial reference P_9, P_{24}, P_{30}. Using (7.2) and (7.3), the error line is found to have the equation

$$y = (8/21)x - 6/21, \quad \text{with} \quad e = -39/21.$$

Since $\max|r_i| = e$, this is also the required L_∞ line, i.e. the exchange method is not needed. If, on the other hand, P_0, P_1, P_2 are chosen as the initial reference, three exchange iterations are required to compute the solution (see Scheid [32, p.271]). //

Table 7.1

x_i	0	1	2	3	4	5	6	7	8	9
y_i	0	1	1	2	1	3	2	2	3	5
r_i	0.1	-0.6	-0.2	-0.8	0.5	-1.1	0.3	0.7	0.1	-1.6

x_i	10	11	12	13	14	15	16	17	18	19
y_i	3	4	5	4	5	6	6	5	7	6
r_i	0.8	0.1	-0.5	0.9	.2	-0.4	-0.0	1.4	-0.3	1.1

x_i	20	21	22	23	24	25	26	27	28	29	30
y_i	8	7	7	8	7	9	11	10	12	11	13
r_i	-0.5	0.8	1.2	0.6	2.0	0.3	-1.3	0.1	1.6	-0.2	-1.8

SUBROUTINE MINMAX(N,X,Y,ITER,ERROR, A,B,C,D) in the appendix is a FORTRAN IV version of the modified exchange method described above. If double precision is required, the REAL declaration should be changed to DOUBLE PRECISION, E to D and ABS to DABS. The formal parameters are as follows

N	Integer	input: number of data points (x_i, y_i)
X	Real array (N)	input: $X(I) = x_i$, $i = 1(1)n$
Y	Real array(N)	input: $Y(I) = y_i$, $i = 1(1)n$
ITER	Integer	output:number of exchange iterations
ERROR	Real	output:minimax error e
A	Real	output:gradient of minimax line
B	Real	output:intercept of minimax line
C	Real	output:gradient of L_2 line
D	Real	output:intercept of L_2 line.

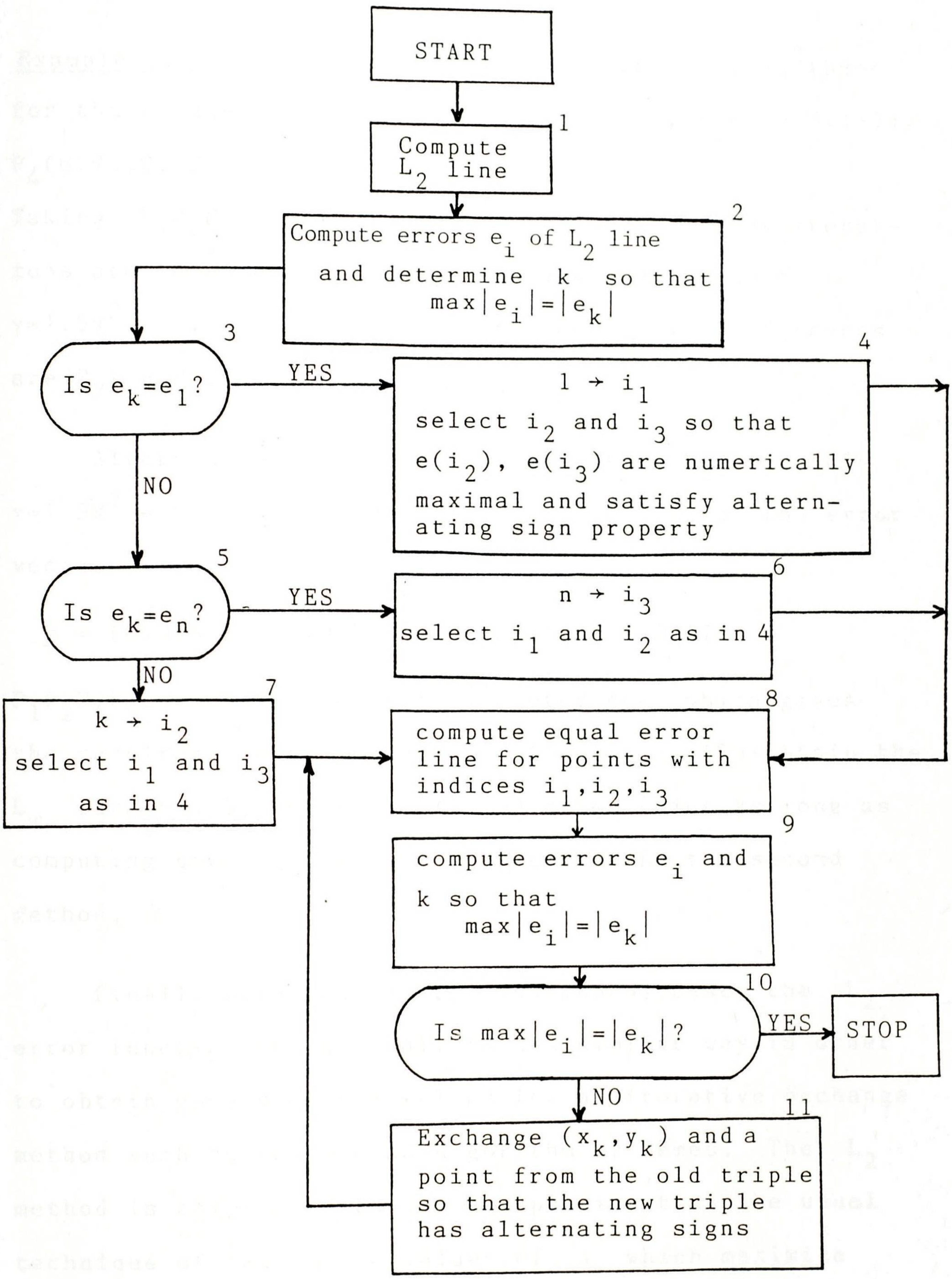
In table 7.2, the running time (in seconds) of a double precision version of MINMAX is compared with that of CHEB, an LP-based subroutine due to Barrodale and Phillips [33]. The 31 points refer to example 1 above, the 201 and 1001 points are given by $y=e^x$, with $x=0(0.01)2$ and $0(0.01)10$, respectively. The figures for MINMAX include CPU time for the L_2 lines. A flowchart for the subroutine is given below.

Table 7.2

Number of points	CHEB	MINMAX
31	0.03	0.01
201	0.19	0.06
1001	0.85	0.33

(My attention has just been drawn by a referee to a recent algorithm by Sklar and Armstrong [71], which appears to be about 5 times faster than Barrodale and Phillips.) See note in pocket.

Flowchart for subroutine MINMAX



Example 7.2 demonstrates that the modified exchange technique of subroutine MINMAX can also be used to obtain best approximating polynomials of higher degree.

Example 7.2 Find the minimax parabola $y=ax^2+bx+c$ for the points $P_1(0,0), P_2(0.25,0.015625)$, $P_3(0.5,0.125)$, $P_4(0.75,0.421875)$, $P_5(1,1)$.
Taking $P_1P_2P_3P_4$ as the initial reference, four iterations are required to obtain the required parabola $y=1.5x^2 - 0.5625x + 0.03125$. The subsequent references are $P_2P_3P_4P_5$, $P_1P_3P_4P_5$, $P_1P_2P_4P_5$.

Alternatively, we first compute the L_2 parabola $y=1.5x^2 - 0.5375x + 0.01875$. By inspection of the error vector

$$\underline{r} = (0.01875, -0.0375, 0, 0.0375, - 0.01875)$$

$P_1P_2P_4P_5$ is chosen as initial reference, which gives the required answer in only one iteration. To obtain the L_∞ parabola by the first method takes twice as long as computing both L_2 and L_∞ parabolas by the second method. //

Finally note that in the continuous case, the L_2 error function can be analyzed in a similar way in order to obtain good starting values for an iterative exchange method such as the second algorithm of Remes. The L_2 method is computationally more expensive than the usual technique of taking the values of x which maximize $|T_{n+1}|$ (n is the order of the approximant and T_{n+1} the Chebyshev polynomial of degree n+1). However, when the approximated function is odd or even, the L_2 method gives better results as the following example shows.

Example 7.3 Minimizing

$$\int_{-1}^{1}[ax^3 + bx^2 + cx + d - \sin(\pi x/2)]^2 dx$$

in the usual way, we find $a = -0.562\ 228$, $b = 0$, $c = 1.553\ 191$, $d = 0$. Searching the error function

$$r(x) = -0.562\ 228x^3 + 1.553\ 191x - \sin(\pi x/2)$$

for maximal absolute values, the reference

$$\{-0.8, -0.3, 0.3, 0.8, 1\} \tag{7.4}$$

is obtained. Alternatively,

$$x_i = \cos[(i-1)\pi/4], \quad i = 1(1)5,$$

defines the initial reference $\{-1, -0.7, 0, 0.7, 1\}$. The next two references are $\{-0.9, -0.4, 0.4, 0.9, 1\}$ and $\{-0.8, -0.3, 0.3, 0.8, 1\}$, i.e. two Remes iterations are needed before reference (7.4) is reached. //

Chapter 8

Segmented Linear Chebyshev Approximation

Segmented approximation provides useful initial estimates for fast and efficient techniques of computing function values. It remains an open question whether there is a general finite-step method of constructing the best approximating polynomial for a given continuous function. In the linear case, such a method exists for a restricted class of functions. The single-variable case is discussed in Natanson [34, p.34 f.], where it is proved that, if a function f can be differentiated twice and if f'' does not alter its sign for $a \leq x \leq b$, then the best linear Chebyshev approximation $g(x) = Ax + B$ over the interval $[a,b]$ is given by

$$A = [f(b) - f(a)]/(b-a) = f'(c) \tag{8.1}$$

$$B = [f(a) + f(c)]/2 - (A/2)(a+c) \tag{8.2}$$

for some $c \varepsilon (a,b)$. We prove a slightly stronger version of Natanson's result.

Theorem 8.1 If f is a strictly convex function which is differentiable on (a,b) and continuous on $[a,b]$, then $g(x) = Ax + B$ as defined by (8.1) and (8.2) is the best linear approximation to f.

To prove the theorem we establish the existence of a number $c \varepsilon (a,b)$ such that

$$[f(b) - f(a)]/(b-a) = f'(c)$$

by the mean value theorem. Now let L be the line parallel to and equidistant from the tangent to f at $P(c,f(c))$ and the chord through the points $Q(a,f(a))$, $R(b,f(b))$. L is determined by its gradient $f'(c)$ and the midpoint $\frac{1}{2}(a + c, f(a) + f(c))$ of PQ, i.e. its equation is

$$y = f'(c)x + [f(a) + f(c)]/2 - f'(c)(a+c)/2,$$

which agrees with (8.1) and (8.2). Since f is convex, the maximum error occurs with alternating signs at $x = a,c,b$. Its absolute value is

$$|f(a) - f(c) - f'(c)(a-c)|/2.$$

To see that the theorem is stronger than Natanson's result we note that the function

$$f(x) = \begin{cases} x^2, & -1 \leq x \leq 0 \\ x^3, & 0 \leq x \leq 1 \end{cases}$$

is convex and differentiable on $[-1,1]$ but $f''(0)$ does not exist.

Before considering a generalization of the above theorem to functions of several variables, we briefly consider an application to computer approximation. (An earlier version of the ideas set out below can be found in M. Planitz[35]). The following square root routine for the now extinct Hewlett-Packard 2000F computer has appeared, without explanations, in Unit 10 of Numerical Computation [36], an Open University text on approximation theory. The process of evaluating $\sqrt{x}$ is carried out in four steps:

(i) Determine a real number $t \in [0.25, 1]$, such that $x = 4^k t$, where k is an integer.

(ii) Use the formula

$$y(t) = \begin{cases} 0.27863 + 0.875t, & t \in [0.25, 0.5) \\ 0.421875 + 0.578125t, & t \in [0.5, 1) \end{cases}$$

to obtain a first approximation for $\sqrt{t}$.

(iii) Apply Newton's method in the form

$$y_{n+1} = (y_n + t/y_n)/2$$

with $y_o = y(t)$ and $n = 0,1$.

(iv) Compute $\sqrt{x} = 2^k y_2$.

This algorithm, which seems cumbersome at first sight, is in fact remarkably efficient. The result is correct to 6 significant figures, and a binary computer requires only 2 "long" operations (i.e. multiplications or divisions). These are needed to compute t/y_n in step (iii). Steps (i) and (iv) as well as the division by 2 in step (iii), only involve shifts. Less obviously, step (ii) can be regarded as a "short" operation, since $0.875 = 0.111_2$ and $0.578125 = 0.100101_2$, i.e. only 4 additions and 3 shifts are required to find $y(t)$. The selection of the function $y(t)$ for step (ii) poses an interesting non-trivial problem. First note that for greater accuracy, the approximation on $[0.25, 1)$ is segmented. Since our computer uses binary arithmetic, a power of 2 is chosen as a point of sub-division. It follows from theorem 6.2, that there is a unique best linear approximation to $\sqrt{t}$ on each of the two subintervals. It is not clear how Hewlett-Packard arrived at the formula in (ii), but the following approach leads to similar, in fact slightly better, results. We first use (8.1) and (8.2) to determine the best segmented approximant

$$y^*(t) = \begin{cases} 0.297\,335 + 0.828\,427t, & t\varepsilon[0.25,0.5) \\ 0.420\,495 + 0.585\,786t, & t\varepsilon[0.5,1), \end{cases}$$

with approximate errors of 0.004 on $[0.25,0.5)$ and 0.006 on $[0.5,1)$. Some of the accuracy of y^* is now sacrificed in order to reduce the execution time of step (ii). This is done by approximating the coefficients of t by numbers whose binary expansions contain only three non-zero bits. The resulting formula is

$$y(t) = \begin{cases} a_o + 0.875t, & t\varepsilon[0.25,0.5) \\ b_o + 0.578\,125t, & t\varepsilon[0.5,1). \end{cases}$$

To adjust the value of a_o we apply theorem 6.1 to the function

$$g(t) = \sqrt{t} - 0.875t.$$

This time the required best approximation is a constant and a simple argument will show that this constant is given by

$$a_o = (m + M)/2,$$

where $m = \min g(t)$ and $M = \max g(t)$ on $[0.25,0.5]$. Since a_o has degree 0, we have to show that the error function alternates on two points. If we define t_1,t_2 by

$m = g(t_1)$ and $M = g(t_2)$, then

$$a_o - g(t_1) = (M - m)/2 \quad \text{and} \quad a_o - g(t_2) = (m - M)/2.$$

Moreover,

$$|a_o - g(t_i)| = \max|a_o - g(t)|, \quad i=1 \text{ or } 2, \qquad t\varepsilon[0.25,0.5],$$

i.e. $a_o = (m + M)/2$ satisfies the alternation property of theorem 6.1. It is now easy to show that

$$m = 0.269\ 068 \quad \text{and} \quad M = 0.285\ 714\ 3.$$

Hence $a_o = 0.277\ 661$. This gives a maximum absolute error of 0.008 on [0.25, 0.5), compared with an error of 0.009 in Hewlett-Packard's original formula. We similarly find $b_o = 0.425\ 008$ with an error of 0.007, which reduces Hewlett-Packard's error by 0.003. Thus the formula in (ii) should be replaced by

$$y(t) = \begin{cases} 0.277\ 661 + 0.875t, & t\varepsilon[0.25,0.5) \\ 0.425\ 008 + 0.578\ 125t, & t\varepsilon[0.5,1). \end{cases}$$

A further reduction in the number of long operations could be achieved by introducing a k-fold segmented approximation to $\sqrt{t}$, with $k>2$, and applying the above technique to each of the k subintervals. The decreasing costs of integrated circuit technology have now made it economically feasible to save CPU time by permanently installing a large number of constants in read-only memory chips. If k is sufficiently large, step (iii) can be eliminated and execution times should approach those of a single multiplication, even for transcendental functions which at present are still computationally expensive.

We now derive a generalization of theorem 8.1 to functions of two variables. Let the strictly convex function f be differentiable on the open rectangle $S = (a,b)\times(c,d)$ and continuous on the corresponding closed rectangle $\bar{S}$. A best approximation

$$g(x,y) = Ax + By + C \tag{8.3}$$

to f on $\bar{S}$ clearly exists. As to uniqueness, we know from the remarks following theorem 6.2 that the Haar theory does not automatically carry over to multivariate approximation. However, for the special case of linear polynomial approximants we have the following result due to L. Collatz [38].

Theorem 8.2 If f has continuous partial derivatives at all interior points of a closed, strictly convex set X of the plane, then there exists a unique linear polynomial $Ax + By + C$ of best approximation to f on X.

In the book by J.R. Rice [58, Vol.II, p.237], theorem 8.2 appears with the weaker hypothesis that X is closed and convex. To disprove this version, consider the convex (but not strictly convex) function

$$f(x,y) = (2y^2 - 1)(1 - x/2),$$

with $0 \leq x \leq 1$ and $-1 \leq y \leq 1$. Then X is convex (but not strictly convex) and $g(x) = kx/2$ is a best approximant to f for any k such that $|k| \leq 1$.

Let L be the best approximating plane (8.3). If $(x,y,f(x,y))$, $(x+h, y+k, f(x+h, y+k))$ are points on the intersection of L with the surface $z=f(x,y)$, then

$$f(x+h, y+k) - f(x,y) = Ah+Bk = (h,k).(A,B).$$

By the mean-value theorem, this expression is equal to

$$(h,k).\underline{\nabla} f(x+\theta h, y+\theta k)$$

for $0<\theta<1$, i.e. there exists a point $(\alpha,\beta) = (x+\theta h, y+\theta k)\varepsilon S$, such that

$$\underline{\nabla} f(\alpha,\beta) = (A,B).$$

Thus the tangent plane T to $z = f(x,y)$ at $P(\alpha,\beta,f(\alpha,\beta))$ is parallel to L. Since f is strictly convex, P is at maximum distance from the best approximation L, and the point (α,β) must be a minus-point, i.e. a point with negative maximum error

$$f(\alpha,\beta) - A\alpha - B\beta - C.$$

Now let L be parallel to and equidistant from the tangent plane T and a third plane U, say. By definition of U, none of the points $P_1(a,c,f(a,c))$, $P_2(b,c,f(b,c))$, $P_3(b,d,f(b,d)$, $P_4(a,d,f(a,d))$ lie above U. Now suppose they all lie below U. Then there exists a plus-point (x_p, y_p) i.e. a point with positive maximum error, which is not one of the Q_i, where Q_i denotes the projection of P_i onto the xy-plane. Suppose (x_p, y_p) lies on the boundary of $\overline{S}$ between Q_1 and Q_2, say. Then $(x_p, y_p, f(x_p, y_p))$ lies above the chord P_1P_2, contradicting the convexity of f. Suppose next $(x_p,y_p)\varepsilon S$ and draw a line from Q_1, say, through (x_p,y_p). If this line meets the boundary of $\bar{S}$ at (x_b,y_b), then $(x_p,y_p,f(x_p,y_p))$ lies above the chord from P_1 to $(x_b,y_b,f(x_b,y_b))$, again contradicting the convexity of f. It follows that at least one of the P_i lies in U. We next prove that at least two more of the points P_i lie in U. First recall the following

<u>Definition 8.1</u> A set of points $M \subset \bar{S}$ will be called a <u>reference</u> of $z = Ax + By + C$ if there is no triple (D,E,F) so that

$$(Dx + Ey + F)[f(x) - Ax - By - C]>0$$

for all $x\varepsilon M$, i.e. there is no plane $z = Dx + Ey + F$ whose sign on M agrees with that of the error $f(x) - Ax - By - C$. The reference is said to be a <u>Chebyshev</u> <u>alternant</u> if for all $x\varepsilon M$

$$|f(x) - Ax - By - C| = ||f(x) - Ax - By - C||_\infty .$$

We also require the following result.

<u>Theorem 8.3</u> $z = Ax + By + C$ is a best Chebyshev approximation to f, if and only if there is a Chebyshev alternant.

For a proof of this theorem, see for example Werner [39, p.141]. If only one of the $P_i(P_1$, say) lies in U, we can clearly determine a plane whose sign is positive for Q_1 and negative for (α,β), contradicting the assumption that the two points form an alternant. The same argument shows that the only possible constellations with two of the P_i in U are P_1, P_3 (or P_2, P_4), with Q_1, Q_3 (or Q_2, Q_4) as plus-points and the minus-point (α,β) on the diagonal $Q_1 Q_3$ (or $Q_2 Q_4$), leading to non-unique approximations. Now assume that there are at least three points in U (P_1, P_2, P_3, say). To determine L, note that, if $z = Ax + By + N$ is the equation of U, then

$$f(a,c) = Aa + Bc + N$$

$$f(b,c) = Ab + Bc + N$$

$$f(b,d) = Ab + Bd + N.$$

Hence

$$A = [f(b,c) - f(a,c)]/(b-a) = f_x(\alpha,\beta) \qquad (8.4)$$

and

$$B = [f(b,d) - f(a,c)]/(d-c) - A(b-a)/(d-c) = f_y(\alpha,\beta) \qquad (8.5)$$

Since U is given by $z = Ax + By + f(a,c) - Aa - Bc$, the vertical distance between U and $P(\alpha,\beta,f(\alpha,\beta))$ is given by

$$d = A\alpha + B\beta + f(a,c) - f(\alpha,\beta) - Aa - Bc.$$

But L is equidistant from T and U. Hence

$$d/2 = A\alpha + B\beta + C - f(\alpha,\beta).$$

Eliminating d from these expressions we find

$$C = \{f(a,c) + f(\alpha,\beta) - A(a+\alpha) - B(c+\beta)\}/2. \qquad (8.6)$$

Equations (8.4), (8.5), (8.6) define L. The maximum error is given by

$$e = \{f(a,c) - f(\alpha,\beta) - A(a-\alpha) - B(c-\beta)\}/2. \tag{8.7}$$

Example 8.1 Determine the best approximation of the form $z = Ax + By + C$ to the function

$$f(x,y) = x^2 + 6y^2 + 4x - 8y - 143$$

on the unit square $[0,1]^2$.

The points $P_1(0,0,-143)$, $P_2(1,0,-138)$, $P_3(1,1,-140)$, $P_4(0,1,-145)$ all lie in the plane U whose equation is

$$z = 5x - 2y - 143.$$

We have $A = 5$, $B = -2$, $\alpha = \beta = 1/2$, and $C = -143.875$.

L is given by

$$z = 5x - 2y - 143.875,$$

with $e = 0.875$. //

Chapter 9

Strict Approximation in the L_1 Norm

We return in this chapter to the problem of linear approximation to a set of data (x_i, y_i), $i = 1(1)n$. In contrast to the L_2 line and L_∞ line, an L_1 line need not be unique even if the x_i are distinct. In fact, if $ax+b$ and $a'x + b'$ are two best linear L_1 approximations, then so is any convex combination

$$\alpha(ax+b) + \beta(a'x+b')$$

for $\alpha, \beta \geqslant 0$ and $\alpha+\beta=1$. This follows from the inequality

$$\Sigma|\alpha(ax_i+b) + \beta(a'x_i+b') - y_i|$$

$$\leqq \alpha\Sigma|ax_i+b-y_i| + \beta\Sigma|a'x_i+b'-y_i|.$$

Thus, if there is more than one L_1 solution, then there are infinitely many. The purpose of this chapter is to develop an algorithm, which determines this infinite solution set and then selects a unique "best" of all best solutions by minimizing $||\underline{r}||_2$ over the L_1 solution set.

We restrict our attention to the non-unique case and assume that an L_1 line

$$L(A_1, x) = a_1 x + b_1$$

has been obtained, using the subroutine L1 by Barrodale and Roberts [40] or any other suitably adapted LP-based package. The subroutine SOLVE (see appendix of programs) is then activated to compute the remaining simplex vertices which represent optimal solutions. Denote these solutions by $L(A_2,x),\ldots,L(A_n,x)$. We know from chapter 6 that any convex combination of the form

$$L(A,x) = \alpha_1 L(A_1,x)+\ldots+\alpha_n L(A_n,x), \tag{9.1}$$

with $\alpha_i \geq 0$ and $\Sigma\alpha_i=1$, is also an L_1 solution and that the locus of all solution parameters $A(a,b)$ is the convex hull H of the points $A_1(a_1,b_1),\ldots,A_n(a_n,b_n)$.

<u>Example 9.1</u> For the data points (0,1), (1,0), (2,0), (3,1), the LP method yields four interpolating L_1 lines: $y=0$, $y=1$, $y=0.5x-0.5$, $y=-0.5x+1$, with $\Sigma|r_i|=2$. The set H is the quadrilateral whose vertices are (-0.5,1), (0,1), (0.5,-0.5), (0,0). //

Contrary to Sadovski's [41, p.245] claim that the L_1 norm fit must pass through at least two data points, we note from the example that $y=0.5$ is an L_1 line which misses all four data points. $y=0.5$ is also an L_∞ and L_2 line and clearly satisfies the additional requirement that $\|\underline{r}\|_2$ should be minimal on H. We shall refer to this line as a strict $L_1(L_2)$ approximation. The term "strict approximation" was first used by J.R. Rice [42] to denote a unique "best" of all best Chebyshev approximations. An exchange algorithm to determine the strict Chebyshev approximation can be found in the paper by Duris and Temple [43].

Example 9.1 is exceptional in that the strict $L_1(L_2)$ approximation coincides with the L_2 and L_∞ approximations. In general, the problem is to minimize the function

$$f(a,b) = \Sigma(ax_i+b-y_i)^2,$$

subject to the constraint $(a,b)\varepsilon H$. We proceed as follows. The subroutine STRICT first computes the (unique) L_2 line $y=cx+d$ and determines whether the point (c,d) lies in H. Two cases arise:

(i) $(c,d)\varepsilon H$. Then $y=cx+d$ is clearly the required strict $L_1(L_2)$ approximation and the algorithm stops (see example 9.1).

(ii) $(c,d)\notin H$. Then f has its global minimum at (c,d). But the convex function f has a positive-definite Hessian matrix

$$\begin{pmatrix} 2\Sigma x_i^2 & 2\Sigma x_i \\ 2\Sigma x_i & 2n \end{pmatrix},$$

since for distinct x_i, $n\Sigma x_i^2 - (\Sigma x_i)^2>0$ by Hölder's inequality. It follows that its constrained minimum is unique and occurs on the boundary of H at (a,b), say (see example 9.2).

In either case, STRICT returns a unique $L_1(L_2)$ approximation.

<u>Example 9.2</u> For the data points (0,2), (1,2.5), (2,2), (3,5), the convex hull H has vertices (1.25,1.25), (1,2), (0.5,2). The L_2 line is given by $y=0.85x + 1.6$, the point (0.85,1.6) lies outside H and the required strict approximation is $y=0.8\bar{3}x + 1.\bar{6}$. //

We now give a description of the subroutines SOLVE and STRICT. Subroutine SOLVE is preceded by a driver program which computes an optimal simplex tableau A and the initial optimal L_1 solution (a_1, b_1). The idea of using linear programming methods to obtain an L_1 approximation for discrete data is due to H.M.Wagner [44]. The LP method is based on the following theory. Set

$$r_i = ax_i + b - y_i, \quad a = \alpha_1 - \alpha_2, \quad b = \beta_1 - \beta_2,$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2 \geqslant 0$. In order to minimize $\Sigma|r_i|$, put $r_i = v_i - u_i$, with $u_i, v_i \geqslant 0$. To ensure non-singularity of the basis matrix, u_i and v_i may not both be present in the basis. It follows that $u_i v_i = 0$ and hence

$$|r_i| = |v_i - u_i| = (u_i^2 \pm 2u_i v_i + v_i^2)^{\frac{1}{2}} = u_i + v_i.$$

Thus the problem can be restated in the form

$$\Sigma(u_i + v_i) = \min!,$$

subject to the constraints

$$y_i = \beta_1 - \beta_2 + (\alpha_1 - \alpha_2)x_i + u_i - v_i,$$

$i=1(1)n$. In the subroutine SOLVE and its driver program, a numerical code is used to identify the variables: the numbers $1, 2, 3, \ldots, n+2$ denote the variables $\alpha_1, \beta_1, u_1, \ldots, u_n$, respectively; $-1, -2, -3, \ldots, -n-2$ denote $\alpha_2, \beta_2, v_1, \ldots, v_n$, respectively. The efficiency of the driver program can be improved by combining the method used in chapter 7 with linear programming techniques. As in subroutine MINMAX, we first compute the L_2 line and then use the errors r_i to estimate the position of two interpolating points of the L_1 line. The following strategy will be employed:

if $|r_j|$, $|r_k|$ are the smallest absolute L_2 errors with $\mathrm{sgn}(r_j r_k) \leq 0$, we apply two LP iterations to ensure that the line goes through the points (x_j, y_j), (x_k, y_k). This step corresponds to phase I of subroutine L1 by Barrodale and Roberts [40]. When the interpolation step is complete, we continue with the usual simplex method or apply phase II of the Barrodale-Roberts algorithm. For the straight line to interpolate (x_j, y_j) and (x_k, y_k) we remove u_j, u_k from the basis without allowing v_j, v_k to enter. Any negative entries in column y are made positive by multiplying the appropriate rows by -1 and making the corresponding u, v-interchanges. The data in the example below appear in Barrodale and Roberts [46].

<u>Example 9.3</u> For the points (1,1), (2,1), (3,2), (4,3), (5,2) we find the L_2 line $y = 0.4x + 0.6$. On inspection of the error vector

$$\underline{r} = (0,\ 0.4,\ -0.2,\ -0.8,\ 0.6),$$

(1,1) and (3,2) are chosen as interpolation points. u_1 and u_3 will therefore be removed from the basis. The condensed tableaux are as follows. (Pivots are indicated by asterisks.)

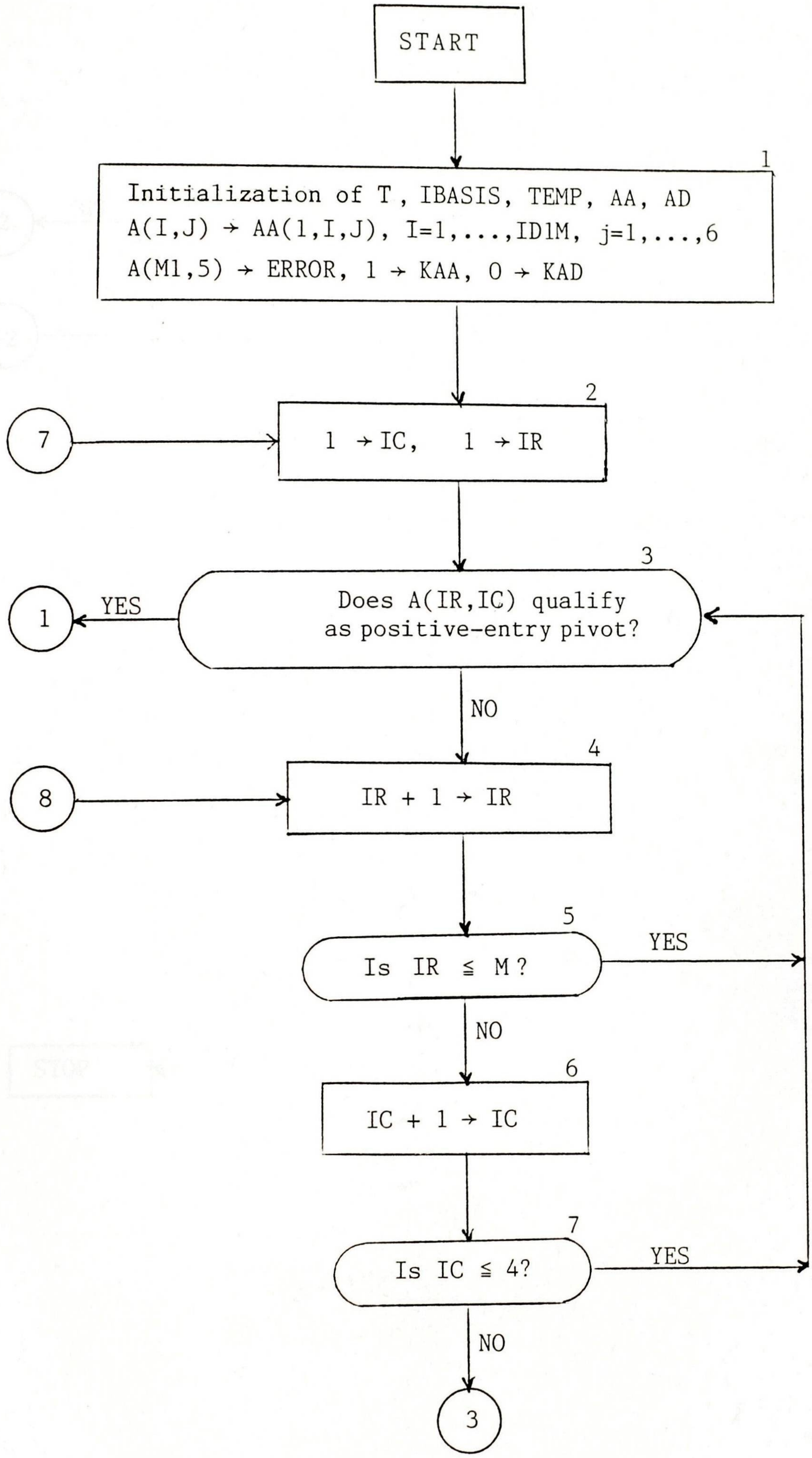
basis	y	β_1	α_1	basis	y	β_1	u_3	basis	y	u_1	u_3
u_1	1	1	1	u_1	1/3	2/3*	-1/3	β_1	1/2	3/2	-1/2
u_2	1	1	2	v_2	1/3	-1/3	2/3	v_2	1/2	1/2	1/2
u_3	2	1	3*	α_1	2/3	1/3	1/3	α_1	1/2	-1/2	1/2
u_4	3	1	4	u_4	1/3	-1/3	-4/3	u_4	1/2	1/2	-3/2
u_5	2	1	5	v_5	4/3	2/3	5/3	v_5	1	- 1	2
	9	5	15		7/3	2/3	-1/3		2	-1	0

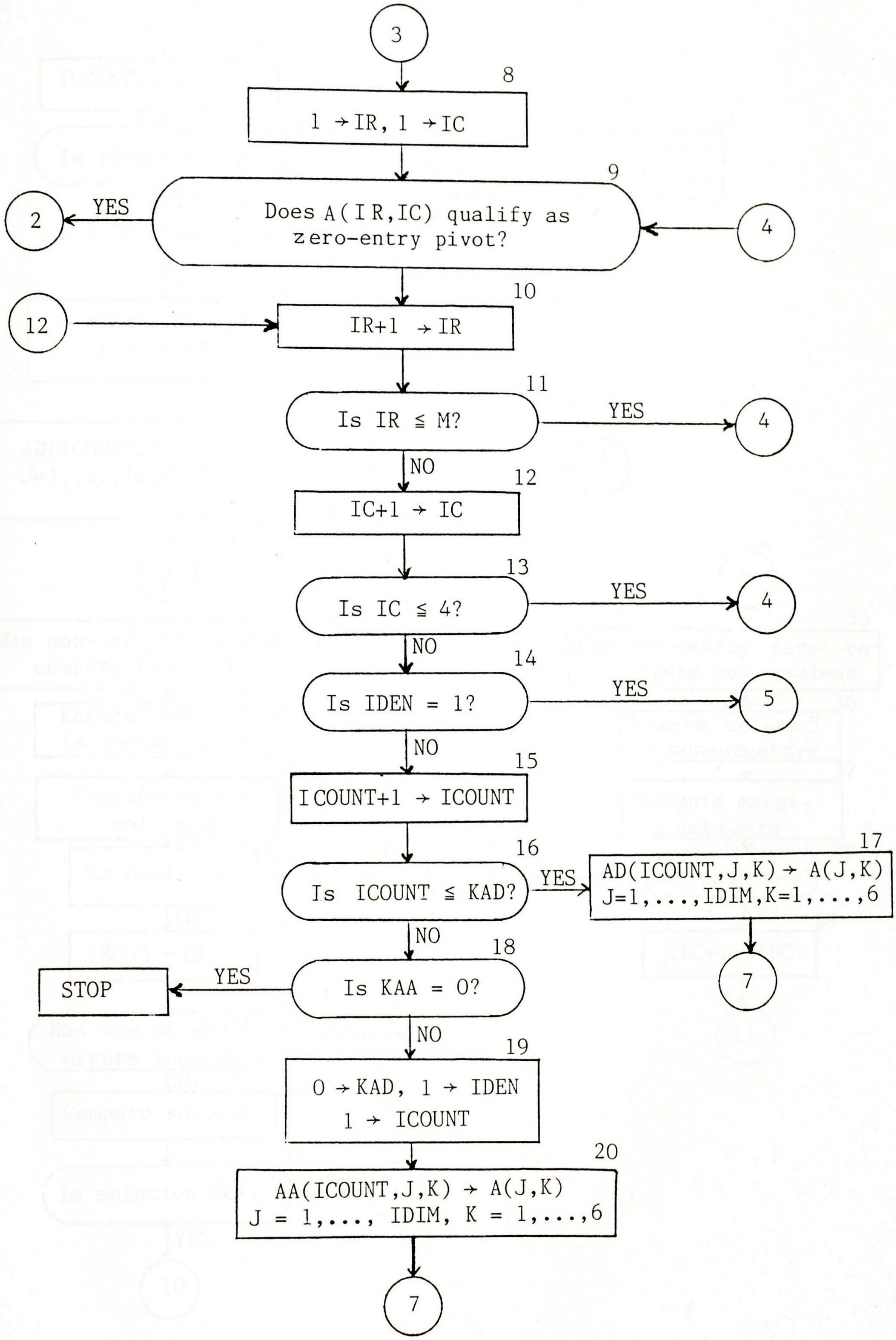
Note that pivot 3* was chosen by applying the usual criteria of the simplex method to rows 1 and 3 of the first tableau. The Barrodale-Roberts technique is computationally more expensive: starting with the usual simplex pivot 5, α_1 is increased until the marginal cost becomes negative. In the above example, the two methods give rise to identical tableaux, which seems fairly typical of small data sets. //

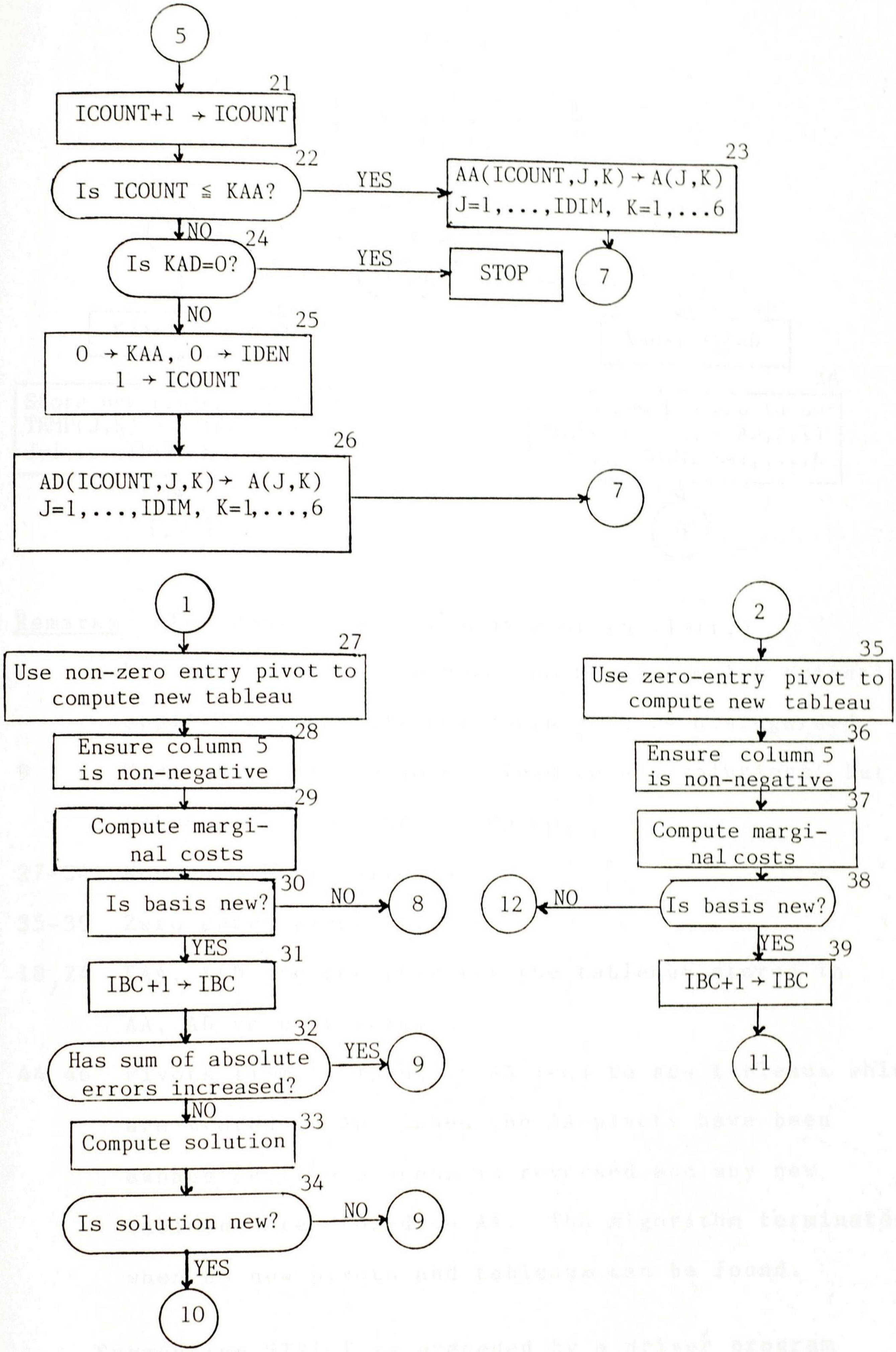
Subroutine SOLVE is summarized in the macroscopic flowchart below; the formal parameters are as follows:

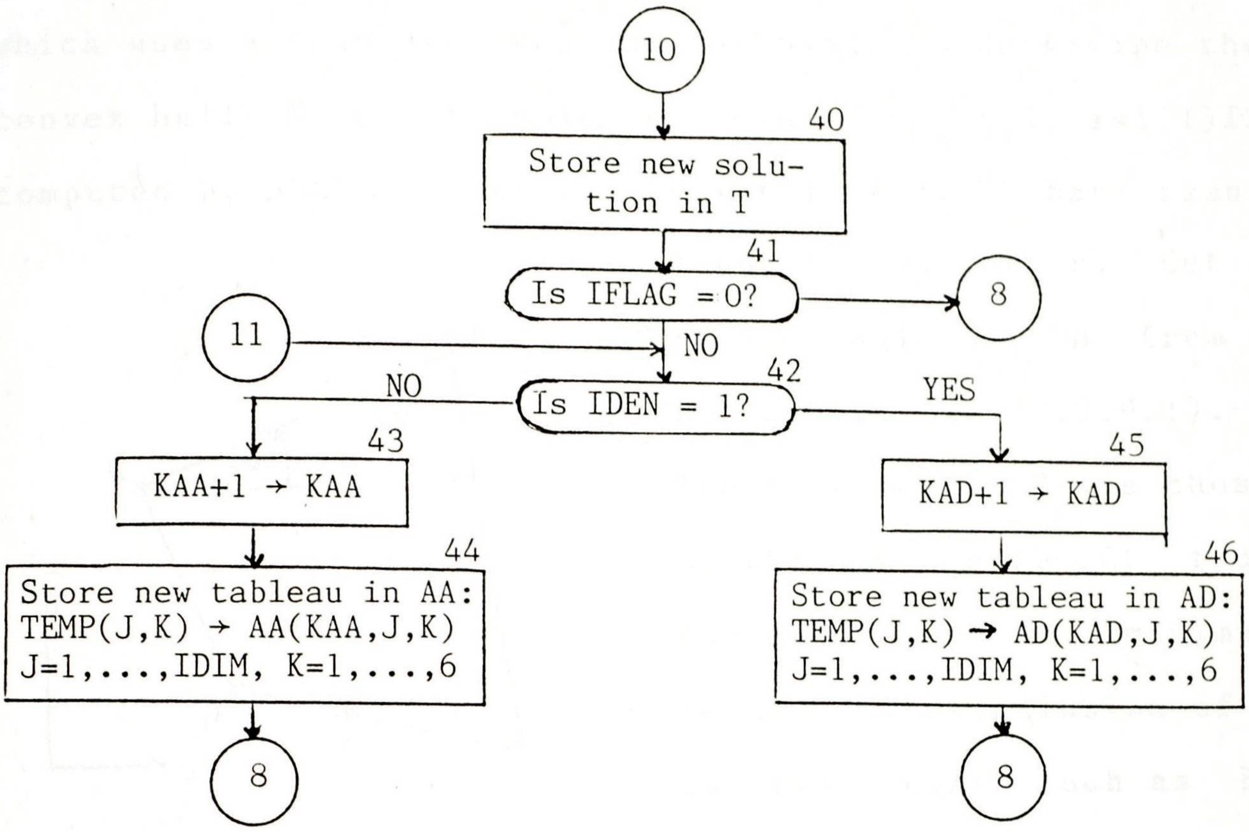
IDIM	Integer	input :	n+2, where n is the number of data points (x_i, y_i)
A	Real array (IDIM,6)	input :	optimal simplex tableau $a_{i,5}$ = residuals, i=1(1)n $a_{n+1,j}$ = marginals, j=1(1)5 $a_{i,6}$ = basis identifiers, i=1(1)n $a_{n+2,j}$ = variable identifiers, j=1(1)4 $a_{n+2,5} = 1$, $a_{n+2,6} = 0$, $a_{n+1,6} = 0$
X	Real array (2)	input :	initial optimal solution $X(1) = a_1$, $X(2) = b_1$
TOLER	Real	input :	1.0 E-D, where D is the number of accurate decimal digits available
IFAIL	Integer	output :	fault indicator equal to 1 increase 1st dimension of AA and AD; 2 increase 1st dimension of IBASIS; 3 increase 2nd dimension of T; 4 pivot is too small; 0 otherwise
ISC	Integer	output :	number of solutions
T	Real array (2,10)	output :	solutions $T(1,I) = a_i$, $T(2,I) = b_i$.

Flowchart for subroutine SOLVE




3
8
1 → IR, 1 → IC
9
2
YES
Does A(IR,IC) qualify as zero-entry pivot?
4
10
12
IR+1 → IR
11
Is IR ≦ M?
YES
4
NO
12
IC+1 → IC
13
Is IC ≦ 4?
YES
4
NO
14
Is IDEN = 1?
YES
5
NO
15
ICOUNT+1 → ICOUNT
16
Is ICOUNT ≦ KAD?
YES
17
AD(ICOUNT,J,K) → A(J,K) J=1,...,IDIM,K=1,...,6
7
NO
18
STOP
YES
Is KAA = 0?
NO
19
0 → KAD, 1 → IDEN 1 → ICOUNT
20
AA(ICOUNT,J,K) → A(J,K) J = 1,..., IDIM, K = 1,...,6
7


5
21
ICOUNT+1 → ICOUNT
22
Is ICOUNT ≤ KAA?
YES
23
AA(ICOUNT,J,K) → A(J,K)
J=1,...,IDIM, K=1,...6
7
NO
24
Is KAD=0?
YES
STOP
NO
25
0 → KAA, 0 → IDEN
1 → ICOUNT
26
AD(ICOUNT,J,K) → A(J,K)
J=1,...,IDIM, K=1,...,6
7
1
27
Use non-zero entry pivot to compute new tableau
28
Ensure column 5 is non-negative
29
Compute marginal costs
30
Is basis new?
NO
8
YES
31
IBC+1 → IBC
32
Has sum of absolute errors increased?
YES
9
NO
33
Compute solution
34
Is solution new?
NO
9
YES
10
2
35
Use zero-entry pivot to compute new tableau
36
Ensure column 5 is non-negative
37
Compute marginal costs
38
Is basis new?
NO
12
YES
39
IBC+1 → IBC
11



<u>Remarks</u> (Box numbers are indicated on the left.)

3 For positive-entry pivots the usual simplex criteria apply; only the minimum-ratio rule is disregarded.

9 Zero-entry pivots do not lead to new solutions, but subsequent tableaux may do so.

27-34 Non-zero entry pivoting.

35-39 Zero entry pivoting.

18, 24 KAA, KAD are counters for the tableaux stored in AA, AD respectively.

44, 46 Pivots from tableaux in AA lead to new tableaux which are stored in AD. When the AA-pivots have been exhausted, the process is reversed and any new tableaux are stored in AA. The algorithm terminates when no new pivots and tableaux can be found.

Subroutine STRICT is preceded by a driver program which uses a standard wrapping technique to determine the convex hull H of the solution points (a_i, b_i), i=1(1)ISC, computed by SOLVE. Suppose the vertices A,B,C have been found in that order. Let α be the angle of CB from the horizontal (see FIG.9.1). The next point P is chosen so that the angle CP from the horizontal is a minimum. To avoid the inclusion of interior points such as E, we ignore angles not greater than α. We also ignore angles not less than 2π. In FIG. 9.1, the next point found in this way is D. Intermediate points such as F are eliminated. Since the point sets encountered in the present context are small, no attempt has been made to include a "quickersort" technique, but a machine-dependent improvement in running time of about 30% was achieved for the driver program by avoiding the function ATAN. Instead of measuring the angle by ATAN(Y/X), where X and Y are the horizontal and vertical steps between consecutive vertices, the "angle" is defined by

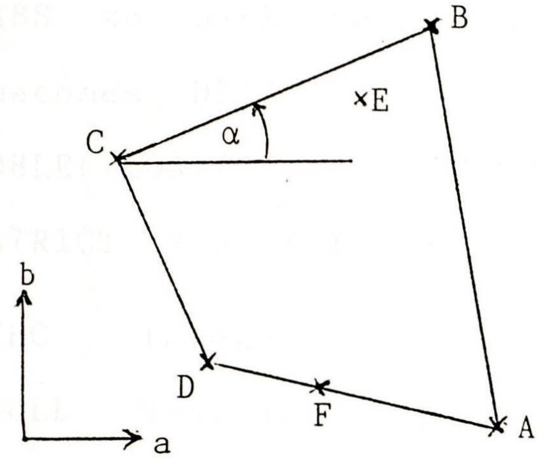


FIG.9.1

$$0.5 * PI*Y/(ABS(X) + ABS(Y)),$$

which preserves the ordering of angles.

Subroutine STRICT first computes the L_2 solution (c,d) for the given data points (x_i, y_i) and then determines whether $(c,d) \varepsilon H$. This is done by considering the intersections of the sides of H with the line segment defined by (c,d) and the centroid (x_o,y_o) of the vertices of H. If double precision is required, the REAL declaration should be changed to DOUBLE PRECISION, E to D and ABS to DABS in either subroutine. In addition, SIGN becomes DSIGN in SOLVE, and FLOAT(.) becomes DBLE(FLOAT(.)) in STRICT. The formal parameters of STRICT are as follows:

IHC	Integer	input :	number of vertices (a_i,b_i)
HULL	Real array(2,IHC)	input :	vertices (a_i,b_i),i=1(1)IHC
M	Integer	input :	number of data points (x_i,y_i)
T1	Real array(M)	input :	T1(I) = x_i, i=1(1)m
T2	Real array (M)	input :	T2(I) = y_i, i=1(1)m
TOLER	Real	input :	as for subroutine MINMAX
ICODE	Integer	output :	indicates status of solution;
		0	strict and L_2 solution are identical;
		1	otherwise
A	Real	output :	gradient of strict L_1 line
B	Real	output :	intercept of strict L_1line
C	Real	output :	gradient of L_2 line
D	Real	output :	intercept of L_2 line.

If $(c,d)\varepsilon H$, this is also the strict solution and the exit code will be set to 0. If $(c,d)\notin H$, the subroutine determines analytically the minimum of

$$f(a,b) = \Sigma(ax_i + b - y_i)^2 \tag{9.2}$$

on the boundary of H. Consider the side with endpoints (a_j, b_j), (a_{j+1}, b_{j+1}). The line through these points is given by

$$b = g(a - a_j) + b_j,$$

where $g = (b_{j+1} - b_j)/(a_{j+1} - a_j)$, $a_{j+1} \neq a_j$. Hence (9.2) becomes

$$f(a) = \Sigma(ax_i + ag - a_j g + b_j - y_i)^2.$$

From $f'(a)$ we find

$$a = \frac{\Sigma[g(a_j x_i + a_j g - b_j + y_i) - b_j x_i + x_i y_i]}{\Sigma(x_i^2 + 2gx_i + g^2)}$$

If $a_j = a_{j+1}$, put $a = a_j$ in (9.2). Then

$$f(b) = \Sigma(a_j x_i + b - y_i)^2 ,$$

and $f'(b) = 0$ gives

$$b = \Sigma(y_i - a_j x_i)/d.$$

In either case, a check is made to ensure that the point (a,b) lies between (a_j, b_j) and (a_{j+1}, b_{j+1}). The local minima found in this way compete with the values of $f(a,b)$ at the vertices of H to determine the global minimum on the boundary.

Note that strict $L_1(L_2)$ approximations can also be defined for continuous approximants as the following example shows.

Example 9.4 The function

$$f(x) = \begin{cases} 0, & -1 \leqq x \leqq 2 \\ -1, & 2 < x \leqq 3 \end{cases}$$

has infinitely many best L_1 approximants of the form $g(x) = ax+b$. These are given by

$$g(x) = tx, \qquad -\tfrac{1}{3} \leqq t \leqq 0.$$

To determine a strict approximation we minimize

$$F(t) = \int_{-1}^{3} [f(x) - tx]^2 \, dx,$$

subject to the constraint $-\frac{1}{3} \leqq t \leqq 0$. From $F'(t) = 0$, $t = -15/52$, i.e. the required strict approximation is $y = (-15/52)x$. //

Chapter 10

An Application to Mineral Processing

It is well known that the general solution of a linear system

$$Ax = b \tag{10.1}$$

is given by

$$x = A^g b + (I - A^g A)w, \tag{10.2}$$

where w is an arbitrary vector in R^n and A^g is any generalized inverse of the $m \times n$ matrix A. If the coefficient matrix A contains inaccurate measurements or observations, we may find there is no solution, i.e. there is no vector x such that $Ax - b = 0$. It then seems natural to consider the following modification of the original problem: choose x such that $\|Ax - b\|$ is a minimum. The most elegant result is obtained if we interpret $\|\cdot\|$ as the Euclidean norm, because x then has the same form as the general solution of the consistent system. Thus (10.2) represents the general solution if the system (10.1) is consistent and the best approximation if it is inconsistent. As has been observed before, the L_2 solution of an inconsistent linear system is not necessarily unique. However, if A^g is interpreted as the Moore-Penrose inverse, then $x = A^g b$ is the unique vector of smallest Euclidean norm minimizing $\|Ax - b\|_2$. (For a proof, see for example M.Planitz [48, p.183].)

A large number of physical and technological applications lead to inconsistent linear systems. Such an application is the problem of balancing the input streams (feeds) and output streams (products) of a mineral processing plant. (Some of the material of this chapter has appeared in the paper by Voller, Planitz and Reid [47].) Following the article by Wiegel [49] in 1972, a number of computer packages have been designed, which determine material balances from sets of inconsistent measurements. A survey of existing packages can be found in the paper by K.J. Reid [50]. Although most of these packages have been designed for mainframe computers, more recently attention has focused on microcomputers implementations.

The purpose of this chapter is to compare existing techniques for the solution of the fundamental material balance problem and to propose alternatives, with particular reference to microcomputer implementation. We consider a single processing unit with a feed stream (1) and two product streams (2) and (3) as shown in fig.10.1.

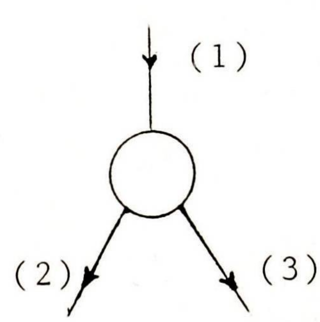


FIG.10.1

It will be assumed that each stream has been assayed for n distinct species. We calculate the mass flow in each stream for the material in the processing unit to balance. This is usually done by obtaining a best least squares solution for the following overdetermined system of n+1 equations:

$$M_1 = M_2 + M_3, \tag{10.3}$$

$$M_1 x_1^k = M_2 x_2^k + M_3 x_3^k, \quad k=1(1)n, \tag{10.4}$$

where M_i denotes the mass flow rate in stream i and x_i^k the assayed percent value of species k in stream i. Eliminating M_3 from (10.3) and (10.4) gives the so-called two-product balance formula

$$M_2 = M_1(x_1^k - x_3^k)/(x_2^k - x_3^k). \tag{10.5}$$

The data in the tables below demonstrate that in practice it is not feasible to use (10.5) in order to determine M_2. Table 10.1 contains a typical set of inconsistent measured assays. Given that $M_1 = 1$, we use (10.5) and (10.3) to obtain the corresponding values of M_2 and M_3 shown in table 10.2.

TABLE 10.1

i	x_i^1	x_i^2
1	23.8	52.1
2	5.3	40.7
3	53.9	63.4

TABLE 10.2

k	M_2	M_3
1	0.6193	0.3807
2	0.4978	0.5022

We therefore modify our problem in the following way.

Denote the unknown exact value of species k in stream i by $\hat{x}_i^k$ and replace the x_i^k by $\hat{x}_i^k$ in equation (10.4). In order to minimize the error in the least squares sense, we require, subject to the constraints (10.3) and (10.4) that

$$J_2 = \sum_{k=1}^{n} J^k = \min! \quad , \tag{10.6}$$

where $J^k = \sum_{j=1}^{3} w_j^k (\hat{x}_j^k - x_j^k)^2$ and w_j^k is a suitable weighting factor. On defining a relative mass flow

$$D = M_2/M_1 \quad ,$$

the $n+1$ constraints reduce to n constraints

$$\hat{x}_1^k = D\hat{x}_2^k + (1-D)\hat{x}_3^k \tag{10.7}$$

There are various ways of solving the problem defined by (10.6) and (10.7). In packages designed for the minerals industry, methods ranging from Lagrange multipliers to direct search techniques have been employed (see Mular [51]). Most solutions start by introducing Lagrange multipliers λ^k, combining (10.6) and (10.7) into a single auxiliary function

$$L = J_2 + \sum_{k=1}^{n} \lambda^k \{ \hat{x}_1{}^k - D\hat{x}_2{}^k - (1-D)\hat{x}_3{}^k \} . \tag{10.8}$$

This approach has been used in a number of large mineral processing material balance packages. These packages then employ a variety of methods to minimize (10.8). Wiegel [49], Cutting [52], and Laguitton and Wilson [53] use a gradient method deriving a set of non-linear equations, which are solved by a linearizing iterative technique. Smith and Ichiyen [54] and Hockings and Callen [55] also employ the gradient method, but combine it with a search over the independent relative mass-flows in the circuit. Hodouin and Everall [56] employ a hierarchical procedure in which the problem is decomposed and a combination of gradient, search, and Newton methods are adopted for maximum efficiency. Setting the partial derivatives of L to zero and re-writing the constraint equations (10.7), we obtain the following $4n+1$ equations:

$$2w_j^k\,(\hat{x}_j^k - x_j^k) - g_j\lambda^k = 0\ , \qquad (10.9a)$$

$$\sum_{k=1}^{n} \lambda^k(\hat{x}_3^k - \hat{x}_2^k) = 0\ , \qquad (10.9b)$$

$$\sum_{j=1}^{3} g_j\hat{x}_j^k = 0\ , \qquad (10.9c)$$

where $g_1 = -1$, $g_2 = D$, $g_3 = 1-D$. In terms of D, equations (10.9a) and (10.9c) give

$$\hat{x}_j^k = x_j^k + g_j r^k/(w_j^k\ h^k), \qquad (10.10)$$

where

$$r^k = x_1^k - Dx_2^k - (1-D)x_3^k \qquad (10.11)$$

is called the residue or imbalance equation and

$$h^k = 1/w_1^k + D^2/w_2^k + (1-D)^2/w_3^k. \qquad (10.12)$$

On substitution of (10.10) into (10.9b), the following polynomial in D is obtained:

$$\sum_{k=1}^{n} (r^k/h^k)\{x_2^k - x_3^k + (r^k/h^k)(D/w_2^k - (1-D)/w_3^k)\} = 0 \quad (10.13)$$

Solving (10.13) iteratively, by Newton's method for example, will give the value of D which minimizes L. The corresponding adjusted assays are then obtained from equation (10.10). This method will be referred to as "LMP" for Lagrange Multiplier Polynomial method.

An alternative method in Voller, Planitz, Reid [47] consists of minimizing

$$J_2^* = \sum_{k=1}^{n} w^{*k}(r^k)^2 , \quad (10.14)$$

where $w^{*k} = 1/h^k$. $\partial J_2^*/\partial D = 0$ leads back to equation (10.13) and the LMP method. If, on the other hand, w^{*k} is treated as a constant by choosing an estimate for D in h^k (via equation (10.5), for example), $\partial J_2^*/\partial D = 0$ gives

$$D = \frac{\sum_{k=1}^{n} w^{*k}(x_2^k - x_3^k)(x_1^k - x_3^k)}{\sum_{k=1}^{n} w^{*k}(x_2^k - x_3^k)^2} . \quad (10.15)$$

The values for D given by (10.15) are substituted into (10.10) in order to obtain the adjusted assay values $\hat{x}_j^k$. This method will be referred to as "MWR" for minimum of weighted residues method. It has obvious computational advantages over LMP, but requires field trials to establish whether it is sufficiently accurate for practical purposes.

Alternatively, we can use penalty functions, an optimization technique which has not yet been employed in the solution of material balance problems. Introducing a large positive constant K, we now minimize

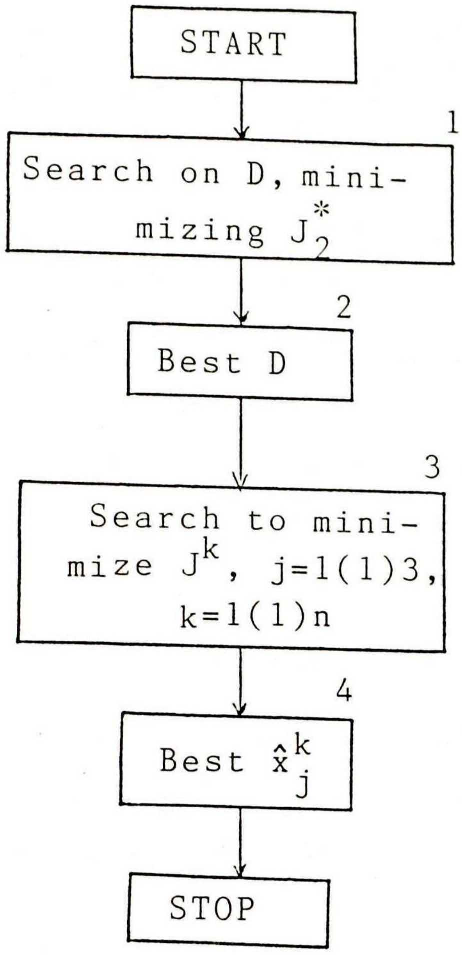
$$L_2^p \equiv J_2 + K \sum_{k=1}^{n} \{\hat{x}_1^k - D\hat{x}_2^k - (1-D)\hat{x}_3^k\}^2 \tag{10.16}$$

The constant K ensures that in the minimization of L_2^p, selections of D and $\hat{x}_j^k$ which violate the mass balance constraints are penalized. The usual gradient method for minimizing L_2^p gives $\hat{x}_j = x_j^k + (g_j r^k / w_j)K/(1+Kh^k)$, (10.17) for the calculation of adjusted assay values, and

$$\sum_{k=1}^{n} Kr^k/(1+Kh^k)\{x_2^k - x_3^k + Kr^k/(1+Kh^k)(D/w_2^k - (1-D)/w_3^k)\} = 0 \tag{10.18}$$

for the calculation of D. For large K, equations (10.17) and (10.18) give values for D and $\hat{x}_j^k$ which are close to those obtained via (10.10), (10.13). Thus for the simple stream process unit, the two methods are roughly equivalent. In the solution of larger problems, the penalty function approach requires further investigation.

The above methods are all gradient methods involving derivatives. In contrast, the flowchart below outlines a hierarchical direct search routine for the solution of the material balance problem defined by equations (10.6) and (10.7). This method will be referred to as "DSM" for direct search method. Steps 1 and 3 were carried out using the Powell quadratic interpolation technique (see G.R. Walsh [57]).



The data of table 10.1 have been reproduced in table 10.3, adding typical percentage standard deviations, σ_j^k, associated with the measurements. The weights w_j^k are inversely proportional to the $(\sigma_j^k)^2$.

TABLE 10.3

i	x_i^1	σ_i^1	x_i^2	σ_i^2
1	23.8	5	52.1	10
2	5.3	5	40.7	10
3	53.9	2	63.4	4

TABLE 10.4

Estimates for D by method

LMP	LMS	MWR	DSM
0.6181	0.6172	0.6181	0.6172

TABLE 10.5

Unadjusted x_j^k	Adjusted $\hat{x}_j^k$				
Input	LMP	LMS	MWR	DSM	ASSAY
23.8	23.85	23.89	23.85	23.89	Type 1
5.3	5.29	5.30	5.29	5.30	
53.9	53.88	53.87	53.88	53.87	
52.1	49.94	49.96	49.95	49.96	Type 2
40.7	41.51	41.51	41.51	41.51	
63.4	63.59	63.59	63.59	63.59	

TABLE 10.6

	LMP	LMS	MWR	DSM
CPU time in seconds	0.4	0.6	0.1	1.0
Number of BASIC lines	40	45	35	70

The four algorithms considered above were coded in BASIC. The results of a comparison between these algorithms are summarized in tables 10.4-10.6. The values of D and $\hat{x}_j^k$ were compatible with those obtained from the mainframe package MATBAL by R.L. Wiegel [49]. For the simple material balance problem, MWR is clearly superior both in CPU time and number of BASIC lines. This is an interesting result, since none of the existing packages use this approach. The BASIC code (MINBAL) for LMS can be found in the appendix of programs. As might be expected, the direct search method (DSM) emerges as the least efficient of the four algorithms. It is unlikely that a more sophisticated search technique would alter the order of merit.

From our results, the MWR method looks promising, and the development along these lines of a full-scale microcomputer package for more complicated processing units seems worthwhile. Such a package could also incorporate adaptive features as suggested in chapter 7. As an example of the use of alternative adjustment criteria, the values of

$$J_1 = \sum_{k=1}^{n} |r^k| \quad \text{and} \quad J_\infty = \max_k |r^k| \tag{10.20}$$

have been minimized, using the test data in table 10.3 to compare various best approximations for the relative mass flow rate D. In table 10.7, these approximations are compared with the values of D obtained by minimizing the weighted sum of squares J_2^* and unweighted sum of squares J_2.

TABLE 10.7

Adjustment criterion	J_1	J_2^*	J_2	J_∞
minimizing value of D	0.6324	0.6181	0.5975	0.5806

The results of table 10.7 indicate that the values of D derived from minimizing J_1 and J_∞ define upper and lower bounds for least squares solutions.

Chapter 11

An Algorithm for Alternative Optimal and Sub-Optimal Solutions in Integer Programming

Standard packages for integer linear programming, such as algorithm HØ2BAF in the N.A.G. library and algorithm 263A in the C.A.C.M. collection, are based on Gomery's cutting plane method and enhanced by a technique known as Wilson's cuts. The purpose of this chapter is to develop an algorithm, which allows the user to search for alternative optimal solutions and for sub-optimal solutions, e.g. all second best solutions, and to solve certain two-stage optimization problems.

More precisely, we wish to determine non-negative integers $x_1,\ldots,x_n$ such that

$$f(\underline{x}) = c_1x_1+\ldots+c_nx_n \tag{11.1}$$

is a minimum (or maximum), subject to linear constraints of the form

$$\underline{A}\ \underline{x} \leq \underline{b} \tag{11.2}$$

where $\underline{x} = (x_1,\ldots,x_n)^T$ and $\underline{A}$ is an m×n matrix. There may also be secondary constraints, e.g. $||x|| = \min!$. The difficulty with this problem lies in the condition that the x_i should be integers, which is equivalent to a non-linear constraint of the form $\sin(\pi x) = 0$. (11.1-2) belongs to a class of so-called NP-complete problems. These are known to be either collectively capable, or collectively incapable, of solution by polynomial-time algorithms. Thus if (11.1-2) could be shown to be polynomial-time soluable, this would be automatically true of other important problems such as Boolean satisfiability or the travelling salesman problem.

We first discuss the existence of an integer solution for the linear diophantine equation

$$c_1x_1+\ldots+c_nx_n = c, \tag{11.3}$$

where $c, c_i \varepsilon Z$, the set of integers. If such a solution exists, then the greatest common divisor $g = (c_1,\ldots,c_n)$ of the c_i must be a factor of c. To show that the converse is also true we require some results from number theory. (Theorems 11.1-4 follow the treatment in Niven and Zuckerman [68].) It will be convenient to begin with the two-variable case.

<u>Theorem 11.1</u> Let $b,c\varepsilon Z$. If $g = (b,c)$, then there exist integers x_o,y_o such that

$$g = bx_o+cy_o.$$

<u>Proof</u> Choose x_o,y_o so that $m = bx_o+cy_o$ is the smallest positive integer of the form $bx+cy$, where $x,y\varepsilon Z$. We show that $m|b$, i.e. m is a factor of b. To obtain a contradiction, assume that $m\nmid b$. Then there are integers q,r such that

$$b = mq+r, \quad 0 < r < m,$$

i.e. $$r = b-mq = b - (bx_o+cy_o)q$$

$$= bx_1+cy_1 < bx_o+cy_o,$$

where $x_1 = 1 - x_o$, $y_1 = -qy_o$.

But this inequality contradicts the definition of m, hence $m|b$. We can similarly show that $m|c$. Since $g = (b,c)$, there are integers k_1, k_2 such that $b = gk_1$, $c = gk_2$ and $m = bx_o+cy_o = g(k_1x_o+k_2y_o)$. It follows that $g|m$, i.e. $g \leqq m$. But $g < m$ contradicts $g = (b,c)$. Hence $g=m$. //

From the above proof we immediately obtain

<u>Theorem 11.2</u> $g = (b,c)$ is the least positive value of $bx+cy$, where x,y range over Z.

The theorem below is a generalization of theorem 11.2 to n variables and will be stated without proof.

<u>Theorem 11.3</u> Given any integers $c_1,\ldots,c_n$ (not all 0), with $g = (c_1,\ldots,c_n)$, there exist integers $x_1,\ldots,x_n$ such that

$$g = \sum_{i=1}^{n} c_i x_i.$$

g is the least positive value of the linear form $\sum_{i=1}^{n} c_i y_i$, with y_i ranging over Z.

Now suppose $g|c$. By the above theorem there exist integers $x_1,\ldots,x_n$ such that

$$g = \sum_{i=1}^{n} c_i x_i$$

Since $g|c$, there exists $g \varepsilon Z$ such that $c=kg$. Hence

$y_i = kx_i$ is a solution of (11.3). We therefore have the following result.

<u>Theorem 11.4</u> The linear diophantine equation

$$c_1x_1+\ldots+c_nx_n = c \tag{11.3}$$

has an integer solution if and only if $(c_1,\ldots,c_n)|c$.

The integer solutions of (11.3) are obtained by reduction to the two-variable case. We therefore first consider the equation

$$ax+by = c. \tag{11.4}$$

Note that if $(a,b) = 1$ and x_o, y_o is any integer solution of (11.4), then all integer solutions are of the form

$$\begin{aligned} x &= x_o - bt \\ y &= y_o + at \end{aligned} \tag{11.5}$$

$t = 0, \pm 1, \pm 2, \ldots$. To see this, let x, y be any other integer solution. Then

$$ax - ax_o + by - by_o = 0$$

i.e. $$y - y_o = (a/b)(x_o - x).$$

Since $(a,b) = 1$, $b|(x_o - x)$, i.e. $x_o - x = bt$, for some t, and $y - y_o = at$. The converse follows by direct substitution of (11.5) into (11.4). The problem of solving (11.4) is now reduced to finding an initial solution x_o, y_o. The algorithm for determining x_o, y_o involves continued fractions. Recall that any rational number a/b $(a,b \in \mathbb{Z}, b \neq 0)$ can be written as a finite continued fraction of the form

$$[a_o,a_1,\ldots,a_n] = a_o + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{\ddots}{\cfrac{1}{a_{n-1} + \cfrac{1}{a_n}}}}}$$

The (n-1)th convergent of $[a_o,a_1,\ldots,a_n]$ is the rational number defined by

$$P_{n-1}/Q_{n-1} = [a_o,a_1,\ldots,a_{n-1}],$$

with P_{n-1}, $Q_{n-1} \varepsilon Z$, $Q_{n-1} \neq 0$.

We assume that $(a,b) = 1$ and apply the Euclidean algorithm:

$$\begin{aligned}
a/b &= a_o + 1/(b/r_1), & 0 < r_1 < b,\\
b/r_1 &= a_1 + 1/(r_1/r_2), & 0 < r_2 < r_1,\\
r_1/r_2 &= a_2 + 1/(r_2/r_3), & 0 < r_3 < r_2,\\
&\vdots\\
r_{n-2}/r_{n-1} &= a_{n-1} + 1/(r_{n-1}/r_n), & 0 < r_n < r_{n-1},\\
r_{n-1}/r_n &= a_n.
\end{aligned}$$

Hence $a/b = [a_o,a_1,\ldots,a_n]$. If we define the convergents

$$\Delta_o = [a_o],\quad \Delta_1 = [a_o,a_1],\quad \ldots,\quad \Delta_k = [a_o,\ \ldots,\ a_k],$$

with $\Delta_k = P_k/Q_k$, $1 \leq k \leq n$,

then

$\Delta_o = a_o$, i.e. $P_o = a_o$ and $Q_o = 1$,

$\Delta_1 = a_o + 1/a_1$, i.e. $P_1 = a_o a_1 + 1$ and $Q_1 = a_1$,

$\Delta_2 = a_o + 1/(a_1 + 1/a_2)$, i.e. $P_2 = a_o a_1 a_2 + a_o + a_2 =$

$a_2 P_1 + a_o$ and $Q_2 = a_1 a_2 + 1 = a_2 Q_1 + a_o$.

Using induction, it is easy to prove that

$$P_k = a_k P_{k-1} + P_{k-2} \quad \text{and} \quad Q_k = a_k Q_{k-1} + Q_{k-2}, \tag{11.6}$$

for $k=2,\ldots,n$. Applying (11.6) repeatedly gives

$$\Delta_k - \Delta_{k-1} = \frac{P_k Q_{k-1} - Q_k P_{k-1}}{Q_k Q_{k-1}} = \frac{(-1)(P_{k-1}Q_{k-2} - Q_{k-1}P_{k-2})}{Q_k Q_{k-1}}$$

$$= \ldots = \frac{(-1)^{k-2}(P_2 Q_1 - Q_2 P_1)}{Q_k Q_{k-1}} = \frac{(-1)^{k-1}}{Q_k Q_{k-1}} \;.$$

Hence $\Delta_n - \Delta_{n-1} = a/b - \Delta_{n-1} = (-1)^{n-1}/(bQ_{n-1})$,

i.e. $aQ_{n-1} - bP_{n-1} = (-1)^{n-1}$

i.e. $a[(-1)^{n-1}cQ_{n-1}] + b[(-1)^n cP_{n-1}] = c$.

It follows that for $a,b \in \mathbb{Z}$ $x_o = (-1)^{n-1}cQ_{n-1}\operatorname{sgn} a$ and $y_o = (-1)^n cP_{n-1}\operatorname{sgn} b$. We therefore have the following result.

<u>Theorem 11.5</u> If $(a,b) = 1$, then all integer solutions of $ax + by = c$ are given by

$$\begin{aligned} x &= (-1)^{n-1}c\, Q_{n-1}\operatorname{sgn} a - bt, \\ y &= (-1)^n c\, P_{n-1}\operatorname{sgn} b + at, \end{aligned} \tag{11.7}$$

with P_{n-1}, Q_{n-1} defined as above.

Example 11.1 Determine all non-negative integer pairs x, y such that $5x + 3y = c$ is minimal subject to the constraints

$$\begin{aligned} 11x + 15y &\leqq 100 \\ -5x - 3y &\leqq -20 \\ 3x - y &\leqq 12. \end{aligned}$$

The N.A.G. routine HØ2BAF gives $c_{min} = 20$ for $(x,y) = (4,0)$. Since $5/3 = [1,1,2]$, we have $n=2$, $P_1=2$, and $Q_1=1$. Hence $x = -20-3t$ and $y = 40+5t$, $t=0,\pm1,\pm2,\ldots$. The constraints $x, y \geqslant 0$ imply $t = -8$ or -7, which gives $(x,y) = (4,0)$ or $(1,5)$. Both points are seen to be feasible. To find any second best, sub-optimal solutions, set $c=21$. Then $x = -21-3t$ and $y = 42+5t$, $t = 0,\pm1,\pm2,\ldots$, and we similarly obtain $(x,y) = (3,2)$ or $(0,7)$. //

Now consider the general case

$$c_1x_1 + \ldots + c_nx_n = c, \tag{11.3}$$

$n>2$. A simple inductive proof can be found in Niven and Zuckerman [68]. We proceed constructively: set

$$x_{n-1} = \alpha_1 v_1 + \alpha_2 v_2, \qquad x_n = \beta_1 v_1 + \beta_2 v_2.$$

If α_1, α_2, β_1, β_2 are chosen so that

$$\alpha_1\beta_2 - \alpha_2\beta_1 = 1, \tag{11.8}$$

then

$$\begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} x_{n-1} \\ x_n \end{pmatrix} \tag{11.9}$$

and

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} \beta_2 & -\alpha_2 \\ -\beta_1 & \alpha_1 \end{pmatrix} \begin{pmatrix} x_{n-1} \\ x_n \end{pmatrix} . \tag{11.10}$$

Putting $\alpha_2 = c_n/(c_{n-1},c_n)$, $\beta_2 = -c_{n-1}/(c_{n-1},c_n)$, we have $(\alpha_2,\beta_2) = 1$ and can use the two-variable method to determine α_1,β_1 so that (11.8) is satisfied.
It then follows that

$$c_{n-1}x_{n-1} + c_n x_n = (c_{n-1}\alpha_1 + c_n\beta_1)v_1,$$

i.e. (11.3) has been reduced to $n-1$ unknowns $x_1,\ldots,x_{n-2}$, v_1. Next put

$$x_{n-2} = \alpha_3 v_3 + \alpha_4 v_4, \quad v_1 = \beta_3 v_3 + \beta_4 v_4$$

to reduce the unknowns to $x_1,\ldots,x_{n-3},v_3$. The process is continued until only two unknowns remain, x_1 and v_{2n-5}. The last two substitutions are as follows

$$x_3 = \alpha_{2n-7}v_{2n-7} + \alpha_{2n-6}v_{2n-6}, \quad v_{2n-9} = \beta_{2n-7}v_{2n-7} + \beta_{2n-6}v_{2n-6},$$

$$x_2 = \alpha_{2n-5}v_{2n-5} + \alpha_{2n-4}v_{2n-4}, \quad v_{2n-7} = \beta_{2n-5}v_{2n-5} + \beta_{2n-4}v_{2n-4}.$$

(11.3) now takes the form

$$ax_1 + bv_{2n-5} = c, \tag{11.11}$$

where a and b are integer coefficients. We apply (11.7) to (11.11) and obtain the general solution

$$x_1 = k - bt_1,$$

$$v_{2n-5} = \ell + at_1,$$

$t_1 = 0, \pm 1, \pm 2, \ldots$. Backsubstitution now gives the solution of (11.3) in terms of n-1 arbitrary parameters $t_1, \ldots, t_{n-1}$. We find

$$x_2 = \alpha_{2n-5} v_{2n-5} + \alpha_{2n-4} v_{2n-4} = \alpha t_1 + \beta t_2 + \gamma,$$

where $\alpha = \alpha_{2n-5} a$, $\beta = \alpha_{2n-4}$, $\gamma = \alpha_{2n-5} \ell$ and $t_2 = v_{2n-4}$.

Similarly x_j is seen to be a linear form in t_1, t_2, t_3, where $t_3 = v_{2n-6}$. Putting $t_4 = v_{2n-8}, \ldots, t_{n-1} = v_2$ and continuing in this way, we find the solution of (11.3) in triangular form

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} d_{11} & 0 & 0 & \cdots & 0 \\ d_{21} & d_{22} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ d_{n-1,1} & d_{n-1,2} & d_{n-1,3} & \cdots & d_{n-1,n-1} \\ d_{n,1} & d_{n,2} & d_{n,3} & \cdots & d_{n,n-1} \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_{n-2} \\ t_{n-1} \end{pmatrix} + \underline{k},$$

where

$d_{11} = -b, \qquad k_1 = k$

$d_{21} = a\alpha_{2n-5}$, $d_{22} = \alpha_{2n-4}$, $k_2 = \alpha_{2n-5}\ell$;

$d_{31} = a\alpha_{2n-7}\beta_{2n-5}$, $d_{32} = \alpha_{2n-7}\beta_{2n-4}$,

$d_{33} = \alpha_{2n-6}$, $k_3 = \alpha_{2n-7}\beta_{2n-5}\ell$;

$\vdots$

$d_{r,1} = a\alpha_{2n-(2r+1)}\beta_{2n-(2r-1)}\beta_{2n-(2r-3)} \cdots \beta_{2n-5}$,

$d_{r,s} = \alpha_{2n-(2r+1)}\beta_{2n-2s}\beta_{2n-(2r-1)}\beta_{2n-(2r-3)} \cdots \beta_{2n-(2s+3)}$,

$s = 2, \ldots, r-1$,

$d_{r,r} = \alpha_{2n-2r}, \quad k_r = d_{r1}\, \ell/a, \qquad r=4,\ldots,n-1;$

$\vdots$

$d_{n,1} = a\beta_1\beta_3\beta_5 \cdots \beta_{2n-5},$

$d_{n,s} = \beta_{2n-2s}\beta_1\beta_3\beta_5 \cdots \beta_{2n-(2s+3)}, \quad s=2,\ldots,n-1,$

$k_n = d_{n,1}\, \ell/a.$

In many operations research problems, the c_i are non-negative, which allows us to determine upper bounds s_i for the x_i :

$$\underline{0} \leqq \underline{x} = \underline{D}\,\underline{t} + \underline{k} \leqq \underline{s} \ ,$$

where $\underline{s} = (c/c_1,\ldots,c/c_n)$. Hence

$$\underline{\ell} \leqq \underline{D}\,\underline{t} \leqq \underline{L} \ ,$$

where $\underline{\ell} = -\underline{k}$ and $\underline{L} = \underline{s} - \underline{k}$. To obtain bounds $\underline{m}$, $\underline{M}$ such that

$$\underline{m} \leqq \underline{t} \leqq \underline{M}$$

we proceed as follows. First assume that $d_{11},\ldots,d_{n-1,n-1}, d_{n,n-1} > 0$; if any of these are negative, upper and lower bounds are interchanged.

From $\ell_1 \leqq d_{11}t_1 \leqq L_1$, we find

$$m_1 = \ell_1/d_{11}, \quad M_1 = L_1/d_{11}.$$

For $k = 2,\ldots,n-1$,

$$(\ell_k - d_{k,1}t_1 - \cdots - d_{k,k-1}t_{k-1})/d_{kk} \leqq t_k \leqq (L_k - d_{k,1}t_1 - \cdots - d_{k,k-1}t_{k-1})/d_{kk}. \tag{11.12}$$

In the LHS (RHS) of (11.12) set

$$t_r = m_r, M_r, \text{ or } 0$$

according as $-d_{kr}(+d_{kr})$ is positive, negative, or zero.

Finally use

$$(\ell_n - d_{n,1}t_1 - \dots - d_{n,n-2}t_{n-2})/d_{n,n-1} \le t_{n-1} \le$$

$$(L_n - d_{n,1}t_1 - \dots - d_{n,n-2}t_{n-2})/d_{n,n-1}$$

to adjust m_{n-1}, M_{n-1} if necessary.

The bounds m_i, M_i found in this way are then used to limit the search for feasible optimal points. The method is demonstrated in the example below.

<u>Example 11.2</u> Solve the equation

$$2x_1 + x_2 + 5x_3 + 3x_4 = 18, \tag{11.13}$$

subject to the constraints

$$\begin{aligned} x_1 - x_2 + 5x_3 + x_4 &\le 10 \\ 3x_1 + x_2 - x_3 + 2x_4 &\le 15 \\ -x_1 + 2x_2 + x_3 - x_4 &\le 5 \\ x_1 + x_2 + x_3 + x_4 &\le 8. \end{aligned}$$

Putting $x_3 = \alpha_1 v_1 + \alpha_2 v_2$, $x_4 = \beta_1 v_1 + \beta_2 v_2$,

$\alpha_2 = 3/(5,3) = 3$, $\beta_2 = -5/(5,3) = -5$, we have

$\alpha_1\beta_2 - \alpha_2\beta_1 = -5\alpha_1 - 3\beta_1 = 1$. Now solve

$$5\alpha_1 + 3\beta_1 = -1.$$

$5/3 = [1,1,2]$, $P_1 = 2$, $Q_1 = 1$,

i.e. $\alpha_1 = 1$, $\beta_1 = -2$. Hence (11.13) becomes

$$2x_1 + x_2 - v_1 = 18. \tag{11.14}$$

Now put $x_2 = \alpha_3 v_3 + \alpha_4 v_4$, $v_1 = \beta_3 v_3 + \beta_4 v_4$,

$\alpha_4 = \beta_4 = -1$, i.e. $\alpha_3\beta_4 - \alpha_4\beta_3 = -\alpha_3 + \beta_3 = 1$.

From $1/1 = [0,1]$, $P_o = 0$, $Q_o = 1$ we obtain

$\alpha = -1$, $\gamma = 0$. Hence (11.14) becomes

$$2x_1 - v_3 = 18 \tag{11.15}$$

$2/1 = [1,1]$, $P_o = 1$, $Q_o = 1$ gives

$$x_1 = 18 + t_1, \quad v_3 = 18 + 2t_1.$$

Backsubstitution with $t_2 = v_4$, $t_3 = v_2$ now gives

$x_2 = -18-2t_1-t_2$, $x_3 = -t_2 + 3t_3$, $x_4 = 2t_2 - 5t_3$.

Using $\qquad 0 \leq x_i \leq 18/c_i$,

We find

$$\begin{pmatrix} -18 \\ 18 \\ 0 \\ 0 \end{pmatrix} \leq \begin{pmatrix} 1 & 0 & 0 \\ -2 & -1 & 0 \\ 0 & -1 & 3 \\ 0 & 2 & -5 \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \leq \begin{pmatrix} -9 \\ 36 \\ 3.6 \\ 6 \end{pmatrix},$$

and hence

$$-18 \leq t_1 \leq -9, \ -18 \leq t_2 \leq 18, \ -8 \leq t_3 \leq 8. \tag{11.16}$$

(11.16) defines a superset of the feasible parameter set, but any infeasible solutions are easily eliminated. The above bounds give 10 feasible solutions (see appendix of programs). //

<u>Example 11.3</u> This problem is a worked example for the N.A.G. library routine HØ2BAF : minimize $c = x_1 + 2x_2$, subject to the constraints $2x_1 + 2x_2 \leq 11$, $-x_1 + 3x_2 \leq 10$, $x_1 - x_2 \leq 2$, $-5x_1 - 15x_2 \leq -33$, $-16x_1 - 8x_2 \leq -33$,

where x_1, x_2 are non-negative integers. The answer given is $c_{min} = 6$ for $(x_1, x_2) = (2,2)$. Using ILP (see appendix), we obtain suboptimal solutions $(x_1, x_2) = (3,2)$, $(1,3)$ for $c = 7$, and $(2,3)$ for $c = 8$. //

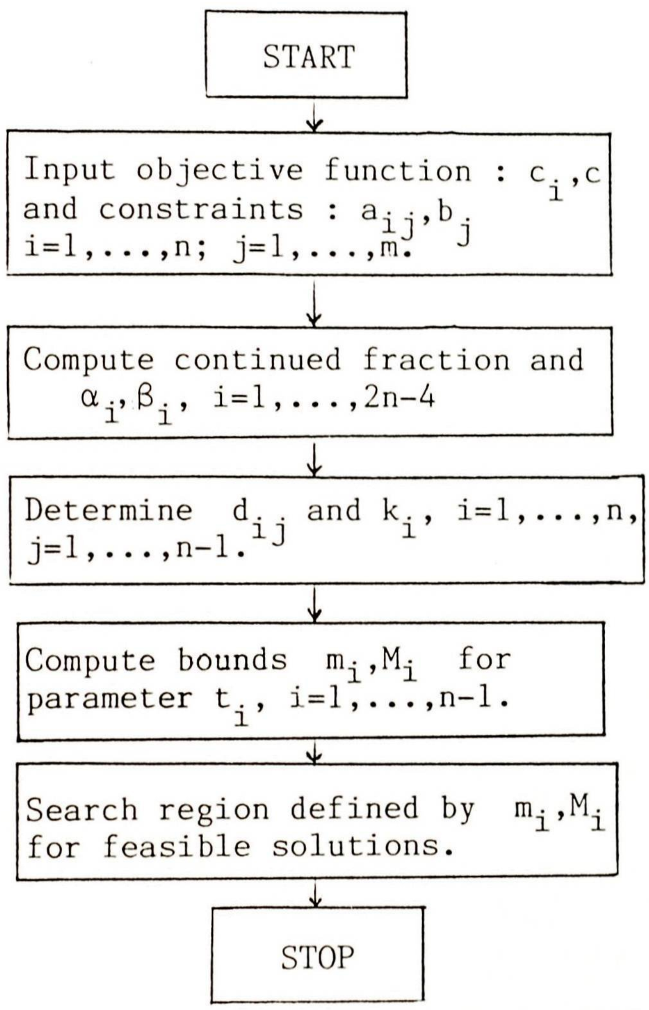
For many applications, secondary constraints of the form $||\underline{x}|| = \min!$ are of interest. Thus, if in example 11.2, we require Σx_i^2 to be minimal, the (unique) solution is $\underline{x} = (0,2,2,2)$.

<u>Example 11.4</u> $c = 2x_1 + x_2 + 5x_3 + 3x_4 = \min!$, subject to the constraints of example 11.2 and additional constraints

$$- x_1, \; - x_2, \; - x_3, \; - x_4 \leqq - 1$$
$$- x_2 - x_4 \leqq - 3$$
$$- x_1 - x_4 \leqq - 5.$$

The N.A.G. library routine HØ2BAF gives $c_{min} = 18$ for $\underline{x} = (4,2,1,1)$. Searching the region defined by (11.16), produces a second optimal solution (3,1,1,2) which is, in fact, the unique minimum-norm solution. //

A FORTRAN version of the algorithm, called ILP (coded by P.J. Watts), is included in the appendix of programs. ILP, like other integer programming routines, is liable to exceed available time resources. An obvious partial remedy lies in speeding up the tree search by parallel processing. Further savings could perhaps be achieved by sharpening the bounds m_i, M_i. It is clear that ILP can also function as an ordinary integer programming routine. A lower bound b for the minimum of $f(\underline{x})$ can sometimes be obtained from physical considerations or by solving the associated continuous problem. ILP is then run with $c = b, b+1, b+2, \ldots$ until an optimal feasible solution is found. For problems with many variables, this is obviously an inefficient process. However, if some estimate $\hat{\underline{x}}$ of the optimal solution $\underline{x}$ is available, we can solve $\hat{\underline{x}} = \underline{D}\,\underline{t}+\underline{k}$ for $\underline{t}$ and then restrict the search to some neighbourhood of $\underline{t}$, keeping within the limits of our time resources. We conclude this chapter with a brief description of ILP.



All variables are integers : XK = k, VL = ℓ, T(I) = t_i, BE(I) = β_i, AL(I) = α_i, IMN(I) = m_i, IMX(I) = M_i, D(I,J) = d_{ij}, CON(I) = k_i.

There are 3 subroutines :

INPUT(M,N,A,B,C), CONVGT(I,J,PN,QN,NC), CONFRA(A,B,E,RN,NC). CONVGT computes the convergents P_n, Q_n; CONFRA determines the continued fraction $A/B = [a_o, \ldots, a_k]$. Formal parameters: M = m, N = n, A(A,J) = a_{ij}, B(I) = b_i, C(I) = c_i, PN = P_n, QN = Q_n, E(I) = a_i, RN = highest common factor, NC = k.

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APPENDIX OF PROGRAMS

```
C
C           SUBROUTINE MINMAX
C           DRIVER PROGRAM
C
      IMPLICIT REAL (A - H, O - Z)
      INTEGER*4 K10, K20
      PARAMETER (N = 1001)
      DIMENSION X(N), Y(N), E(N)
      COMMON X, Y, E
5     WRITE(1, 1)
1     FORMAT(//'INPUT NUMBER OF POINTS'/)
      READ(1, *) NPTS
6     WRITE(1, 7)
7     FORMAT(//'TYPE 1 TO INPUT INTERACTIVELY'/
     *         'ELSE TYPE 2 FOR EXPONENTIAL FUNCTION')
      READ(1, *, ERR = 6) IREPLY
      IF(IREPLY .EQ. 2) GO TO 9
      IF(IREPLY .NE. 1) GO TO 6
      CALL INTER(X, Y, NPTS)
      GO TO 11
9     DO 10 I = 1, NPTS
      X(I) = 0.01 * FLOAT(I - 1)
      P = X(I)
      Y(I) = EXP(P)
10    CONTINUE
11    CALL CTIM£A(K10)
      CALL MINMAX(NPTS, X, Y, E, ITER, ERROR, A, B, C, D)
      CALL CTIM£A(K20)
      TI = FLOAT(K20 - K10) / 1000.
      WRITE(1, 20) C, D, A, B, ERROR, ITER, TI
20    FORMAT(/'L2 LINE'/'GRADIENT: ', 1PE12.3/
     *        'INTERCEPT: ', 1PE12.3//
     *        'MINMAX LINE'/'GRADIENT: ',
     *        1PE12.3/'INTERCEPT: ', 1PE12.3/
     *        'MAXIMUM ERROR: ', 1PE12.3//
     *        'NUMBER OF ITERATIONS: ', I4/
     *        'CPU TIME IN SECONDS: ', 1PE9.2)
25    WRITE(1, 30)
30    FORMAT(///'DO YOU WISH TO CONTINUE'/'TYPE Y OR N')
      READ(1, 35) IREPLY
35    FORMAT(A1)
      IF (IREPLY .EQ. 'Y') GO TO 5
      IF (IREPLY .EQ. 'N') STOP
      GO TO 25
      END
C
C
C
C
C
      SUBROUTINE MINMAX(N, X, Y, E, ITER, ERROR,
     *                  A, B, C, D)
C
C        THIS SUBROUTINE COMPUTES THE L2 LINE
C        FOR A GIVEN SET OF DATA AND THEN USES
C        A MODIFIED EXCHANGE ALGORITHM TO OBTAIN
C        THE MINMAX LINE FOR THE SAME DATA
C
      REAL X(N), Y(N), E(N), A, C, SX, SY, SXY,
     *     SXX, D, C, AMAX, TEST, ERROR, B,
     *     SIZE, SGNIND, SGNONE
      LOGICAL L1, L2, L3, L4
C
C        FIND THE LEAST SQUARES LINE
C
      SX = 0.0
      SY = 0.0
      SXY = 0.0
      SXX = 0.0
      DO 40 I = 1, N
      SX = SX + X(I)
      SY = SY + Y(I)
      SXY = SXY + X(I) * Y(I)
      SXX = SXX + X(I) * X(I)
40    CONTINUE
      D = (SY * SXX - SX * SXY) / (N * SXX - SX * SX)
      C = (N * SXY - SX * SY) / (N * SXX - SX * SX)
C
C        THIS GIVES THE L2 LINE Y = C*X + D
C        NEXT OBTAIN ERRORS OF L2 LINE
```

```
C
      DO 60 I = 1, N
      E(I) = D + C * X(I) - Y(I)
60    CONTINUE
C
C        THE NUMERICALLY LARGEST ERRORS OBEYING
C        SIGN PROPERTY ARE CHOSEN
C
C        CASE 1: MAX ABS ERROR IS NEITHER E(1) NOR E(N),
C        CASE 2: ABS(E(1)) IS MAX,
C        CASE 3: ABS(E(N)) IS MAX.
C        FIRST OBTAIN MAX ERROR
C
      AMAX = ABS(E(1))
      IND = 1
      DO 70 I = 2, N
      TEST = ABS(E(I))
      IF (AMAX .GE. TEST) GO TO 70
      AMAX = TEST
      IND = I
70    CONTINUE
      IF (IND .EQ. 1) GO TO 200
      IF (IND .EQ. N) GO TO 300
C
C       CASE 1: NEITHER E(1) NOR E(N) GIVE MAX ABS ERROR
C
      I2 = IND
      AMAX =  - 1.0
      IFIRST = IND + 1
      DO 80 I = IFIRST, N
      TEST = ABS(E(IND) - E(I))
      IF (AMAX .GE. TEST) GO TO 80
      AMAX = TEST
      I3 = I
80    CONTINUE
      AMAX =  - 1.0
      ILAST = IND - 1
      DO 90 I = 1, ILAST
      TEST = ABS(E(IND) - E(I))
      IF (AMAX .GE. TEST) GO TO 90
      AMAX = TEST
      I1 = I
90    CONTINUE
      GO TO 320
C
C       CASE 2: E(1) GIVES MAX ABS ERROR
C
200   I1 = 1
      AMAX =  - 1.0
      DO 100 I = 2, N
      TEST = ABS(E(1) - E(I))
      IF (AMAX .GE. TEST) GO TO 100
      AMAX = TEST
      I2 = I
100   CONTINUE
      AMAX =  - 1.0
      IFIRST = I2 + 1
      DO 110 I = IFIRST, N
      TEST = ABS(E(I2) - E(I))
      IF (AMAX .GE. TEST) GO TO 110
      AMAX = TEST
      I3 = I
110   CONTINUE
      GO TO 320
C
C        CASE 3: E(N) GIVES MAX ABS ERROR
C
300   I3 = N
      AMAX =  - 1.0
      ILAST = N - 1
      DO 310 I = 2, ILAST
      TEST = ABS(E(N) - E(I))
      IF (AMAX .GE. TEST) GO TO 310
      AMAX = TEST
      I2 = I
310   CONTINUE
      AMAX =  - 1.0
      ILAST = I2 - 1
      DO 315 I = 2, ILAST
      TEST = ABS(E(I2) - E(I))
```

```
      IF (AMAX .GE. TEST) GO TO 315
      AMAX = TEST
      I1 = I
315   CONTINUE
C
C        THE INITIAL TRIPLE IS X(I1), Y(I1); X(I2), Y(I2);
C        X(I3), Y(I3). THE FIRST EQUAL ERROR LINE WILL
C        NOW BE FOUND. ITER IS THE NUMBER OF EQUAL ERROR
C        LINES NEEDED TO OBTAIN THE MINIMAX LINE Y = A*X + B
320   ITER = 0
330   ERROR = 0.5 * ((X(I1) - X(I2)) * (Y(I2) - Y(I3)) +
     *        (X(I3) - X(I2)) * (Y(I1) - Y(I2))) /
     *        (X(I1) - X(I3))
      ITER = ITER + 1
      A = (Y(I3) - Y(I1)) / (X(I3) - X(I1))
      B = Y(I1) + ERROR - A * X(I1)
      AMAX =  - 1.0
      DO 350 I = 1, N
      E(I) = B + A * X(I) - Y(I)
      SIZE = ABS(E(I))
      IF (AMAX .GE. SIZE) GO TO 350
      AMAX = SIZE
      IND = I
350   CONTINUE
      IF (IND. EQ. I1 .OR. IND .EQ. I2 .OR.
     *    IND .EQ. I3) GO TO 500
C
C        THE ABOVE DETERMINES IF THE MINIMAX LINE
C        HAS BEEN FOUND. IF NOT, THE EXCHANGE
C        ALGORITHM WILL NOW BE ACTIVATED
C
      SGNIND = DSIGN(1.0, E(IND))
      SGNONE = DSIGN(1.0, E(I1))
C
C        X(IND) TO LEFT OF X(I1)
C
      L1 = X(IND) .LT. X(I1)
C
C        X(IND) BETWEEN X(I1) AND X(I2)
C
      L2 = X(IND) .GT. X(I1) .AND. X(IND) .LT. X(I2)
C
C        X(IND) BETWEEN X(I2) AND X(I3)
C
      L3 = X(IND) .GT. X(I2) .AND. X(IND) .LT. X(I3)
C
C              X(IND) TO RIGHT OF X(I3)
C
      L4 = X(IND) .GT. X(I3)
      IF (SGNIND .EQ. SGNONE) GO TO 400
C
C        E(IND) AND E(I1) HAVE THE SAME SIGN
C
      IF (.NOT. L1) GO TO 380
      I3 = I2
      I2 = I1
      I1 = IND
      GO TO 330
380   IF (L4) GO TO 390
      I2 = IND
      GO TO 330
390   I1 = I2
      I2 = I3
      I3 = IND
      GO TO 330
C
C        E(IND) AND E(I1) HAVE SAME SIGN
C
400   IF (L3 .OR. L4) GO TO 410
      I1 = IND
      GO TO 330
410   I3 = IND
      GO TO 330
C
C        EXCHANGE IS NOW COMPLETE
C
500   ERROR = ABS(ERROR)
      RETURN
      END
C
```

```
C
C         END OF SUBROUTINE MINMAX
C
C
      SUBROUTINE INTER(X, Y, NPTS)
      IMPLICIT REAL (A - H, O - Z)
      DIMENSION X(NPTS), Y(NPTS)
      WRITE(1, 1) NPTS
1     FORMAT('TYPE IN ', I3, ' PAIRS')
      DO 12 I = 1, NPTS
      WRITE(1, 2)I
2     FORMAT(T12, I4)
      READ(1,  *) X(I), Y(I)
12    CONTINUE
      RETURN
      END


INPUT NUMBER OF POINTS
31


TYPE 1 TO INPUT INTERACTIVELY
ELSE TYPE 2 FOR EXPONENTIAL FUNCTION
1
TYPE IN  31 PAIRS
           1
0. 0.
           2
1. 1.
           3
2. 1.
           4
3. 2.
           5
4. 1.
           6
5. 3.
           7
6. 2.
           8
7. 2.
           9
8. 3.
          10
9. 5.
          11
10. 3.
          12
11. 4.
          13
12. 5.
          14
13. 4.
          15
14. 5.
          16
15. 6.
          17
16. 6.
          18
17. 5.
          19
18. 7.
          20
19. 6.
          21
20. 8.
          22
21. 7.
          23
22. 7.
          24
23. 8.
          25
24. 7.
          26
```

```
25. 9.
              27
26. 11.
              28
27. 10.
              29
28. 12.
              30
29. 11.
              31
30. 13.

L2 LINE
GRADIENT:       3.706E-01
INTERCEPT:       5.444E-02

MINMAX LINE
GRADIENT:       3.810E-01
INTERCEPT:      -2.857E-01
MAXIMUM ERROR:        1.857E 00

NUMBER OF ITERATIONS:      1
CPU TIME IN SECONDS:   1.00E-03


DO YOU WISH TO CONTINUE
TYPE Y OR N
Y


INPUT NUMBER OF POINTS
210


TYPE 1 TO INPUT INTERACTIVELY
ELSE TYPE 2 FOR EXPONENTIAL FUNCTION
2

L2 LINE
GRADIENT:       3.169E 00
INTERCEPT:       8.332E-02

MINMAX LINE
GRADIENT:       3.390E 00
INTERCEPT:       1.257E-01
MAXIMUM ERROR:        8.743E-01

NUMBER OF ITERATIONS:      3
CPU TIME IN SECONDS:   6.00E-03


DO YOU WISH TO CONTINUE
TYPE Y OR N
Y


INPUT NUMBER OF POINTS
1001


TYPE 1 TO INPUT INTERACTIVELY
ELSE TYPE 2 FOR EXPONENTIAL FUNCTION
2

L2 LINE
GRADIENT:       1.061E 03
INTERCEPT:      -3.092E 03

MINMAX LINE
GRADIENT:       2.203E 03
INTERCEPT:      -7.375E 03
MAXIMUM ERROR:        7.376E 03

NUMBER OF ITERATIONS:      3
CPU TIME IN SECONDS:   2.70E-02
```

```
C             SUBROUTINE EXTRAP
C             DRIVER ROUTINE
C
        WRITE(1,10)
10      FORMAT(/'TYPE IN GRADIENT AND INTERCEPT OF',
     +        ' L1, L2 AND MINIMAX LINES')
        READ(1,*) A,B,C,D,E,F
        WRITE(1,20)
20      FORMAT(/'TYPE IN VALUE OF X')
        READ(1,*) X
        CALL EXTRAP(A,B,C,D,E,F,X,YMIN,YMAX,ICODE,JCODE)
        WRITE(1,30) YMIN,ICODE,YMAX,JCODE
30      FORMAT(/'YMIN= ',1PE12.3/'CODE= ',I1//
     +        'YMAX= ', E12.3/'CODE= ', I1)
        WRITE(1,40)
40      FORMAT(/'CODE = 1, 2, 3 DENOTES L1, L2, MINIMAX LINE'
     +        ' RESPECTIVELY')
        STOP
        END
C
C
C
C
C
        SUBROUTINE EXTRAP(A,B,C,D,E,F,X,
     +                    YMIN,YMAX,ICODE,JCODE)
        ICODE = 1
        YMIN = A*X + B
        TEMP = C*X + D
        IF (YMIN .LE. TEMP) GO TO 10
        YMIN = TEMP
        ICODE = 2
10      TEMP = E*X + F
        IF (YMIN .LE. TEMP) GO TO 20
        YMIN = TEMP
        ICODE = 3
20      JCODE = 1
        YMAX = A*X + B
        TEMP = C*X + D
        IF (YMAX .GE. TEMP) GO TO 30
        YMAX = TEMP
        JCODE = 2
30      TEMP = E*X + F
        IF (YMAX .GE. TEMP) GO TO 40
        YMAX = TEMP
        JCODE = 3
40      RETURN
        END
```

```
TYPE IN GRADIENT AND INTERCEPT OF L1, L2 AND MINIMAX LINES
.5 0. .5 -.1566667 .5 -.25

TYPE IN VALUE OF X
3

YMIN=    1.250E 00
CODE= 3

YMAX=    1.500E 00
CODE= 1

CODE = 1, 2, 3 DENOTES L1, L2, MINIMAX LINE RESPECTIVELY
```

```
C        SUBROUTINE SOLVE
C        DRIVER PROGRAM
C
      PARAMETER (IDIM = 6, TOLER = 1.E-6)
C
C        ADJUST IDIM = M + 2, WHERE M IS THE
C        NUMBER OF DATA POINTS
C
      DIMENSION A(IDIM, 6), X(2), T(2, 10),
     *          TEMP(IDIM, 6), RATIO(IDIM)
      DATA BIG /1.E30/
      M = IDIM - 2
      M1 = IDIM -1
      DO 20 I = 1, M
      WRITE(1, 10) I
10    FORMAT('TYPE IN POINT NUMBER ', I5)
      READ(1, *) A(I, 2), A(I, 5)
      A(I, 1) = 1.
      A(I, 3) = -1.
      A(I, 4) = - A(I, 2)
      A(I, 6) = FLOAT(I + 2)
20    CONTINUE
C
C        ENSURE THAT COLUMN 5 IS NON - NEGATIVE
C
      DO 40 I = 1, M
      IF (A(I, 5) .GE. 0.) GO TO 40
      DO 30 J = 1, 6
      A(I, J) = - A(I, J)
30    CONTINUE
40    CONTINUE
C
C        COMPUTE MARGINAL COSTS
C
      DO 60 J = 1, 5
      SUM = 0.
      DO 50 I = 1, M
      SUM = SUM + A(I, J)
50    CONTINUE
      A(M1, J) = SUM
60    CONTINUE
      A(IDIM, 5) = 1.
      A(IDIM, 6) = 0.
      A(M1, 6) = 0.
C
C        IDENTIFY COLUMNS
C
      A(IDIM, 1) = 1.
      A(IDIM, 2) = 2.
      A(IDIM, 3) = -1.
      A(IDIM, 4) = -2.
C
C        CHOOSE PIVOT
C
65    IN = 1
      DO 70 J = 2, 4
      IF (A(M1, IN) .LT. A(M1, J)) IN = J
70    CONTINUE
      IF (A(M1, IN) .LE. 0.) GO TO 330
      DO 80 I = 1, M
      IF (A(I, IN) .LE. 0. .OR. A(I, 5) .EQ. 0.)
     *    RATIO(I) = BIG
      IF (A(I, IN) .GT. 0.)
     *    RATIO(I) = A(I, 5) / A(I, IN)
80    CONTINUE
      IOUT = 1
      DO 90 I = 2, M
      IF (RATIO(I) .LT. RATIO(IOUT)) IOUT = I
90    CONTINUE
      PIV = A(IOUT, IN)
      IF (PIV .GT. TOLER) GO TO 95
      IFAIL = 4
      GO TO 330
C
C        COPY A INTO TEMP
C
95    DO 100 I = 1, IDIM
      DO 100 J = 1, 6
```

```
100   TEMP(I, J) = A(I, J)
C
C        COMPUTE TABLEAU USING PIVOT PIV
C
      DO 110 J = 1, 5
      IF (J .EQ. IN) GO TO 110
      TEMP(IOUT, J) = A(IOUT, J) / PIV
110   CONTINUE
      DO 130 I = 1, M
      IF (I .EQ. IOUT) GO TO 130
      D = A(I, IN)
      DO 120 J = 1, 5
      IF (J .EQ. IN) GO TO 120
      TEMP(I, J) = A(I, J) - D * TEMP(IOUT, J)
120   CONTINUE
130   CONTINUE
      DO 140 I = 1, M
      IF (I .EQ. IOUT) GO TO 140
      TEMP(I, IN) = - A(I, IN) / PIV
140   CONTINUE
      TEMP(IOUT, IN) = 1. / PIV
      TEMP(IOUT, 6) = A(IDIM, IN)
      TEMP(IDIM, IN) = A(IOUT, 6)
      DO 160 J = 1, 4
      IF (A(IDIM, J) .NE. - A(IDIM,IN)) GO TO 160
      DO 150 I = 1, IDIM
      TEMP(I, J) = - TEMP(I, IN)
150   CONTINUE
160   CONTINUE
C
C        COLUMN 5 MUST BE NON - NEGATIVE
C
      DO 180 I = 1, M
      IF (TEMP(I, 5) .GE. 0.) GO TO 180
      DO 170 J = 1, 6
      TEMP(I, J) = - TEMP(I, J)
170   CONTINUE
180   CONTINUE
C
C        COMPUTE MARGINAL COSTS
C
      DO 200 J = 1, 5
      SUM = 0.
      DO 190 I = 1, M
      CR = 1.
      IF (ABS(TEMP(I, 6)) .EQ. 1. .OR.
     *    ABS(TEMP(I, 6)) .EQ. 2.) CR = 0.
      SUM = SUM + TEMP(I, J) * CR
190   CONTINUE
      CR = 1.
      IF (ABS(TEMP(IDIM, J)) .EQ. 1. .OR.
     *    ABS(TEMP(IDIM, J)) .EQ. 2.) CR = 0.
      TEMP(M1, J) = SUM - CR
200   CONTINUE
C
C        COPY TEMP INTO A
C
      DO 210 I = 1, IDIM
      DO 210 J = 1, 6
210   A(I, J) = TEMP(I, J)
C
C        CHECK IF TABLEAU IS OPTIMAL
C
      IOPT = 0
      DO 220 J = 1, 4
      IF (A(M1, J) .GT. TOLER) IOPT = 1
220   CONTINUE
      IF (IOPT .EQ. 1) GO TO 65
C
C        TABLEAU IS OPTIMAL
C        STORE SOLUTION IN X
C
      IFLAG1 = 0
      IFLAG2 = 0
      DO 270 I = 1, M
      IF (ABS(A(I, 6)) .NE. 1.) GO TO 240
      D = SIGN(A(I, 5), A(I, 6))
      X(1) = D
      IFLAG1 = 1
240   IF (ABS(A(I, 6)) .NE. 2.) GO TO 270
```

```
      D = SIGN(A(I, 5), A(I, 6))
      X(2) = D
      IFLAG2 = 1
270   CONTINUE
      IF (IFLAG1 .EQ. 0) X(1) = 0.
      IF (IFLAG2 .EQ. 0) X(2) = 0.
300   CALL SOLVE(IDIM, A, X, TOLER, IFAIL, ISC, T)
330   WRITE(1, 360) IFAIL
360   FORMAT('IFAIL = ', I1)
      IF (IFAIL .NE. 0) STOP
      WRITE(1,370) ISC
370   FORMAT ('NUMBER OF SOLUTIONS: ', I3)
      DO 380 J = 1, ISC
380   WRITE(1,390) T(1,J), T(2,J)
390   FORMAT(1P2E14.6)
      STOP
      END
C
C
C
C
C
      SUBROUTINE SOLVE(IDIM, A, X, TOLER, IFAIL, ISC, T)
C
C        GIVEN THE L1 LINE OF A SET OF DATA,
C        THIS ALGORITHM COMPUTES ANY OTHER
C        L1 LINE WHICH MAY EXIST
C
      REAL A(IDIM, 6), X(2), TOLER, T(2, 10),
     *     AA(300, 102, 6), AD(300, 102, 6),
     *     TEMP(102, 6), CR, PIV, SUM
      INTEGER IDIM, IFAIL, ISC, IBASIS(200, 102),
     *        IB, IBC, IC, ICOUNT, IDEN, IFLAG,
     *        IFLAG1, IFLAG2, IN, IOUT, IR, KAA,
     *        KAD, M, M1
      COMMON / BLK / AA, AD, IBASIS, TEMP
      DATA BIG /1.E30/
      M = IDIM - 2
      M1 = IDIM - 1
      IFAIL = 0
C
C        INITIALIZE T
C
      ISC = 1
      T(1, 1) = X(1)
      T(2, 1) = X(2)
      DO 5000 I = 1, 2
      DO 5000 J = 2, 10
5000  T(I, J) = BIG
C
C        INITIALIZE BASIS
C
      IBC = 1
      DO 5050 I = 1, 200
      DO 5050 J = 1, IDIM
5050  IBASIS(I, J) = 0
      DO 5100 I = 1, M
      IB = A(I, 6)
      IBASIS(1, IABS(IB)) = ISIGN(1, IB)
5100  CONTINUE
C
C        COPY INTO AA(1, I, J),
C        INITIALIZE TEMP AND AD(1, I, J)
C
      DO 5200 J = 1, 6
      DO 5200 I = 1, IDIM
      D = A(I, J)
      AA(1, I, J) = D
      TEMP(I, J) = 0.
5200  CONTINUE
C
C        INITIALIZE AA AND AD
C
      DO 5600 I = 2, 300
      DO 5600 J = 1, IDIM
      DO 5600 K = 1, 6
      AA(I, J,K) = 0.
      AD(I, J,K) = 0.
5600  CONTINUE
      ERROR = A(M1, 5)
```

```
      KAA = 1
      KAD = 0
      IDEN = 1
C
C        ICOUNT IS TABLEAU COUNTER
C
      ICOUNT = 1
      GO TO 5755
C
C        INITIALIZATION COMPLETE
C        SEARCH AA AND STORE IN AD
C
5670  KAD = 0
      IDEN = 1
      ICOUNT = 1
5675  DO 5750 J = 1, IDIM
      DO 5750 K = 1, 6
      D = AA(ICOUNT, J, K)
      A(J, K) = D
5750  CONTINUE
5755  GO TO 7040
5760  ICOUNT = ICOUNT + 1
      IF (ICOUNT .GT. 300) IFAIL = 1
      IF (IFAIL .EQ. 1) RETURN
      IF (ICOUNT .LE. KAA) GO TO 5675
      IF (KAD .EQ. 0) RETURN
C
C        SEARCH AD AND STORE IN AA
C
5770  KAA = 0
      IDEN = 0
      ICOUNT = 1
5775  DO 5850 J = 1, IDIM
      DO 5850 K = 1, 6
      D = AD(ICOUNT, J, K)
      A(J, K) = D
5850  CONTINUE
      GO TO 7040
5855  ICOUNT = ICOUNT + 1
      IF (ICOUNT .GT. 300) IFAIL  =  1
      IF (IFAIL .EQ. 1) RETURN
      IF(ICOUNT .LE. KAD) GO TO 5775
      IF (KAA .EQ. 0) RETURN
      GO TO 5670
C                                ENTRY
C        SEARCH FOR POSITIVE PIVOTS
C
7040  IC = 1
7050  IR = 1
7055  IF (ABS(A(M1, IC)) .GT. TOLER .OR.
     *     ABS(A(IR,5)) .LE. TOLER .OR.
     *     A(IR, IC) .LE. 0) GO TO 7070
      IOUT = IR
      IN = IC
      IF (A(IOUT, IN) .GT. TOLER) GO TO 8010
      IFAIL = 4
      RETURN
7070  IR = IR + 1
      IF(IR .LE. M) GO TO 7055
      IC = IC + 1
      IF (IC .LE. 4) GO TO 7050
C
C        SEARCH FOR ZERO ENTRY PIVOTS
C
      IC = 1
7100  IR = 1
7150  IF (A(IR, IC) .EQ. 0. .OR.
     *     ABS(A(IR, 5)) .GT. TOLER) GO TO 7170
      IOUT = IR
      IN = IC
      IF (ABS(A(IOUT, IN)) .GT. TOLER) GO TO 9010
      IFAIL = 4
      RETURN
7170  IR = IR + 1
      IF (IR .LE. M) GO TO 7150
      IC = IC + 1
7180  IF (IC .LE. 4) GO TO 7100
      IF (IDEN .EQ. 1) GO TO 5760
      IF (IDEN .EQ. 0) GO TO 5855
C
```

```
C          NON-ZERO ENTRY PIVOTING
C
8010    PIV=A(ICUT, IN)
C
C          COPY A INTO TEMP
C
        DO 8020 I = 1, IDIM
        DO 8020 J = 1, 6
8020     TEMP(I, J) = A(I, J)
C
C          COMPUTE TABLEAU USING PIVOT PIV
C
        DO 8025 J = 1, 5
        IF(J .EQ. IN) GO TO 8025
        TEMP(IOUT, J) = A(IOUT, J) / PIV
8025    CONTINUE
        DO 8100 I = 1, M
        IF(I .EQ. IOUT) GO TO 8100
        D = A(I, IN)
        DO 8050 J = 1, 5
        IF (J .EQ. IN) GO TO 8050
        TEMP(I, J) = A(I, J)-D * TEMP(IOUT, J)
8050    CONTINUE
8100    CONTINUE
        DO 8150 I = 1, M
        IF (I .EQ. IOUT) GO TO 8150
        TEMP(I, IN) = -A(I, IN) / PIV
8150    CONTINUE
        TEMP(IOUT, IN) = 1. / PIV
        TEMP(IOUT, 6) = A(IDIM, IN)
        TEMP(IDIM, IN) = A(IOUT, 6)
        DO 8160 J = 1, 4
        IF (A(IDIM, J) .NE. -A(IDIM, IN)) GO TO 8160
        DO 8155 I = 1, IDIM
        TEMP(I, J) = -TEMP(I, IN)
8155    CONTINUE
8160    CONTINUE
C
C          COLUMN 5 MUST BE NON-NEGATIVE
C
        DO 8200 I = 1, M
        IF (TEMP(I, 5) .GE. 0.) GO TO 8200
        DO 8170 J = 1, 6
        TEMP(I, J) = -TEMP(I, J)
8170    CONTINUE
8200    CONTINUE
C
C          COMPUTE MARGINAL COSTS
C
        DO 8300 J = 1, 5
        SUM = 0.
        DO 8250 I = 1, M
        CR = 1.
        IF (ABS(TEMP(I, 6)) .EQ. 1. .OR.
     +      ABS(TEMP(I, 6)) .EQ. 2) CR = 0.
        SUM = SUM + TEMP(I, J) * CR
8250    CONTINUE
        CR = 1.
        IF (ABS(TEMP(IDIM, J)) .EQ. 1. .OR.
     +      ABS(TEMP(IDIM, J)) .EQ. 2.) CR = 0.
        TEMP(M1, J) = SUM - CR
8300    CONTINUE
C
C          CHECK IF BASIS IS NEW
C
        DO 8301 I = 1, IDIM
8301    IBASIS(IBC + 1, I) = 0
        DO 8303 I = 1, M
        IB = IFIX(TEMP(I, 6))
        IBASIS(IBC + 1, IABS(IB)) = ISIGN(1, IB)
8303    CONTINUE
        DO 8307 I = 1, IBC
        DO 8305 J = 1, IDIM
        IF (IBASIS(IBC + 1, J) - IBASIS(I, J) .NE. 0) GO TO 83(
8305    CONTINUE
C
C          CONTINUE SEARCH FOR PIVOTS
C
        GO TO 7070
8307    CONTINUE
```

```
8309  IBC = IBC+1
      IF (IBC .GT. 200) IFAIL = 2
      IF (IFAIL .EQ. 2) RETURN
C
C        SUM OF ABSOLUTE ERRORS SHOULD NOT INCREASE
C
      IF (TEMP(M1, 5) - ERROR .GT. TOLER)
     *   GO TO 8500
C
C        DETERMINE SOLUTION
C
      IFLAG1 = 0
      IFLAG2 = 0
      DO 8350 I = 1, M
      IF (ABS(TEMP(I, 6)) .NE. 1.) GO TO 8320
      D = SIGN(TEMP(I, 5), TEMP(I, 6))
      X(1) = D
      IFLAG1 = 1
8320  IF (ABS(TEMP(I, 6)) .NE. 2.) GO TO 8350
      D = SIGN(TEMP(I, 5), TEMP(I, 6))
      X(2) = D
      IFLAG2 = 1
8350  CONTINUE
      IF (IFLAG1 .EQ. 0) X(1) = 0.
      IF (IFLAG2 .EQ. 0) X(2) = 0.
C
C        CHECK IF X CONTAINS NEW SOLUTION
C
      DO 8400 J = 1, ISC
      IF (ABS(T(1, J) - X(1)) .LT. TOLER .AND.
     *    ABS(T(2, J) - X(2)) .LT. TOLER) GO TO 8500
8400  CONTINUE
C
C        STORE NEW SOLUTION IN T
C
      IFLAG = 1
      ISC = ISC + 1
      IF (ISC .GT. 10) IFAIL = 3
      IF (IFAIL .EQ. 3) RETURN
      D = X(1)
      T(1, ISC) = D
      D = X(2)
      T(2, ISC) = D
      GO TO 8550
C
C        IFLAG = 0 MEANS PIVOT IS NO USE
C
8500  IFLAG = 0
8550  IF (IFLAG .EQ. 0) GO TO 7070
C
C        IF IDEN = 0 TEMP IS STORED IN AA
C        IF IDEN = 1 TEMP IS STORED IN AD
C
      IF (IDEN .EQ. 1) GO TO 8700
C
C        STORE IN AA
C
      KAA = KAA + 1
      IF (KAA .GT. 300) IFAIL = 1
      IF (IFAIL .EQ. 1) RETURN
      DO 8650 J = 1, IDIM
      DO 8650 K = 1, 6
      D = TEMP(J, K)
      AA(KAA, J, K) = D
8650  CONTINUE
C
C        CONTINUE SEARCH FOR PIVOTS
C
      GO TO 7070
C
C        STORE IN AD
C
8700  KAD = KAD + 1
      IF (KAD .GT. 300) IFAIL = 1
      IF (IFAIL .EQ. 1) RETURN
      DO 8750 J = 1, IDIM
      DO 8750 K = 1, 6
      D = TEMP(J, K)
      AD(KAD, J, K) = D
8750  CONTINUE
```

```
C
C         CONTINUE SEARCH FOR PIVOTS
C
8900   GO TO 7070
C
C         ZERO-ENTRY PIVOTING
C
9010   PIV = A(IOUT, IN)
C
C         COPY A INTO TEMP
C
       DO 9020 I = 1, IDIM
       DO 9020 J = 1, 6
       TEMP(I, J) = A(I, J)
9020   CONTINUE
C
C         COMPUTE TABLEAU USING PIVOT PIV
C
       DO 9025 J = 1, 5
       IF (J .EQ. IN) GO TO 9025
       TEMP(IOUT, J) = A(IOUT, J) / PIV
9025   CONTINUE
       DO 9100 I = 1, M
       IF(I .EQ. IOUT) GO TO 9100
       D = A(I, IN)
       DO 9050 J = 1, 5
       IF (J .EQ. IN) GO TO 9050
       TEMP(I, J) = A(I, J) - D * TEMP(IOUT,J)
9050   CONTINUE
9100   CONTINUE
       DO 9150 I = 1, M
       IF(I .EQ. IOUT) GO TO 9150
       TEMP(I, IN) =  - A(I, IN) / PIV
9150   CONTINUE
       TEMP(IOUT, IN) = 1. / PIV
       TEMP(IOUT, 6) = A(IDIM, IN)
       TEMP(IDIM, IN) = A(IOUT, 6)
       DO 9160 J = 1, 4
       IF (A(IDIM, J) .NE. - A(IDIM, IN)) GO TO 9160
       DO 9155 I = 1, IDIM
       TEMP(I, J) =  - TEMP(I, IN)
9155   CONTINUE
9160   CONTINUE
C
C         COLUMN 5  MUST BE NON - NEGATIVE
C
       DO 9200 I = 1, M
       IF (TEMP(I, 5) .GE. 0.) GO TO 9200
       DO 9170 J = 1, 6
       TEMP(I, J) =  - TEMP(I,J)
9170   CONTINUE
9200   CONTINUE
C
C         COMPUTE MARGINAL COSTS
C
       DO 9300 J = 1, 5
       SUM = 0.
       DO 9250 I = 1, M
       CR = 1.
       IF (ABS(TEMP(I, 6)) .EQ. 1. .OR.
     *     ABS(TEMP(I, 6)) .EQ. 2.) CR = 0.
       SUM = SUM + TEMP(I, J) * CR
9250   CONTINUE
       CR = 1.
       IF (ABS(TEMP(IDIM, J)) .EQ. 1. .OR.
     *     ABS(TEMP(IDIM, J)) .EQ. 2.) CR = 0.
       TEMP(M1, J) = SUM - CR
9300   CONTINUE
C
C         CHECK IF BASIS IS NEW
C
       DO 9301 I = 1, IDIM
       IBASIS(IBC + 1, I) = 0
9301   CONTINUE
       DO 9303 I = 1, M
       IB = IFIX(TEMP(I, 6))
       IBASIS(IBC + 1, IABS(IB)) = ISIGN(1, IB)
9303   CONTINUE
       DO 9307 I = 1, IBC
       DO 9305 J = 1, IDIM
```

```
      IF (IBASIS(IBC + 1, J) - IBASIS(I, J) .NE. 0)
     *   GO TO 9307
9305  CONTINUE
C
C        CONTINUE SEARCH FOR PIVOTS
C
      GO TO 7170
9307  CONTINUE
9309  IBC = IBC + 1
      IF (IBC .GT. 200) IFAIL = 2
      IF (IFAIL .EQ. 2) RETURN
C
C        IF IDEN = 0, TEMP IS STORED IN AA
C        IF IDEN = 1, TEMP IS STORED IN AD
C
      IF (IDEN .EQ. 1) GO TO 9700
C
C        STORE IN AA
C
      KAA = KAA + 1
      IF (KAA .GT. 300) IFAIL = 1
      IF (IFAIL .EQ. 1) RETURN
      DO 9650 J = 1, IDIM
      DO 9650 K = 1, 6
      D = TEMP(J, K)
      AA(KAA, J, K) = D
9650  CONTINUE
C
C        CONTINUE SEARCH FOR PIVOTS
C
      GO TO 7170
C
C        STORE IN AD
C
9700  KAD = KAD + 1
      IF (KAD .GT. 300) IFAIL = 1
      IF (IFAIL .EQ. 1) RETURN
      DO 9750 J = 1, IDIM
      DO 9750 K = 1, 6
      D = TEMP(J, K)
      AD(KAD, J, K) = D
9750  CONTINUE
C
C        CONTINUE SEARCH FOR PIVOTS
C
9900  GO TO 7170
      END
OK, SEG SOLVE
TYPE IN POINT NUMBER       1
0. 1.
TYPE IN POINT NUMBER       2
1. 0.
TYPE IN POINT NUMBER       3
2. 0.
TYPE IN POINT NUMBER       4
3. 1.
IFAIL = 0
NUMBER OF SOLUTIONS:     5
  0.000000E-01  0.000000E-01
  1.000000E 00 -5.000000E-01
  0.000000E-01  3.333333E-01
  1.000000E 00  0.000000E-01
 -5.000000E-01  5.000000E-01

**** STOP
OK,


SEG SOLVE
TYPE IN POINT NUMBER       1
0. 2.
TYPE IN POINT NUMBER       2
1. 2.5
TYPE IN POINT NUMBER       3
2. 2.
TYPE IN POINT NUMBER       4
3. 5.
IFAIL = 0
NUMBER OF SOLUTIONS:     3
  2.000000E 00  5.000000E-01
```

```
C
C          SUBROUTINE STRICT
C          DRIVER PROGRAM
C
      PARAMETER(M = 5, TOLER = 1.E-6)
C
C          M SHOULD EQUAL THE NUMBER OF
C          DATA POINTS
C
      DIMENSION HULL(2,26), T1(M), T2(M)
5     WRITE(1, 10)
10    FORMAT('TYPE IN ISC>1, THE NUMBER OF SOLUTIONS')
      READ(1, *) ISC
      IF (ISC .LE. 1) GO TO 5
      DO 30 J = 1, ISC
      WRITE(1, 20) J
20    FORMAT('TYPE IN SOLUTION POINT NUMBER ', I5)
30    READ(1, *) HULL(1, J), HULL(2, J)
      DO 36 I = 1, M
      WRITE(1, 34) I
34    FORMAT('TYPE IN DATA POINT NUMBER ', I5)
36    READ(1, *) T1(I), T2(I)
C
C          INITIALIZE COLUMNS ISC + 1 TO 26
C
      ISCP1 = ISC + 1
      DO 40 J = ISCP1, 26
      DO 40 I = 1, 2
40    HULL(I, J) = 0.
C
C          CHOOSE MINIMUM B
C
      MIN = 1
      DO 50 J = 2, ISC
      IF (HULL(2, J) .GE. HULL(2, MIN)) GO TO 50
      MIN = J
50    CONTINUE
C
C          IHC IS THE NUMBER OF POINTS IN THE HULL
C
      IHC = 0
      HULL(1, ISC + 1) = HULL(1, MIN)
      HULL(2, ISC + 1) = HULL(2, MIN)
      ANGMIN = -1.
C
C           CHOOSE MINIMUM ANGLE
C
      PI = ATAN(1.0) * 4.0
60    IHC = IHC + 1
      TEMP1 = HULL(1, IHC)
      TEMP2 = HULL(2, IHC)
      HULL(1, IHC) = HULL(1, MIN)
      HULL(2, IHC) = HULL(2, MIN)
      HULL(1, MIN) = TEMP1
      HULL(2, MIN) = TEMP2
      MIN = ISC + 1
      ALPHA = ANGMIN
      ANGMIN = PI * 2.0
      ISCP1 = ISC + 1
      DO 70 J = IHC, ISCP1
      X = HULL(1, J) - HULL(1, IHC)
      Y = HULL(2, J) - HULL(2, IHC)
      CALL ANGLE(X, Y, ANG)
      IF (ANG .LE. ALPHA) GO TO 70
      IF (ANG .GE. ANGMIN) GO TO 70
      MIN = J
      X = HULL(1, MIN) - HULL(1, IHC)
      Y = HULL(2, MIN) - HULL(2, IHC)
      CALL ANGLE(X, Y, ANG)
      ANGMIN = ANG
70    CONTINUE
C
C          ELIMINATE INTERMEDIATE POINTS
C
      X = HULL(1, MIN) - HULL(1, IHC)
      Y = HULL(2, MIN) - HULL(2, IHC)
      AGL = ANGMIN
      DIS = X * X + Y * Y
      IHCP1 = IHC + 1
      DO 80 J = IHCP1, ISCP1
```

```
      X = HULL(1, J) - HULL(1, IHC)
      Y = HULL(2, J) - HULL(2, IHC)
      CALL ANGLE(X, Y, ANG)
      X2Y2 = X * X + Y * Y
      IF (ANG .NE. AGL) GO TO 80
      IF (X2Y2 .LE. DIS) GO TO 80
      DIS = X2Y2
      MIN = J
80    CONTINUE
      IF (MIN .LT. ISCP1) GO TO 60
C
C         PREPARE OUTPUT FOR HULL
C
      WRITE(1, 90) IHC
90    FORMAT(/'NUMBER OF VERTICES OF HULL: ', I5)
      WRITE(1, 100)
100   FORMAT('COORDINATES OF VERTICES: ')
      DO 110 J = 1, IHC
110   WRITE(1, 120) HULL(1, J), HULL(2, J)
120   FORMAT(1P2E14.6)
C
C         COMPUTE STRICT APPROXIMATION
C
      CALL STRICT(IHC, HULL, M, T1, T2, TOLER,
     *            ICODE, A, B, C, D)
      WRITE(1, 130) C, D
130   FORMAT(/'THE L2 APPROXIMATION IS GIVEN BY'/
     *       'GRADIENT: ', 1PE14.6/
     *       'INTERCEPT: ', 1PE14.6)
      IF (ICODE .EQ. 0) GO TO 150
      WRITE(1, 140) A, B
140   FORMAT(/'THE STRICT APPROXIMATION IS GIVEN BY'/
     *       'GRADIENT: ', 1PE14.6/
     *       'INTERCEPT: ', 1PE14.6)
      GO TO 170
150   WRITE(1, 160)
160   FORMAT(/'L2 AND STRICT APPROXIMATION ARE IDENTICAL')
170   STOP
      END
C
C         COMPUTE ANGLE ANG
C
      SUBROUTINE ANGLE(X, Y, ANG)
      IF (X .EQ. 0.0 .AND. Y .EQ. 0.0) A = 4.0
      IF (X .NE. 0.0 .OR.  Y .NE. 0.0) A = Y /
     *    (ABS(X) + ABS(Y))
      IF (X .LT. 0.0) A = 2.0 - A
      IF (X .GE. 0.0 .AND. Y .LT. 0.0) A = A + 4.0
      ANG = A * 2.0 * ATAN(1.0)
      RETURN
      END
C
C
C
C
C         END OF DRIVER PROGRAM
C
C
C
C
      SUBROUTINE STRICT(IHC, HULL, M, T1, T2, TOLER,
     *                  ICODE, A, B, C, D)
      REAL HULL(2, IHC), T1(M), T2(M), A, SB, C, D,
     *     SX, SY, SXY, SXX, DENOM, X0, Y0, DENOM0,
     *     DENOM1, G0, G1, X2, Y2, DENOM2, SMIN, A,
     *     SB, ANUM, GRD, TEMPM, TEMPB, SUM
C
C         DETERMINE L2 LINE WITH
C         GRADIENT C AND INTERCEPT D
C
      SX = 0.0
      SY = 0.0
      SXY = 0.0
      SXX = 0.0
      DO 10 I = 1, M
      SX = SX + T1(I)
      SY = SY + T2(I)
      SXY = SXY + T1(I) * T2(I)
      SXX = SXX + T1(I) * T1(I)
10    CONTINUE
      DENOM = FLOAT(M) * SXX - SX * SX
      D = (SY * SXX - SX * SXY) / DENOM
```

```
      C = (FLOAT(M) * SXY - SX * SY) / DENOM
      IF (IHC .EQ. 2) GO TO 70
C
C        DETERMINE CENTROID (X0, Y0) OF HULL
C
      X0 = 0.0
      Y0 = 0.0
      DO 20 I = 1, M
      X0 = X0 + HULL(1, I)
      Y0 = Y0 + HULL(2, I)
20    CONTINUE
      X0 = X0 / FLOAT(IHC)
      Y0 = Y0 / FLOAT(IHC)
C
C        DETERMINE INTERSECTION (X2, Y2) OF SIDES OF
C        HULL WITH LINE THROUGH (X0, Y0) AND (C, D)
C
      ICODE = 0
      KOUNT = 0
30    KOUNT = KOUNT + 1
      ITOP = KOUNT + 1
      IF (KOUNT .LE. IHC) GO TO 40
      RETURN
40    IF (KOUNT .EQ. IHC) ITOP = 1
      DENOM0 = C - X0
      DENOM1 = HULL(1, ITOP) - HULL(1, KOUNT)
      IF (DENOM0 .EQ. 0.0 .AND. DENOM1 .EQ. 0.0) GO TO 30
      IF (DENOM0 .EQ. 0.0) GO TO 55
      IF (DENOM1 .EQ. 0.0) GO TO 50
      G0 = (D - Y0) / DENOM0
      G1 = (HULL(2, ITOP) - HULL(2, KOUNT)) / DENOM1
      DENOM = G1 - G0
      IF (DENOM .EQ. 0.0) GO TO 30
      X2 = (G1 * HULL(1, KOUNT) - HULL(2, KOUNT) -
     *     G0 * X0 + Y0) / DENOM
      Y2 = G0 * (X2 - X0) + Y0
      GO TO 52
C
C        CASE: INFINITE G1 AND FINITE G0
C
50    G0 = (D - Y0) / DENOM0
      X2 = HULL(1, KOUNT)
      Y2 = G0 * (X2 - X0) + Y0
C
C        TEST IF (C, D) IS INSIDE HULL
C
52    IF (X2 .LT. X0 .AND. X2 .GT. C .OR.
     *     X2 .LT. C  .AND. X2 .GT. X0) GO TO 53
      GO TO 30
53    IF (X2 .LE. HULL(1, KOUNT) .AND. X2 .GE.
     *    HULL(1, ITOP) .OR. X2 .LE. HULL(1, ITOP)
     *   .AND. X2 .GE. HULL(1, KOUNT))
     *   GO TO 110
      GO TO 30
C
C        CASE: INFINITE G0 AND FINITE G1
C
55    G1 = (HULL(2, ITOP) - HULL(2, KOUNT)) / DENOM1
      X2 = X0
      Y2 = G1 * (X2 - HULL(1, KOUNT)) + HULL(2, KOUNT)
C
C        TEST IF (C, D) IS INSIDE HULL
C
57    IF (X2 .LE. X0 .AND. X2 .GE. C .OR.
     *     X2 .LE. C  .AND. X2 .GE. X0) GO TO 60
      GO TO 30
60    IF (Y2 .LT. D  .AND. Y2 .GT. Y0 .OR.
     *     Y2 .LT. Y0 .AND. Y2 .GT. D) GO TO 110
      GO TO 30
C
C        CASE: IHC = 2
C
70    DENOM2 = HULL(1, 2) - HULL(1, 1)
      IF (DENOM2 .EQ. 0.0) GO TO 90
      G2 = (HULL(2, 2) - HULL(2, 1)) / DENOM2
      DDD = G2 * (C - HULL(1, 1)) + HULL(2, 1)
      IF (ABS(D - DDD) .GT. TOLER) GO TO 110
80    IF (C .LE. HULL(1, 2) .AND. C .GE. HULL(1, 1) .OR.
     *    C .GE. HULL(1, 2) .AND. C .LE. HULL(1, 1))
     *   RETURN
```

```
      GO TO 110
C
C        CASE: IHC = 2 AND GRADIENT G2 IS INFINITE
C
90    IF (ABS(C - HULL(1, 1)) .GT. TOLER) GO TO 110
100   IF (D .LE. HULL(2, 2) .AND. D .GE. HULL(2, 1) .OR.
     *    D .GE. HULL(2, 2) .AND. D .LE. HULL(2, 1))
     *  RETURN
110   ICODE = 1
C
C        COMPUTE STRICT SOLUTION
C
      SMIN = 1.0E30
      A = 0.0
      B = 0.0
      DO 160 J = 1, IHC
      ITOP = J + 1
      IF (J .EQ. IHC) ITOP = 1
C
C        CHECK IF GRADIENT IS FINITE
C
      IF (HULL(1, ITOP) - HULL(1, J) .EQ. 0.0) GO TO 130
      GRD = (HULL(2, ITOP) - HULL(2, J)) /
     *      (HULL(1, ITOP) - HULL(1, J))
      ANUM = 0.0
      DENOM = 0.0
      DO 120 I = 1, M
      ANUM = ANUM + GRD *
     *       (HULL(1, J) * T1(I) + GRD * HULL(1, J)
     *        - HULL(2, J) + T2(I)) - HULL(2, J) *
     *        T1(I) + T1(I) * T2(I)
      DENOM = DENOM + T1(I) * T1(I) + 2.0 * T1(I) *
     *        GRD + GRD * GRD
120   CONTINUE
      TEMPM = ANUM / DENOM
      TEMPB = GRD * (TEMPM - HULL(1, J)) + HULL(2, J)
C
C        CHECK IF LOCAL MINIMUM LIES ON CURRENT SIDE
C
      IF (TEMPM .GT. HULL(1, J) .AND. TEMPM .GT.
     *    HULL(1, ITOP) .OR. TEMPM .LT.
     *    HULL(1, J) .AND. TEMPM .LT.
     *    HULL(1, ITOP)) GO TO 150
      SUM = 0.0
      DO 125 K = 1, M
125   SUM = SUM + (TEMPM * T1(K) + TEMPB - T2(K)) ** 2
      IF (SUM .GE. SMIN) GO TO 150
      SMIN = SUM
      A = TEMPM
      B = TEMPB
      GO TO 150
C
C        CASE: GRADIENT GRD IS INFINITE
C
130   TEMPM = HULL(1, J)
      TEMPB = 0.0
      DO 140 I = 1, M
      TEMPB = TEMPB + T2(I) - T1(I) * HULL(1, J)
140   CONTINUE
      TEMPB = TEMPB / FLOAT(M)
C
C        CHECK IF LOCAL MINIMUM LIES ON CURRENT SIDE
C
      IF (TEMPB .GT. HULL(2, J) .AND. TEMPB .GT.
     *    HULL(2, ITOP) .OR. TEMPB .LT. HULL(2, J)
     *    .AND. TEMPB .LT. HULL(2, ITOP))
     *   GO TO 150
      SUM = 0.0
      DO 145 K = 1, M
145   SUM = SUM + (TEMPM * T1(K) + TEMPB - T2(K)) ** 2
      IF (SUM .GE. SMIN) GO TO 150
      SMIN = SUM
      A = TEMPM
      B = TEMPB
C
C        TEST VERTEX J + 1
C
150   TEMPM = HULL(1, ITOP)
      TEMPB = HULL(2, ITOP)
      SUM = 0.0
```

```
      DO 155 K = 1, M
155   SUM = SUM + (TEMPM * T1(K) + TEMPB - T2(K)) ** 2
      IF (SUM .GE. SMIN) GO TO 160
      SMIN = SUM
      A = TEMPM
      B = TEMPB
160   CONTINUE
      RETURN
      END
C
C
C
C          OUTPUT
C          EXAMPLE 1
C
C
C
TYPE IN ISC>1, THE NUMBER OF SOLUTIONS
5
TYPE IN SOLUTION POINT NUMBER        1
0. 0.
TYPE IN SOLUTION POINT NUMBER        2
0.5 -0.5
TYPE IN SOLUTION POINT NUMBER        3
0. 1.
TYPE IN SOLUTION POINT NUMBER        4
-0.5 1.
TYPE IN SOLUTION POINT NUMBER        5
.3333333 1.
TYPE IN DATA POINT NUMBER        1
0. 1.
TYPE IN DATA POINT NUMBER        2
1. 0.
TYPE IN DATA POINT NUMBER        3
2. 0.
TYPE IN DATA POINT NUMBER        4
3. 1.

NUMBER OF VERTICES OF HULL:        4
COORDINATES OF VERTICES:
   5.000000E-01 -5.000000E-01
   3.333333E-01  1.000000E 00
  -5.000000E-01  1.000000E 00
   0.000000E-01  0.000000E-01

THE L2 APPROXIMATION IS GIVEN BY
GRADIENT:     0.000000E-01
INTERCEPT:     5.000000E-01

L2 AND STRICT APPROXIMATION ARE IDENTICAL

C
C
C
C          EXAMPLE 2
C
C
C
TYPE IN ISC>1, THE NUMBER OF SOLUTIONS
3
TYPE IN SOLUTION POINT NUMBER        1
0.5 2.
TYPE IN SOLUTION POINT NUMBER        2
1.25 1.25
TYPE IN SOLUTION POINT NUMBER        3
1. 2.
TYPE IN DATA POINT NUMBER        1
0. 2.
TYPE IN DATA POINT NUMBER        2
1. 2.5
TYPE IN DATA POINT NUMBER        3
2. 2.
TYPE IN DATA POINT NUMBER        4
3. 5.

NUMBER OF VERTICES OF HULL:        3
COORDINATES OF VERTICES:
   1.250000E 00  1.250000E 00
   1.000000E 00  2.000000E 00
   5.000000E-01  2.000000E 00
```

```
THE L2 APPROXIMATION IS GIVEN BY
GRADIENT:     8.499999E-01
INTERCEPT:     1.600000E 00

THE STRICT APPROXIMATION IS GIVEN BY
GRADIENT:     8.333333E-01
INTERCEPT:     1.666667E 00


C
C
C
C           EXAMPLE 3
C           SET M = 5
C
C
C
TYPE IN ISC>1, THE NUMBER OF SOLUTIONS
2
TYPE IN SOLUTION POINT NUMBER       1
0.5 2.5
TYPE IN SOLUTION POINT NUMBER       2
0.25  2.75
TYPE IN DATA POINT NUMBER       1
1. 3.
TYPE IN DATA POINT NUMBER       2
2. 3.
TYPE IN DATA POINT NUMBER       3
3. 4.
TYPE IN DATA POINT NUMBER       4
4. 5.
TYPE IN DATA POINT NUMBER       5
5. 4.

NUMBER OF VERTICES OF HULL:       2
COORDINATES OF VERTICES:
   5.000000E-01  2.500000E 00
   2.500000E-01  2.750000E 00

THE L2 APPROXIMATION IS GIVEN BY
GRADIENT:     4.000000E-01
INTERCEPT:     2.600000E 00

L2 AND STRICT APPROXIMATION ARE IDENTICAL
```

```
10 REM SUBROUTINE "MINBAL"
20 REM ------------------
30 @%=10
40 F0=0
50 DIM A(3,10)
60 DIM E(3,10)
70 DIM X(3,10)
80 DIM P(3)
90 DIM W(3)
100 REM INPUT ROUTINES
110 REM -------------
120 FOR I%=1 TO 3
130 PRINT"INPUT DIRECTION OF STREAM ";I%
140 INPUT P(I%)
150 NEXT I%
160 PRINT
170 PRINT "INPUT MASS FLOW RATE"
180 INPUT "DEFAULT RATE 100", W(1)
190 PRINT
200 INPUT "INPUT NUMBER OF ASSAYS",N
210 PRINT
220 FOR J%=1 TO N
230 FOR I%=1 TO 3
240 PRINT "STREAM ";I%;" ASSAY ";J%;
250 INPUT A(I%,J%)
260 INPUT "INPUT ASSOCIATED ERROR (PERCENT)",E(I%,J%)
270 E(I%,J%)=(E(I%,J%)*A(I%,J%)/100)^2/2
280 PRINT
290 NEXT I%
300 PRINT:PRINT
310 NEXTJ%
320 TEMPUS=TIME
330 A=1:B=1
340 W(2)=W(1)*(A(1,1)-A(3,1))/(A(2,1)-A(3,1))
350
360 REM MINIMIZATION ROUTINE FOR W(2) GUESS
370 REM ---------------------------------
380 F=0
390 FORJ%=1 TO N
400 S1=0:S2=0
410 FORI%=1 TO 3
420 S1=S1+E(I%,J%)*W(I%)^2
430 S2=S2+P(I%)*W(I%)*A(I%,J%)
440 NEXTI%
450 FORI%=1 TO 3
460 X(I%,J%)=A(I%,J%)-P(I%)*E(I%,J%)*W(I%)*S2/S1
470 F=F+(X(I%,J%)-A(I%,J%))^2*2/E(I%,J%)
480 NEXTI%
490 NEXTJ%
500 IF F0=0 OR F<=F0 THEN GOTO 590
```

```
530 REM SEARCH ROUTINE ON W(2)
540 REM ----------------------
550 W(2)=W(2)-B*A
560 A=A/2
570 B=-B
580 IF A<.009 GOTO 620
590 FO=F
600 W(2)=W(2)+B*A
610 GOTO 360
620 REM OUTPUT
630 REM ------
640 FOR J%=1 TO N
650 @%=10
660 PRINT "ASSAY TYPE ";J%
670 PRINT "STREAM","MEASURED","ADJUSTED", "MASSFLOW"
680 PRINT
690 @%=&0002030A
700 FOR I%=1 TO 3
710 PRINT;I%;TAB(10)A(I%,J%);TAB(19)X(I%,J%);TAB(30)W(I%)
720 NEXT I%
730 PRINT
740 NEXT J%
750 @%=10
760 PRINT"RUNNING TIME IN CSEC: ";TIME-TEMPUS
770 END
```

```
INPUT DIRECTION OF STREAM 1
?-1
INPUT DIRECTION OF STREAM 2
?1
INPUT DIRECTION OF STREAM 3
?1

INPUT MASS FLOW RATE
DEFAULT RATE 100?100

INPUT NUMBER OF ASSAYS?2

STREAM 1 ASSAY 1?23.8
INPUT ASSOCIATED ERROR (PERCENT)?5

STREAM 2 ASSAY 1?5.3
INPUT ASSOCIATED ERROR (PERCENT)?5

STREAM 3 ASSAY 1?53.9
INPUT ASSOCIATED ERROR (PERCENT)?2


STREAM 1 ASSAY 2?52.1
INPUT ASSOCIATED ERROR (PERCENT)?10

STREAM 2 ASSAY 2?40.7
INPUT ASSOCIATED ERROR (PERCENT)?10

STREAM 3 ASSAY 2?63.4
INPUT ASSOCIATED ERROR (PERCENT)?4


ASSAY TYPE 1
STREAM      MEASURED   ADJUSTED   MASSFLOW

1.000       23.800     22.297     100.000
2.000       5.300      5.597      398.356
3.000       53.900     53.900     0.000

ASSAY TYPE 2
STREAM      MEASURED   ADJUSTED   MASSFLOW

1.000       52.100     62.398     100.000
2.000       40.700     15.663     398.356
3.000       63.400     63.400     0.000

RUNNING TIME IN CSEC: 8676
```

```
C ILP
C ------------------------------------------------
C A PROGRAM TO DETERMINE ALTERNATIVE OPTIMAL
C AND SUB-OPTIMAL INTEGER SOLUTIONS OF
C A LINEAR OBJECTIVE FUNCTION SUBJECT TO
C LINEAR CONSTRAINTS
C ------------------------------------------------
C
      IMPLICIT INTEGER(A-Z)
      REAL MN,MX,P,Q,MC,PF,QF,FS,QS,MNA,MXA,MA,MB
      DIMENSION C(20),AL(10),BE(10),D(20,20),CON(20),
     @          MN(20),MX(20),PF(20),QF(20),P(20,20),
     @          G(20,20),IMN(20),IMX(20),T(20),NT(20)
     @          A(20,20),B(20),S(20,20),X(20),E(20),
     @          F(20)
C
C  INITIALIZE ARRAYS
C  ----------------
      DO 8 J=1,20
      DO 8 I=1,20
      D(I,J)=0
      S(I,J)=0
8     CONTINUE
      CALL INPUT(M,N,A,B,C)
      IF(N.NE.2)GO TO 15
      D(1,1)=-C(2)
      D(2,1)=C(1)
      KAP1=C(1)
      KAP2=C(2)
      GO TO 58
C
C  FIND ALPHA AND BETA ARRAYS
C  -------------------------
15    ND=2 N-4
      KAP2=C(N)
      KAP1=C(N-1)
      M2=N-2
      DO 10 M3=1,M2
         M4=N+1-M3
         M5=M3 2
         CALL CONFPA(KAP2,KAP1,E,RN,NC)
         AL(M5)=KAP2/RN
         BE(M5)=-KAP1/RN
         ALF=-AL(M5)
         BET=BE(M5)
         CALL CONVGT(BET,ALF,PN,QN,NC)
         AL(M5-1)=((-1)**NC)*QN
         IF(BET.LT.0)AL(M5-1)=-AL(M5-1)
         BE(M5-1)=((-1)**(NC-1))*PN
         IF(ALF.LT.0)BE(M5-1)=-BE(M5-1)
         KAP2=KAP1 AL(M5-1)+KAP2 BE(M5-1)
         KAP1=C(M4-2)
10    CONTINUE
C
C  NOW COMPUTE MATRIX D
C  --------------------
      BE(2*N-2)=KAP1
      D(1,1)=-KAP2
      DO 120 K1=2,N
         K2=K1-1
         K3=K2-1
         IF(K1.EQ.2)K3=1
         DO 110 R1=1,K3
            IF(R1.EQ.1) GO TO 88
            R2=R1-1
            F(R2)=1
88          IF(K1.EQ.2) GO TO 100
            DO 90 S1=R1,K3
```

```
      IF(S1.NE.1) GO TO 89
      F(1)=BE(2*N-(2*S1+3))
      GO TO 90
89       F(S1)=F(S1-1)*BE(2*N-(2*S1+3))
90    CONTINUE
      IF(K1.EQ.N) GO TO 105
100   D(K1,R1)=AL(2*N-(2*K1+1))*BE(2*N-2*R1)*F(K2
      GO TO 110
105   D(N,R1)=BE(2*N-2*R1)*F(K3)
110   CONTINUE
      IF(K1.EQ.N) GO TO 115
      D(K1,K2)=AL(2*N-(2*K1+1))*BE(2*N-2*K2)
      D(K1,K1)=AL(2*N-2*K1)
      GO TO 120
115   D(K1,K2)=BE(2*N-2*K2)
120   CONTINUE
      N1=N-1
      DO 49 I=1,N
49    CONTINUE
50    WRITE(1,31)
31    FORMAT(/'INPUT C')
      READ(1,*)Z
      IF(Z.NE.-9999) GO TO 32
      STOP
C
C   FIND XK,VL, THE INITIAL SOLUTIONS
C   -------------------------------
32    CALL CONVGT(KAP1,KAP2,PN,QN,NC)
      XK=((-1)**NC)*QN*Z
      IF(KAP1.LT.0)XK=-XK
      VL=((-1)**(NC+1))*PN*Z
      IF(KAP2.LT.0)VL=-VL
C
C   FIND THE CONSTANT VECTOR K
C   -------------------------
      CON(1)=XK
      DO 210 K1=2,N
         CON(K1)=D(K1,1)*VL/KAP1
210    CONTINUE
C
C   DETERMINE BOUNDS OF T
C   ---------------------
      MN(1)=-FLOAT(CON(1))/D(1,1)
      MX(1)=(FLOAT(Z)/C(1)-FLOAT(CON(1)))/D(1,1)
      IF(MN(1).LE.MX(1)) GO TO 310
      MS=MN(1)
      MN(1)=MX(1)
      MX(1)=MS
      IF(N.EQ.2) GO TO 351
310   DO 350 K=2,N
         N6=K-1
         IF(K.EQ.N)N6=N6-1
         DD=D(K,K)
         K1=K-1
         IF(K.EQ.N)DD=D(K,K1)
         DO 340  J=1,N6
            P(K,J)=-D(K,J)*MN(J)/DD
            Q(K,J)=-D(K,J)*MX(J)/DD
            IF(P(K,J).LE.Q(K,J)) GO TO 330
            MS=P(K,J)
            P(K,J)=Q(K,J)
            Q(K,J)=MS
            J1=J-1
330         IF(J1.GT.0) GO TO 335
            PS=0.
            QS=0.
            GO TO 336
335         PS=P(K,J1)
```

```
                  QS=Q(K,J1)
336               PF(K)=P(K,J)+PS
                  QF(K)=Q(K,J)+QS
340         CONTINUE
            MNA=PF(K)
            MXA=QF(K)
            IF(DD.GE.0) GO TO 345
            MNA=QF(K)
            MXA=PF(K)
            MN(K)=-FLOAT(CON(K))/DD+MNA
            MX(K)=(FLOAT(Z)/C(K)-FLOAT(CON(K)))/DD+MX
345          IF(MN(K).LE.MX(K)) GO TO 350
            MS=MN(K)
            MN(K)=MX(K)
            MX(K)=MS
350    CONTINUE
       IF(MN(N).LT.MN(N-1))MN(N-1)=MN(N)
       IF(MX(N).GT.MX(N-1))MX(N-1)=MX(N)
       N1=N-1
351     DO 365 J=1,N1
            DO 365 K=1,2
               MA=MN(J)
               IF(K.EQ.2) MA=MX(J)
               MB=ABS(MA)
C
C   TEST IF BOUND IS ALREADY INTEGER
C   --------------------------------
            IF((MA-IFIX(MA)).EQ.0.) GO TO 352
C
C   IF MIN IS POSITIVE OR MAX IS NEGATIVE
C   ROUND DOWN
C   -------------------------------------
            IF((K.EQ.1).AND.(MA.GE.0.)) GO TO 352
            IF((K.EQ.2).AND.(MA.LT.0.)) GO TO 352
            MB=MB+1.0
352          MI=IFIX(MB)
               IF(K.EQ.2)GO TO 360
               IMN(J)=-MI
               IF(MA.GE.0)IMN(J)=MI
               GO TO 365
360            IMX(J)=-MI
               IF(MA.GE.0)IMX(J)=MI
365      CONTINUE
C
C   SET INITIAL T VALUES AND COUNT T-SET
C   ------------------------------------
       N1=N-1
       N10=1
       DO 70 J=1,N1
            T(J)=IMN(J)
            NT(J)=IMX(J)-IMN(J)+1
            N10=N10*NT(J)
70     CONTINUE
       WRITE(1,71)N10
71     FORMAT(/'NUMBER OF POINTS SEARCHED'/I1 )
       T(N1)=IMN(N1)-1
C
C   COMPUTE SOLUTION X AND CHECK FEASIBILITY
C   ----------------------------------------
       WRITE(1,402)
402    FORMAT(/'FEASIBLE SOLUTIONS X(I)')
       J1=0
       DO 85 J10=1,N10
       IT  =1
405    IF(T(IT).GT.IMX(IT)) GO TO 420
       IT=IT+1
       IF(IT.NE.N1) GO TO 405
       T(IT)=T(IT)+1
```

```
      IF(T(IT).LE.IMX(IT)) GO TO 430
420   T(IT)=IMN(IT)
      IT=IT-1
      T(IT)=T(IT)+1
      IF(T(IT).GT.IMX(IT)) GO TO 405
430   CONTINUE
      FE=0
C
C  SETS FEASIBILITY INDICATOR
C  --------------------------
      T(N)=0
      DO 520 J=1,N
            XA=0
            DO 510 K=1,J
                      XA=XA+D(J,K)*T(K)
510         CONTINUE
            X(J)=CON(J)+XA
            IF(X(J).GE.0) GO TO 520
      J=N
      GO TO 525
520    CONTINUE
      FE=1
525    CONTINUE
            IF(FE.EQ.0)GO TO 80
C
C  FE=1 IF SOLUTIONS IS FEASIBLE
C  FE=0 OTHERWISE
C  -----------------------------
      FE=0
      DO 620 I=1,M
            S(I,1)=A(I,1)*X(1)
             DO 610 J=2,N
                      S(I,J)=S(I,J-1)+A(I,J)*X(J)
610           CONTINUE
            IF(S(I,N).LE.B(I)) GO TO 620
            I=M
            GO TO 630
620    CONTINUE
      FE=1
630    CONTINUE
            IF(FE.EQ.0) GO TO 80
C
C  PRINT IF FEASIBLE
C  -----------------
            WRITE(1,75)(X(K),K=1,N)
75          FORMAT(/10(2X,I1 )/)
80          J1=J1+1
            IF(J1.LT.100000) GO TO 85
            J1=0
85    CONTINUE
      GO TO 50
      END
      SUBROUTINE CONVGT(I,J,PN,QN,NC)
C
C  THIS FINDS FIRST THE CONTINUED FRACTION OF I,J
C  THEN THE (N-1)TH CONVERGENT OF P,Q
C  ----------------------------------------------
      IMPLICIT INTEGER(A-Z)
      DIMENSION P(20),Q(20),E(20)
      IF(IABS(J).EQ.1) GO TO 26
      IF(IABS(I).EQ.1) GO TO 27
      CALL CONFRA(I,J,E,PN,NC)
C
C  CONVERGENTS
C  -----------
      P(1)=E(1)
      Q(1)=1
      P(2)=E(2)*E(1)+1
```

```
      Q(2)=E(2)
      IF(NC.GT.3) GO TO 20
      PN=P(2)
      QN=Q(2)
      GO TO 30
20    N5=NC-1
      DO 25 M1=3,N5
         P(M1)=E(M1)*P(M1-1)+P(M1-2)
         Q(M1)=E(M1)*Q(M1-1)+Q(M1-2)
25    CONTINUE
      PN=P(M1)
      QN=Q(M1)
      GO TO 30
26    PN=IABS(I/J)-1
      QN=1
      NC=2
      GO TO 30
27    PN=0
      QN=1
      NC=2
30    RETURN
      END
      SUBROUTINE CONFRA(A,B,E,RN,NC)
C
C   FINDS HCF OF A,B AND CONTINUED FRACTION OF A/B
C   ----------------------------------------------
      IMPLICIT INTEGER(A-Z)
      DIMENSION E(20),R(20)
      NC=1
      I1=IABS(A)
      J1=IABS(B)
      R(1)=J1
      IF((I1.EQ.1).OR.(J1.EQ.1)) GO TO 45
C
C   CONTINUED FRACTIONS
C   -------------------
C
      IF(I1.LE.J1) GO TO 35
      E(1)=I1/J1
      R(2)=I1-E(1)*J1
      GO TO 40
35    E(1)=0
      R(2)=I1
40    NC=NC+1
      E(NC)=R(NC-1)/R(NC)
      R(NC+1)=R(NC-1)-E(NC)*R(NC)
      IF(R(NC+1).NE.0) GO TO 40
      RN=R(NC)
      GO TO 50
45    RN=1
50    RETURN
      END
      SUBROUTINE INPUT(M,N,A,B,C)
C
C   INPUTS AX<=B
C   A IS AN M BY N MATRIX
C   C'X IS THE OBJECTIVE FUNCTION
C   -----------------------------
      IMPLICIT INTEGER(A-Z)
      DIMENSION A(20,20),B(20),C(20)
4     WRITE(1,5)
5     FORMAT(//'ENTER NO. OF VARIABLES')
      READ(1,*)N
      WRITE(1,10)
10    FORMAT(/'ENTER COEFFICIENTS C(J)')
      READ(1,*)(C(J),J=1,N)
      WRITE(1,25)
25    FORMAT(/'HOW MANY CONSTRAINTS')
```

```
      Q(2)=E(2)
      IF(NC.GT.3) GO TO 20
      PN=P(2)
      QN=Q(2)
      GO TO 30
20    N5=NC-1
      DO 25 M1=3,N5
         P(M1)=E(M1)*P(M1-1)+P(M1-2)
         Q(M1)=E(M1)*Q(M1-1)+Q(M1-2)
25    CONTINUE
      PN=P(M1)
      QN=Q(M1)
      GO TO 30
26    PN=IABS(I/J)-1
      QN=1
      NC=2
      GO TO 30
27    PN=0
      QN=1
      NC=2
30    RETURN
      END
      SUBROUTINE CONFRA(A,B,E,RN,NC)
C
C   FINDS HCF OF A,B AND CONTINUED FRACTION OF A/B
C   ---------------------------------------------
      IMPLICIT INTEGER(A-Z)
      DIMENSION E(20),R(20)
      NC=1
      I1=IABS(A)
      J1=IABS(B)
      R(1)=J1
      IF((I1.EQ.1).OR.(J1.EQ.1)) GO TO 45
C
C   CONTINUED FRACTIONS
C   -------------------
C
      IF(I1.LE.J1) GO TO 35
      E(1)=I1/J1
      R(2)=I1-E(1)*J1
      GO TO 40
35    E(1)=0
      R(2)=I1
40    NC=NC+1
      E(NC)=R(NC-1)/R(NC)
      R(NC+1)=R(NC-1)-E(NC)*R(NC)
      IF(R(NC+1).NE.0) GO TO 40
      RN=R(NC)
      GO TO 50
45    RN=1
50    RETURN
      END
      SUBROUTINE INPUT(M,N,A,B,C)
C
C   INPUTS AX<=B
C   A IS AN M BY N MATRIX
C   C*X IS THE OBJECTIVE FUNCTION
C   -----------------------------
      IMPLICIT INTEGER(A-Z)
      DIMENSION A(20,20),B(20),C(20)
4     WRITE(1,5)
5     FORMAT(//'ENTER NO. OF VARIABLES')
      READ(1,*)N
      WRITE(1,10)
10    FORMAT(/'ENTER COEFFICIENTS C(J)')
      READ(1,*)(C(J),J=1,N)
      WRITE(1,25)
25    FORMAT(/'HOW MANY CONSTRAINTS')
```

```
      READ(1,*)M
      WRITE(1,30)
30    FORMAT(/'ENTER COEFFICIENTS A(I,J)')
      DO 35 I=1,M
35    READ(1,*)(A(I,J),J=1,N)
      WRITE(1,40)
40    FORMAT(/'TYPE IN COEFFICIENTS B(I)')
      READ(1,*)(B(I),I=1,M)
      WRITE(1,55)
55    FORMAT(/'IS INPUT O.K.  ENTER "Y" OR "N" ')
      READ(1,60)X
60    FORMAT(A1)
      IF(X.EQ.'N') GO TO 4
      RETURN
      END
```

```
ENTER NO. OF VARIABLES
4

ENTER COEFFICIENTS C(J)
2 1 5 3

HOW MANY CONSTRAINTS
4

ENTER COEFFICIENTS A(I,J)
  1 -1 5 1
3 1 -1 2
-1 2 1 -1
1 1 1 1

TYPE IN COEFFICIENTS B(I)
10 15 5 8

IS INPUT O.K.  ENTER "Y" OR "N"
Y

INPUT C
18

NUMBER OF POINTS SEARCHED
      6669

FEASIBLE SOLUTIONS X(I)
```

0	3	0	5
0	2	2	2
0	1	1	4
0	0	0	6
1	2	1	3
1	1	0	5
2	3	1	2
2	0	1	3
3	1	1	2
4	2	1	1

86, -2. The referee's estimate was not confirmed by a direct comparison of MINMAX with subroutine LINES by Sklar and Armstrong. In order to clarify the role of the advanced L_2 start, a third program (subroutine SHORT) was included in this comparison. SHORT is a subset of MINMAX which works without the L_2 start. The following CPU times in csec are representative for small and large data sets, respectively. The figures in brackets denote the number of statements in each subroutine.

Number of points	MINMAX(121)	SHORT(47)	LINES(149)
31	0.5	0.6	0.7
450	12	6	10

The figures show that, in general, no time advantage is gained by applying the L_2 start to large data sets. An optimal code (usually faster than LINES) would combine MINMAX and SHORT, activating the SHORT option for large data sets.

The integration of this, and the numerical series which ensue, provide exercises for the interested reader.

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A square root algorithm

MAX PLANITZ

Although the approximation of elementary functions is a well-researched area of mathematics, very little has been published on built-in routines in any particular calculator or computer. Computer manufacturers are, understandably perhaps, reluctant to publicise details about their algorithms. Hewlett-Packard have been less secretive than most and allowed an occasional glimpse behind the scene in their own Journal and various other sources. The following square root routine for one of their machines, the now extinct 2000F series, has appeared in an Open University text on numerical computation [1]. The process of evaluating $\sqrt{x}$ is carried out in four steps:

(i) Determine a real number $t \in [0{\cdot}25, 1]$, such that $x = 4^k t$, where k is an integer.

(ii) Use the formula

$$y(t) = \begin{cases} 0{\cdot}27863 \quad + 0{\cdot}875t & t \in [0{\cdot}25, 0{\cdot}5) \\ 0{\cdot}421875 + 0{\cdot}578125t & t \in [0{\cdot}5, 1) \end{cases}$$

to obtain a first approximation for $\sqrt{t}$.

(iii) Apply Newton's method in the form

$$y_{n+1} = (y_n + t/y_n)/2$$

with $y_0 = y(t)$ and $n = 0, 1$.

(iv) Compute $\sqrt{x} = 2^k y_2$. The result is correct to 6 significant figures!!

This algorithm, which seems cumbersome at first sight, is in fact remarkably efficient. To obtain $\sqrt{x}$ to 6 significant figures, a binary computer requires only 2 "long" operations (i.e. multiplications or divisions). These are needed to compute t/y_n in step (iii). Steps (i) and (iv), as well as the division by 2 in step (iii), only involve shifts. Less obviously, step (ii) can be called a "short" operation, since $0{\cdot}875 = 0{\cdot}111_2$ and $0{\cdot}578125 = 0{\cdot}100101_2$, i.e. only 4 additions and 3 shifts are required to find $y(t)$.

The selection of an approximating function for step (ii) is an interesting, non-trivial problem. First note that for greater accuracy, the approximation on $[0{\cdot}25,\ 1)$ is segmented. Since our computer is assumed to use binary arithmetic, a power of 2 is chosen as the point of subdivision. We require the best linear approximation for $\sqrt{t}$ on each subinterval. The precise meaning of "best approximation" depends on the norm used to measure the "distance" between two functions. For the purposes of evaluating a function on a closed interval, an appoximation is as good as its maximum error on that interval. It therefore makes sense to minimize the Chebyshev norm of $y(t) - \sqrt{t}$, i.e. the expression

$$\max_{a \leqslant t \leqslant b} |y(t) - \sqrt{t}|.$$

More generally, we make the following

DEFINITION. Let $y(t)$ belong to the set P_{n-1} of polynomials whose degree does not exceed $n - 1$. If

$$\max_{a \leqslant t \leqslant b} |y(t) - f(t)| \leqslant \max_{a \leqslant t \leqslant b} |x(t) - f(t)|$$

for all x in P_{n-1}, then y is called a *polynomial of best approximation* to $f(t)$.

Polynomials of best approximation are characterised by an alternation property, which was discovered by Chebychev in the 1850s. We state this property for polynomials in P_{n-1}; for a proof the reader is referred to [2, p. 75].

THEOREM. *Let $f \in C[a, b]$ and $y \in P_{n-1}$. Then y is a polynomial of best approximation to f on $[a, b]$ if and only if there are $n + 1$ points $t_1, \ldots, t_{n+1} \in [a, b]$, with $t_1 < \ldots < t_{n+1}$, such that*

$$|y(t_i) - f(t_i)| = \max_{a \leqslant t \leqslant b} |y(t) - f(t)|$$

and $y(t_i) - f(t_i)$ alternates in sign for $i = 1, \ldots, n + 1$.

Although y is known to exist, uniquely in fact, for any continuous f, it remains an open question whether there is a general finite-step algorithm for the construction of best approximations. (An iterative method can be found in the book by Cheney [2, p.96].) Such a construction is feasible, however, if f has a second derivative whose sign does not alter on $[a, b]$ and if y is linear. These conditions are satisfied by $f(t) = \sqrt{t}$ and $y(t) = a_0 + a_1 t$, and we proceed to deduce the values of a_0 and a_1 from the alternation property. First consider the interval $[0{\cdot}25,\ 0{\cdot}5]$. The theorem tells us that the error function

$$y(t) - f(t) = a_0 + a_1 t - \sqrt{t}$$

attains its extrema for three values $t_1, t_2, t_3 \in [0{\cdot}25, 0{\cdot}5]$, with $t_1 < t_2 < t_3$. It follows that

$$y'(t_2) - f'(t_2) = a_1 - 1/(2\sqrt{t_2}) = 0$$

i.e.

$$a_1 = 1/(2\sqrt{t_2}).$$

Since $f''(t) < 0$ on $[0{\cdot}25, 0{\cdot}5]$, $y'(t) - f'(t)$ cannot vanish for a second value of t inside the interval, i.e. $t_1 = 0{\cdot}25$ and $t_3 = 0{\cdot}5$. Using the alternation property, we can now write

$$a_0 + 0{\cdot}25a_1 - 0{\cdot}5 = a_0 + 0{\cdot}5a_1 - \sqrt{0{\cdot}5} = \sqrt{t_2} - a_0 - t_2 a_1,$$

(where $a_1 = 1/(2\sqrt{t_2})$. Solving, we find $a_0 = 0{\cdot}297335$, $a_1 = 0{\cdot}828427$, $t_2 = 0{\cdot}363277$. We then apply the same technique to the interval $[0{\cdot}5, 1]$. The approximation formula obtained in this way is

$$y^*(t) = \begin{cases} 0{\cdot}297335 + 0{\cdot}828427t & t \in [0{\cdot}25, 0{\cdot}5) \\ 0{\cdot}420495 + 0{\cdot}585786t & t \in [0{\cdot}5, 1), \end{cases}$$

with approximate errors of $0{\cdot}004$ on $[0{\cdot}25, 0{\cdot}5)$ and $0{\cdot}006$ on $[0{\cdot}5, 1)$.

Some of the accuracy of y^* is now sacrificed in order to reduce the execution time of step (ii). This is done by approximating the coefficients of t by numbers whose binary expansions contain only three non-zero bits. The resulting formula is

$$y(t) = \begin{cases} a_0 + 0{\cdot}875t & t \in [0{\cdot}25, 0{\cdot}5) \\ b_0 + 0{\cdot}578125t & t \in [0{\cdot}5, 1). \end{cases}$$

It is not clear how the coefficients a_0, b_0 were originally obtained, but the following approach leads to similar, in fact slightly better, results. To adjust first the value of a_0, we apply our theorem to the function

$$g(t) = \sqrt{t} - 0{\cdot}875t.$$

This time, the best approximation is a constant, and a simple argument will show that this constant is given by

$$a_0 = (m + M)/2,$$

where $m = \min g(t)$ and $M = \max g(t)$ on $[0{\cdot}25, 0{\cdot}5]$. Since $n = 1$, we have to show that the error function alternates on two points. If we define t_1, t_2 by $m = g(t_1)$ and $M = g(t_2)$, then

$$a_0 - g(t_1) = (M - m)/2 \quad \text{and} \quad a_0 - g(t_2) = (m - M)/2.$$

Moreover,

$$|a_0 - g(t_i)| = \max|a_0 - g(t)|, \quad i = 1 \text{ or } 2, \quad 0{\cdot}25 \leqslant t \leqslant 0{\cdot}5,$$

i.e. $a_0 = (m + M)/2$ satisfies the alternation property of the theorem. It is now easy to show that $m = 0{\cdot}2696068$ and $M = 0{\cdot}2857143$. Hence $a_0 = 0{\cdot}277661$. This gives a maximum absolute error of $0{\cdot}008$ on $[0{\cdot}25, 0{\cdot}5)$, compared with an error of $0{\cdot}009$ in Hewlett-Packard's original formula. We similarly find $b_0 = 0{\cdot}425008$ with an error of $0{\cdot}007$, which represents an improvement by $0{\cdot}003$. A further reduction in the number of long operations could be achieved by introducing a k-fold segmented approximation to $\sqrt{t}$, with $k > 2$.

The basic strategy of our square root routine is to reduce execution time by using shifts, additions and recall of prestored constants in preference to long operations. With the dramatic fall in the cost of computer memory, this technique has become widely used, especially in a group of algorithms referred to as "CORDIC". The **Co**ordinate **R**otation **Di**gital **C**omputer was designed by J. E. Volder [3] in the 1950s. Its purpose was to perform real-time navigational calculations at high speed. We conclude this article by outlining a CORDIC algorithm for tan x.

Let $x = \sigma_1\alpha_1 + \cdots + \sigma_n\alpha_n + \varepsilon_n$ $(0 < x < \pi/2)$, where $\sigma_i = \pm 1$ and ε_n is small. The angles $\alpha_1, \ldots, \alpha_n$ (n depends on the accuracy required) will be defined later; they represent the rotations from which the method takes its name. Using the usual addition formulae for the sine and cosine functions, we obtain

$$\begin{pmatrix}\cos x\\ \sin x\end{pmatrix} = \cos\alpha_1\begin{pmatrix}1 & -\tan\alpha_1\\ \tan\alpha_1 & 1\end{pmatrix}\begin{pmatrix}\cos(x-\alpha_1)\\ \sin(x-\alpha_1)\end{pmatrix}$$

and

$$\begin{pmatrix}\cos(x-\alpha_1)\\ \sin(x-\alpha_1)\end{pmatrix} = \cos\alpha_2\begin{pmatrix}1 & -\tan\alpha_2\\ \tan\alpha_2 & 1\end{pmatrix}\begin{pmatrix}\cos(x-\alpha_1-\alpha_2)\\ \sin(x-\alpha_1-\alpha_2)\end{pmatrix}.$$

Denoting $\cos\alpha_i$ by c_i, $\tan\alpha_i$ by t_i and $\begin{pmatrix}1 & -t_i\\ t_i & 1\end{pmatrix}$ by T_i, we can write

$$\begin{pmatrix}\cos x\\ \sin x\end{pmatrix} = c_1c_2T_1T_2\begin{pmatrix}\cos(x-\alpha_1-\alpha_2)\\ \sin(x-\alpha_1-\alpha_2)\end{pmatrix}.$$

Continuing this process we find

$$\begin{pmatrix}\cos x\\ \sin x\end{pmatrix} = c_1\ldots c_nT_1\ldots T_n\begin{pmatrix}\cos\varepsilon_n\\ \sin\varepsilon_n\end{pmatrix} \quad \text{or}$$

$$\begin{pmatrix}(\cos x)/c\\ (\sin x)/c\end{pmatrix} = T_1\ldots T_n\begin{pmatrix}\cos\varepsilon_n\\ \sin\varepsilon_n\end{pmatrix},$$

where $c = c_1\ldots c_n$ and $\begin{pmatrix}\cos\varepsilon_n\\ \sin\varepsilon_n\end{pmatrix} \approx \begin{pmatrix}1\\ 0\end{pmatrix}$. Note that c need not be evaluated

since tan x = sin x/cos

clever choice of the angles

$\alpha_i = \tan^{-1} 2^{1-i}$,

$i = 1, \ldots, n$, which enable

if the values of t_i and α_i ar

CORDIC techniques

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Data permutation t

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Example 1. A horticultu

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since $\tan x = \sin x/\cos x$. The power of the CORDIC method lies in the clever choice of the angles $\alpha_1, \ldots, \alpha_n$. We define

$$\alpha_i = \tan^{-1} 2^{1-i},$$

$i = 1, \ldots, n$, which enables us to compute $\tan x$ by shifts and additions only, if the values of t_i and α_i are prestored in read-only memory.

CORDIC techniques have been developed for other elementary functions, including the square root function. An interesting unified CORDIC algorithm can be found in a paper by J. S. Walther [4]. By constructing a special processor with three parallel adders, Walther achieved the same maximum execution time of 100 μsec for square roots, multiplications and divisions.

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Data permutation tests

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This article is about a powerful method of carrying out tests of statistical significance. Its rationale depends on simple ideas of probability and is suitable for pupils at school. Practical applications require a considerable amount of computation but now that schools are equipped with computers this should not be a problem.

Systematic data permutation

The method is introduced by means of examples; in these the sample sizes are kept unrealistically small so that the method used can be more easily perceived. Examples 1 to 3 illustrate different types of data permutation appropriate to three common situations.

Example 1. A horticulturalist has managed to raise 5 seeds of a rare plant and wishes to compare two methods of feeding the plants. He assigns at random 2 seeds to method A and 3 to method B, and finds that the percentage increases in heights of the plants are 53, 97 for method A, and 3, 6, 11 for method B.

There are 10 ways in which the 5 seeds could have been divided into two groups of sizes 2 and 3; since the sampling was random all 10 ways are equally likely. On the null hypothesis that the percentage increase in height is independent of the method of feeding, each of the following results is equally likely. Here n_A, n_B are the numbers in groups A and B; m_A, m_B are the means of the groups; $\sum X_A, \sum X_B$ are the totals for the two groups and t is calculated from the formulae

$$t = (m_A - m_B)\Big/\left(\frac{s^2}{n_A} + \frac{s^2}{n_B}\right)^{\frac{1}{2}}$$

$$\text{where } s^2 = \left(\sum(X_A - m_A)^2 + \sum(X_B - m_B)^2\right)/(n_A + n_B - 2)$$

Method A	Method B	$m_A - m_B$	t	$\sum X_A$	$\sum X_B$
3 6	11 53 97	−49·2	−1·53	9	161
3 11	6 53 97	−45·0	−1·32	14	156
6 11	3 53 97	−42·5	−1·21	17	153
3 53	6 11 97	−10·0	−0·24	56	114
6 53	33 11 97	−7·5	−0·18	59	111
11 53	3 6 97	−3·3	−0·08	64	106
3 97	6 11 53	26·7	0·67	100	70
6 97	3 11 53	29·2	0·74	103	67
11 97	3 6 53	33·3	0·87	108	62
53 97	3 6 11	68·3	4·10	150	20

The observed result has the largest value of $t = 4{\cdot}10$, and so the probability that t should be as large as this (or greater) is 1/10. One would expect the experimenter to specify in advance a level of probability at which to reject the null hypothesis. However, the examples are artificial and we shall not pretend to do this. The experimenter should also be clear whether a one- or two-tailed test is appropriate but in this case a two-tailed test, and a one-tailed test in favour of method A, have the same probability.

It was not necessary to list the results in full but the table does help to illustrate some of the following points:

(1) We considered every possible pair of samples of the specified sizes which could have been drawn from the 5 values of the variate. This is one example of *systematic data permutation*.

(2) We made *no* assumption that the original sample was random, only that the assignment to the methods was made on a random basis. The test which followed is an example of a *randomisation test*. As really random samples are very rare, there is a clear advantage in such tests.

A COMPARISON OF THE ALGORITHMS FOR AUTOMATED DATA ADJUSTMENT AND MATERIAL BALANCE AROUND MINERAL PROCESSING EQUIPMENT

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Abstract. The data adjustment problem that occurs in the mass balance of a mineral processing plant is outlined. By means of a simple problem of one process unit, with one feed and two output streams, the basic techniques of data adjustment and material balance are presented. Algorithms that employ the varying techniques are then examined from the programming point of view, with particular emphasis on microcomputer applications.

Keywords. Automated material balance; Computer aided circuit analysis; Minerals industries; Optimisation.

INTRODUCTION

One area where the increasing availability of micro-computers can make a large impact is in the automation of tedious engineering calculations. An example is the calculation of a material balance in a mineral processing plant (ie. what flows where and how much of it flows there). The problem associated with this task is that the measured data give rise to an overdetermined inconsistent set of equations. Therefore in a large process flow-sheet, consisting of multiple process streams and equipment, achieving a reliable material balance depends on the mineral engineer's experience in making the necessary adjustments to the measured assay data. For complicated flowsheets this may demand many man hours of work.

Since the early 70's,following in the wake of the work of Wiegel (1972), there have been a number of computer packages designed to produce a material balance around a mineral processing circuit from inconsistent measurements (see Reid et al (1982) for a review). The basic principle in all of these packages is the automated adjustment of the input data via the minimisation of a weighted sum of squares.

It is true to say that the majority of available packages are intended for implementation on main frame computers. There is, however, a strong argument to be made for fitting data adjustment and material balance routines on to microcomputers. For relatively simple problems this has already been achieved, Reid and Voller (1983). In fact, a data adjustment algorithm for hydrocyclone size data has been implemented on a hand held programmable calculator, Voller and Ryan (1983).

The aim of this paper is to return to the "fundamental" material balance problem, that is the balance around a single three stream (one feed,two products) process unit. In this way the basic engineering and mathematical problems can be clearly stated and examined. Furthermore, a comparative study of the possible techniques for solving the data adjustment and material balance problem in terms of computer and engineering requirements can be made.

THE MATERIAL BALANCE PROBLEM

Consider a single processing unit with a feed stream (1) and two product streams (2) and (3) shown schematically in Fig. 1.

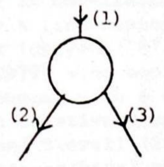

Fig. 1. A three stream process unit.

Further, assume that each stream has been assayed for n distinct species (eg % copper, % weight of particles with size less than 100μ etc.,). In order to close the material balance around this process unit, ie. calculate the mass flows in each stream n+1 mass balance equations have to be satisfied, viz,

$$M_1 - M_2 - M_3 = 0 \tag{1}$$

and

$$M_1X_1^k - M_2X_2^k - M_3X_3^k = 0 \quad (k=1(1)n) \qquad (2)$$

where M_i is the mass flow in stream i and X_i^k is the assayed value of species k on stream i. In terms of the feed mass flow rate M_1 solutions to equations (1) and (2) will be of the form

$$M_2 = M_1 \ (X_1^k - X_3^k)/X_2^k - X_3^k) \qquad (3)$$

the so called "two product balance" formula. The major drawback in using equation (3) is that due to sampling errors etc. the values of M_2 and M_3 will depend on the assay species used. The data in Table 1 represents a typical set of inconsistent measured assays. Using

TABLE 1 Assay Data

Stream	Assay type 1	2
(1)	23.8	52.1
(2)	5.3	40.7
(3)	53.9	63.4

each of the two assay species in turn in two product balance formula will give marked differences in the estimates for M_2 and M_3, see Table 2.

TABLE 2 Two Product Balance Massflow Estimates.

Assay Type	Mass flows as a fraction of M_1 M_2	M_3
1	.6192	.3808
2	.4976	.5024

To solve this system of overdetermined inconsistent equations the measured assayed data need to be adjusted. A technique that adjusts the assayed data would have to perform in a constant manner, ie., the criteria by which adjustments are made should be independent of the problem. A suitable criterion for adjustment would be one in which the adjusted assays: (1) satisfied all the mass balance equations; and (2) the adjustments made were in some sense the minimum possible. In addition, adjustments of the assays would also have to take account of the relative errors generated in the sampling and assaying. Errors of this type are often assumed to be normal, unbiased and independent. With these assumptions the minimum adjustment may be taken to occur when

$$J = \sum_1^n J^k = \text{a minimum} \qquad (4)$$

In the case of a single three stream process unit we have

$$J^k = \sum_1^3 W_j^k(\hat{X}_j^k - X_j^k)^2 \qquad (5)$$

where $\hat{X}_j^k$ is the adjusted assay on stream j and W_j^k is a weighting factor. The material balance problem may be stated as:- find the set of assays $\hat{X}_j^k$ (j=1(1)3, k=1(1)n) that minimise J subject to the mass balance constraints equations (1) and (2). On defining a relative mass flowrate D to be

$$D = M_1/M_2$$

the n+1 constraints on the minimisation of J can be reduced to the n constraints

$$\hat{X}_1^k - D\hat{X}_2^k - (1 - D)\hat{X}_3^k = 0 \qquad (6)$$

THE METHODS

There are a number of alternative approaches for solving the optimisation problem defined by equations (4)-(6). In packages designed for the minerals industry methods ranging from Lagrange multipliers to direct search techniques have been employed, Mular (1980). In applications to the simple one process test problem some of the subtlety of these methods is lost. Nevertheless the basic differences of the varying approaches can be clearly illustrated.

The most common approach of solving equations (4)-(6) is by the introduction of Lagrange multipliers, λ^k, such that the mass balance constraints and functional J are combined in a single functional, viz

$$L = J + \lambda^k(\hat{X}_1^k - D\hat{X}_2^k - (1-D)\hat{X}_3^k) \qquad (7)$$

which requires minimisation. This approach has been used in a number of large mineral processing material balance packages. These packages, however, employ a variety of methods to minimise equation (7). Wiegel (1972), Cutting (1976) and Laguitton and Wilson (1979) use a gradient method deriving a set of non-linear equations which are solved by a linearising iterative technique. Smith and Ichiyen (1973) and Hockings and Callen (1977) also employ the gradient method coupled with a search over the independent relative massflows in the circuit. Hodouin and Everell (1980) employ a so-called "hierarchical procedure" in which the problem is decomposed and a combination of gradient, search, and Newton-Raphson methods are adopted for maximum efficiency.

For the case of a balance around a single process unit application of a gradient method (ie differentiation w.r.t. each unknown) results in a set of 4n+1 equations viz,

$$2W_j^k(\hat{X}_j^k - X_j^k) - g_j\lambda^k = 0 \qquad (8a)$$

$$\sum_1^3 g_j\hat{X}_j^k = 0 \qquad (8b)$$

$$\sum_1^n \lambda^k(\hat{x}_3^k - \hat{x}_2^k) = 0 \tag{8c}$$

where $g_1 = -1$, $g_2 = D$, and $g_3 = 1-D$. In terms of D equations (8) give

$$\hat{x}_j^k = x_j^k + g_j r^k/(W_j h^k) \tag{9}$$

where

$$r^k = x_1^k - Dx_2^k - (1-D)x_3^k \tag{10}$$

is referred to as the residue or imbalance equation and

$$h^k = 1/W_1^k + D^2/W_2^k + (1-D)^2/W_3^k \tag{11}$$

On substitution of equation (9) into equation (8) the following polynomial in D is obtained

$$\sum_1^n \left(\frac{r^k}{h^k}\right)\left[(x_2^k - x_3^k) + \left(\frac{r^k}{h^k}\right)\left(\frac{D}{W_2^k} - \frac{(1-D)}{W_3^k}\right)\right] = 0 \tag{12}$$

Solution of this polynomial, via Newton-Raphson for example, will give the value of D that minimises L. The corresponding adjusted assays may then be calculated from equation (9). This method will be referred to as LMP for Lagrange Multiplier Polynomial.

The value of D that minimises L may alternatively be found via a search technique. For any choice of D corresponding minimum adjusted assays may be calculated from equation (9). Therefore on performing a search on D calculating adjusted assays at each step the values of D and $\hat{x}_j^k$ that minimise L may be found. This method will be referred to as LMS for Lagrange Multiplier Search.

Minimisation of the weighted sum of squares

$$J^* = \sum_1^n W^{*k}(r^k)^2 \tag{13}$$

where the weighting factor $W^{*k} = 1/h^k$ provides yet one more way of determining a "best" value for D. A gradient method to minimise J^* gives

$$D = \frac{\sum_1^n W^{*k}(x_2^k - x_3^k)(x_1^k - x_3^k)}{\sum_1^n W^{*k}(x_2^k - x_3^k)^2} \tag{14}$$

and this value may be substituted into equation (9) to calculate the set of adjusted assays that along with D minimise L and hence solve the material balance problem. This method will be referred to as MWR for minimum of weighted residues.

An alternative, but similar, approach to using Lagrange multipliers is the use of penalty functions, Walsh (1976). An optimisation technique that has not yet been employed in the solution of material balance problems. Using penalty functions the solution of the material balance problem defined by equations (4)-(6) reduces to minimising the functional

$$L^* = J + K\sum_1^n(\hat{x}_1^k - D\hat{x}_2^k - (1-D)\hat{x}_3^k)^2 \tag{15}$$

where K is a large positive constant. The constant K may be regarded as a "numerical" Lagrange multiplier. Its role is to ensure that in the minimisation of L^* selections of D and $\hat{x}_j^k$ that contravene the mass balance constraints are penalised by introducing a large constant in L^*. The major advantage in the penalty function approach is that the number of unknowns in the problem are reduced by n (ie. there are no unknown multipliers). In a large problem this could be significant. In the single process unit balance under consideration here, however, a gradient method to minimise L^* gives equations for the adjusted assays in the form

$$\hat{x}_j^k = x_j^k + g_j r^k/W_j\left(\frac{K}{1+Kh^k}\right) \tag{16}$$

with the "best" value for D calculated from the polynomial

$$\sum_1^n \left(\frac{Kr^k}{1+Kh^k}\right)\left[(x_2^k - x_3^k) + \left(\frac{Kr^k}{1+Kh^k}\right)\left(\frac{D}{W_2^k} - \frac{(1-D)}{W_3^k}\right)\right] \tag{17}$$

For large K, equations (16) and (17) will give values for D and x_j^k very close to those obtained from equations (9) and (12). Hence for the single three stream process unit there is no advantage in using penalty functions.

TABLE 3 Hierarchical Search Technique

STEP 1 search on D to minimise J^* (Powell Quadratic Interpolation PQI Walsh (1976))

↓

"Best" D

STEP 2 for each of the n assays one variable at a time PQI search to minimise J^k subject to mass balance constraint Eq(6)

↓

"Best" $\hat{x}_j^k$

↓

Solution to Problem.

All the above techniques for solution of the material balance problem employ differentiation. This problem may be solved without resorting to derivatives. Table 3 shows the main steps in a hierarchical direct search routine for the solution of the material balance problem defined by equations (4)-(6). This method will be referred to as DSM for direct search method.

RESULTS

The data of Table 1 is reproduced in Table 4 along with a typical error model, consisting of the percent relative standard deviations associated with each measurement, σ_j^k. It is this value which is used to determine the weighting factors, ie, $W_j^k = \sigma_j^k x_j^k/100$

TABLE 4 Assay Data and Error Model

Stream	Assay 1 X	Assay 1 σ	Assay 2 X	Assay 2 σ
(1)	23.8	5	52.1	10
(2)	5.3	5	40.7	10
(3)	53.9	2	63.4	4

BASIC+ programs suitable for implementation on a microcomputer have been written for each of the above data adjustment and material balance methods (LMP, LMS, MWR and DSM). Using the Data in Table 4 as a test problem each of these programs has been run. The results along with a comparison of CPU time requirements and program size are given in Table 5.

TABLE 5 Results

Estimates for relative flowrate D

LMP	LMS	MWR	DSM
.6181	.6172	.6181	.6172

Assays

Input	Adjusted LMP	LMS	MWR	DSM
23.8	23.85	23.89	23.85	23.89
5.3	5.29	5.30	5.29	5.30
53.9	53.88	53.87	53.88	53.87
52.1	49.94	49.96	49.95	49.96
40.7	41.51	41.51	41.51	41.51
63.4	63.59	63.59	63.59	63.59

CPU time (seconds)

LMP	LMS	MWR	DSM
0.4	0.6	0.1	1.0

Number of BASIC+ lines

LMP	LMS	MWR	DSM
40	45	35	70

All the methods, as might be expected, give similar results, in agreement with results obtained on running the test problem on the MATBAL main frame package, Weigel (1972).

For the simple material balance problem examined the MWR method is clearly superior in the CPU time taken and in number of programming lines required. This is an interesting result because none of the available mineral processing automated material balance packages use this approach.

The direct search method, ie, DSM, is inferior in all departments. Obviously the search technique used in this method could be improved. It is difficult, however, to see a ten fold improvement in CPU time on using an alternative search technique.

DISCUSSION

From the results the MWR method looks promising. The limiting nature of the test problem must be considered, however. It is possible that alternative approaches may be more appropriate for large scale problems. This point requires some investigation before the MWR method can be confidently used in a full scale microcomputer package.

Another area of interest worth exploring is the choice of adjustment criteria. In all methods so far discussed the criterion has been that of minimisation of a sum of squares. In a case where the errors in the measured data are not normally distributed, it may be more appropriate to find a "minimax" or "least absolute sum" solution. As an example of the use of these criteria the values

$$J_a = \sum_{1}^{n} |r^k| \quad \text{and} \quad J_m = \max |r^k|$$

have been minimised, using the test data in Table 4, to find "best" values for the relative mass flow rate D. These values are compared with the values of D obtained by minimising the weighted sum of squares J^* and an unweighted sum of squares in Table 6.

TABLE 6 Comparison of adjustment criteria

Min J_a	.6324
Min J^*	.6181
Unweighted Sum squr.	.5975
Min J_m	.5806

The results in Table 6 indicate that the values of D derived from minimising J_a and J_m bound the sum of squares solutions which suggests that use of these alternative criteria provides upper and lower bounds on the least squares results.

CONCLUSIONS

In this paper techniques of solving a simple mineral processing material balance problem have been investigated. Some of the optimisation techniques tested are currently used in automated material balance computer packages. Others (eg. penalty functions) have not been used in the solution of mineral processing material balance problems before. The main conclusion that can be drawn from the study is that there are efficient means of solving material balance problems that as of yet have not been exploited. It is these methods, in particular the MWR method coupled with the penalty function approach that need to be developed in building microcomputer software for solution of material balance problems in the minerals industry.

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