NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

Technical Memorandum 33-724

An Initial Feasibility Stage for Stoer's Constrained Least Squares Algorithm

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(NASA-CR-142189) AN INITIAL FEASIBILITY STAGE FOR STOER'S CONSTRAINED LEAST SQUARES ALGORITHM (Jet Propulsion Lab.) 19 p HC $3.25 CSCL 12A
N75-22025
Unclas
G3/64 19428

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PASADENA, CALIFORNIA

April 15, 1975

Prepared Under Contract No. NAS 7-100
National Aeronautics and Space Administration

PREFACE

The work described in this report was performed by the Data Systems Division of the Jet Propulsion Laboratory.

ACKNOWLEDGMENTS

The author has benefited from discussions with Prof. Bartels at the symposium cited in [1] and also from access to an Algol code for Stoer's algorithm written by Mr. P. Patzelt and kindly provided by Prof. Stoer.

CONTENTS

1. Introduction 1

2. Computing an initial feasible vector x_0 3

3. Partial triangularization of N 6

4. Initialization of Stoer's state variables 11

References 12

ABSTRACT

A procedure is described for computing an initial feasible vector, x_0, for Stoer's algorithm for solving the linear least squares problem subject to linear equality and inequality constraints. The procedure described fits well with Stoer's algorithm since much of the computation performed to determine x_0 accomplishes initializing transformations of the problem data, which would otherwise be done in Stoer's algorithm after being given an x_0.

AN INITIAL FEASIBILITY STAGE FOR STOER'S CONSTRAINED LEAST SQUARES ALGORITHM

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1. Introduction.

Denoting real matrices and vectors by upper and lower case letters respectively, introduce the following constrained least squares problems:

(1) Problem LSIE   Least squares with inequality and equality constraints.

(1a) $$\text{Minimize } \|Ex - f\|$$

subject to

(1b) $$Cx = d$$

and

(1c) $$Gx \geq h$$

(2) Problem LSE   Least squares with equality constraints [Eq (1a) and (1b)].

(3) Problem LSI   Least squares with inequality constraints [Eq (1a) and (1c)].

(4) Problem NNLS   Nonnegative least squares.

(4a) $$\text{Minimize } \|Ex - f\|$$

subject to

(4b) $$x \geq 0$$

(5) Problem LDP Least distance programming.

(5a) Minimize $\|x\|$

subject to

(5b) $Gx \geq h$

Stoer [3], Lawson and Hanson [2, Chapter 23] and Bartels [1] have given algorithms for Problem LSIE which work directly with the matrix E rather than with the nonnegative-definite symmetric matrix E^TE which is used in most quadratic programming algorithms.*

Although the algorithms described by Lawson and Hanson and by Bartels are different, they have the common feature that Problem LSIE is transformed via duality relations to a Problem NNLS. (Note that in this context the symbols E, x, and f of Eq (4a) do not denote the same quantities as in Eq (1a)). Problem NNLS is then solved by a descent algorithm having finite convergence.

One feature of these dual approaches is that there is no special problem of finding an initial feasible vector. The vector $x = 0$ is feasible for Problem NNLS.

In contrast the Stoer algorithm may be classified as a primal algorithm. It deals directly with the objective function of Problem LSIE, also by a descent algorithm having finite convergence. The Stoer algorithm requires an initial feasible vector, x_0, satisfying the constraints of Eq (1b) and (1c).

Two possibilities are mentioned in [3] regarding the determination of x_0. One is that a feasible vector may be known a priori. The other is that if the LSIE algorithm is extended to include a linear programming capability (such

*More precisely Bartels discusses the problem with generality which encompasses either working with E or with E^TE.

an extension is included in loc. cit.) then a special preliminary linear programming problem could be solved to determine x_0. This latter approach would apparently require the temporary introduction of some artificial variables with an associated requirement for some additional two-dimensional arrays of working storage, however this storage question is not detailed in loc. cit.

The purpose of this paper is to show how the LDP algorithm of [2] can be adapted for use as an initial feasibility stage for Stoer's algorithm. This approach requires only one additional row and/or column in some of the two-dimensional arrays already present in Stoer's algorithm. Furthermore it blends conveniently with the initialization phase of his algorithm in the following sense: The initialization phase triangularizes the rows of the constraint equations (1b) and (1c) which are satisfied as equations by the given x_0. The proposed use of algorithm LDP will do most of the work of this triangularization as a by-product of determining x_0.

2. Computing an initial feasible vector x_0.

Assume the data denoted by E, f, C, d, G, and h in Eq (1a)-(1c) is given, specifying a Problem LSIE. Assume the matrix C has m rows and n columns. To avoid complications in the exposition assume further that $m < n$ and Rank $(C) = m$.

Let K be an $n \times n$ orthogonal matrix that triangularizes C from the right, thus

$$\begin{bmatrix} C \\ G \end{bmatrix} K = \begin{bmatrix} L_1 & 0 \\ M & N \end{bmatrix} \tag{6}$$

where L_1 is an $m \times m$ lower triangular nonsingular matrix.

With the change of variables

(7) $$x = K y$$

Eq (1b) and (1c) are respectively transformed to

(8) $$[L_1 : 0]\ y = d$$

and

(9) $$[M : N]\ y \geq h$$

Let y_1 denote the first m components of y, and y_2 denote the remaining n - m components. Equation (8) determines a unique value for y_1, say $\hat{y}_1$, as the solution of

(10) $$L_1 y_1 = d$$

Substituting $\hat{y}_1$ into Eq (9) gives

(11) $$N y_2 \geq h - M \hat{y}_1$$

Define

(12) $$p = h - M \hat{y}_1$$

so that Eq (11) may be written as

(13) $$N y_2 \geq p$$

We now seek an (n - m)-vector y_2 satisfying Eq (13). We will impose the additional condition of seeking the y_2 of least Euclidean norm satisfying

Eq (13). This is an LDP problem. As is shown in Chapter 23 of [2] the solution to this problem can be extracted from the residual vector of a dual NNLS problem.

The NNLS problem to be solved is

$$\text{(14)} \qquad \text{minimize } \|[0, \ldots, 0, 1] - v^T[N : p]\|$$

subject to

$$\text{(15)} \qquad v \geq 0$$

Letting $\hat{v}$ be the solution vector determined by Algorithm NNLS [2, p. 161] for this problem, define the residual $(n - m + 1)$-vector

$$\text{(16)} \qquad \hat{r}^T = [0, \cdots, 0, 1] - \hat{v}^T[N : p]$$

and let $\hat{\rho}$ denote the last component of $\hat{r}^T$. Theoretically $\hat{\rho}$ will be zero if and only if $\|\hat{r}\| = 0$ which will occur if and only if the constraint system of Eq (13) is inconsistent. Otherwise with $\hat{\rho} \neq 0$ define the $(n - m)$-vector $\hat{y}_2$ by

$$\text{(17)} \qquad \begin{bmatrix} \hat{y}_2 \\ -1 \end{bmatrix} = -\hat{r}/\hat{\rho}$$

It can be shown [e.g., 2, Chap. 23] that $\hat{y}_2$ is the minimal norm solution of Eq (13). Furthermore using the transformation of Eq (7) it follows that the n-vector

$$\text{(18)} \qquad \hat{x} = K\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \end{bmatrix}$$

satisfies the constraints of Eq (1b) and (1c) and thus is suitable for use as an initial feasible vector x_0 in Stoer's algorithm.

3. Partial triangularization of N.

To initialize Stoer's algorithm we next wish to transform N to a partially triangularized form. Specifically let I denote the set of row indices of G for which $\hat{x}$ satisfies Eq (1c) with equality. To initialize Stoer's algorithm, we must triangularize the rows of N with indices $i \in I$. Note that I is also the set of row indices of N for which $\hat{y}_2$ satisfies Eq (13) with equality.

The key observation is that generally most of the work needed to achieve this triangularization will already have been done by Algorithm NNLS.

To provide the details supporting this observation we must summarize some properties of Algorithm NNLS. Algorithm NNLS induces a partition of the row indices of $[N : p]$ into two sets, say $\hat{I}$ and its complement. Suppose $\hat{I}$ contains $\hat{k}$ indices and, by relabeling if necessary, assume these indices are $1, 2, \cdots, \hat{k}$. Partition $[N : p]$ into its first $\hat{k}$ rows and the remaining rows as

(19) $$[N : p] = \begin{bmatrix} N_1 & p_1 \\ N_2 & p_2 \end{bmatrix}$$

Algorithm NNLS generates an $(n - m + 1) \times (n - m + 1)$ orthogonal matrix U satisfying

(20) $$\begin{bmatrix} N_1 & p_1 \\ N_2 & p_2 \\ 0 & 1 \end{bmatrix} U = \begin{bmatrix} L_2 & 0 & 0 \\ A_2 & B_2 & \tilde{p}_2 \\ s_1^T & s_2^T & \sigma \end{bmatrix}$$

where L_2 is a $\hat{k} \times \hat{k}$ lower triangular nonsingular matrix. If the solution vector $\hat{v}$ produced by Algorithm NNLS is also partitioned into $\hat{v}_1$ and $\hat{v}_2$ where $\hat{v}_1$ denotes the first $\hat{k}$ components, then these subvectors satisfy

(21) $$\hat{v}_1^T L_2 = s_1^T$$

(22) $$\hat{v}_1^T > 0$$

(23) $$\hat{v}_2^T = 0$$

and $\hat{y}_2$ satisfies

(24) $$N_1 \hat{y}_2 = p_1$$

and

(25) $$N_2 \hat{y}_2 \geq p_2$$

From these last two equations it follows that $\hat{I} \subset I$. In other words all rows of $[N : p]$ which have been triangularized by Algorithm NNLS are rows that needed to be triangularized to initialize Stoer's algorithm. In addition however, $\hat{y}_2$ may "accidentally" satisfy some of the rows of Eq (25) with equality. If so these rows must eventually be brought into the triangularization to complete the initialization.

First however we attend to eliminating the effect of p_1 in Eq (20) since p_1 is extraneous for the triangularization of N_1 that we need. The method will be similar to Row Removal Method 1 given in Chap. 27 of [2]. Apply Givens rotations from the right to Eq (20) to transform the vectors s_2 and s_1 to zero. This will necessarily transform σ to 1 or -1 since the row vector $[s_1^T, s_2^T, \sigma]$

has unit norm. These Givens rotations should operate on pairs of columns in the order $(n - m + 1, n - m)$, $(n - m + 1, n - m - 1), \ldots, (n - m + 1, 1)$, to preserve the zero structure of the first two blocks of the first block-row of the right-side matrix in Eq (20).

Calling the product of these $n - m$ rotations V this transforms Eq (20) to

$$\begin{bmatrix} N_1 & p_1 \\ N_2 & p_2 \\ 0 & 1 \end{bmatrix} UV = \begin{bmatrix} L_3 & 0 & t_1 \\ A_3 & B_3 & t_2 \\ 0 & 0 & \pm 1 \end{bmatrix} \tag{26}$$

where L_3 is a $\hat{k} \times \hat{k}$ lower triangular nonsingular matrix. Since $[0 \cdots 0, 1]\ UV = [0 \cdots 0, \pm 1]$ it follows that the last column of UV is $[0 \cdots 0, \pm 1]^T$. Since UV is orthogonal this implies that the last row of UV must be $[0 \cdots 0, \pm 1]$. Thus UV is of the form

$$UV = \begin{bmatrix} W & 0 \\ 0 & \pm 1 \end{bmatrix} \tag{27}$$

with W orthogonal. Substituting Eq (27) into Eq (26) we observe that

$$\begin{bmatrix} t_1 \\ t_2 \end{bmatrix} = \pm p \tag{28}$$

and

$$\begin{bmatrix} N_1 \\ N_2 \end{bmatrix} W = \begin{bmatrix} L_3 & 0 \\ A_3 & B_3 \end{bmatrix} \tag{29}$$

This gives our desired triangularization of N_1.

Define $\hat{z}$ by

$$\hat{y}_2 = W\hat{z} \tag{30}$$

Then from Eq (24) - (25) $\hat{z}$ satisfies

$$[L_3 : 0]\ \hat{z} = p_1 \tag{31}$$

and

$$[A_3 : B_3]\ \hat{z} \geq p_2 \tag{32}$$

We return now to consideration of the possibility (probably rare in practice) that $\hat{I} \neq I$. If there are k indices in I and $k > \hat{k}$ this would be evidenced by $\hat{z}$ satisfying $k - \hat{k}$ rows of Eq (32) with equality. By relabeling if necessary we assume these are the leading $k - \hat{k}$ rows of Eq (32). Let W_2 be an orthogonal matrix that brings these additional rows into the triangularization. Thus

$$\begin{bmatrix} L_3 & 0 \\ A_3 & B_3 \end{bmatrix} W_2 = \begin{bmatrix} L_4 & 0 \\ A_4 & B_4 \end{bmatrix} \tag{33}$$

where L_4 is $k \times k$ lower triangular. In general L_4 could be singular however the nondegeneracy assumption which Stoer invokes [3, p. 384] would imply that L_4 is nonsingular.

Define $\hat{w}$ by

$$\hat{z} = W_2\ \hat{w} \tag{34}$$

Then $\hat{w}$ satisfies

(35) $$[L_4 : 0]\ \hat{w} = \bar{p}_1$$

and

(36) $$[A_4 : B_4]\ \hat{w} > \bar{p}_2$$

where $\bar{p}_1$ denotes the first k components of p and $\bar{p}_2$ denotes the remaining subvector of p.

Combining the various orthogonal transformation matrices we may define the $n \times n$ orthogonal matrix Q by

(37) $$\begin{bmatrix} Q & 0 \\ 0 & \pm 1 \end{bmatrix} = \begin{bmatrix} K & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & U \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} K & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & W & 0 \\ 0 & 0 & \pm 1 \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & W_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

This matrix Q triangularizes C and the first k rows of G as follows.

(38) $$\begin{bmatrix} C \\ G \end{bmatrix} Q = \begin{bmatrix} L_1 & 0 & 0 \\ M_1 & L_4 & 0 \\ M_2 & A_4 & B_4 \end{bmatrix}$$

where

$$\begin{bmatrix} M_1 \\ M_2 \end{bmatrix}$$

is a partitioning of M of Eq (6) into its first k rows and the remaining rows.

4. Initialization of Stoer's state variables.

The Stoer algorithm is described in [3] in terms of transformations of a 7-tuple denoted by $\{\dot{x}, \dot{J}; \dot{Q}, \dot{L}, \dot{G}, \dot{R}, \dot{h}\}$ where the dots are added here to preclude confusion with symbols used in the present paper. The first four of these items may be initialized as

$$\dot{x} := \hat{x}$$

$$\dot{J} := I$$

$$\dot{Q} := Q$$

and

$$\dot{L} := \begin{bmatrix} L_1 & 0 \\ M_1 & L_4 \end{bmatrix}$$

The items $\dot{G}$, $\dot{R}$, and $\dot{h}$ depend upon E and f of Eq (1a) and would be computed as in [3].

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