# ALGORITHM 587 <br> Two Algorithms for the Linearly Constrained Least Squares Problem 

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#### Abstract

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General Terms. Algorithms Additional Key Words and Phrases: linear least squares solution, equality constraints, inequality constraints, nonnegativity constraints, inconsistent constraints, covarıance matrix


## 1. INTRODUCTION

This paper discusses subroutines for computing numerical solutions of the following two linearly constrained linear least squares problems.

| Problem NNLSE | $E \mathbf{x}=\mathbf{f}$ | (equations to be exactly satisfied) |
| :---: | :---: | :---: |
|  | $A \mathbf{x} \cong \mathbf{b}$ | (equations to be approximately satisfied, least squares sense) |
|  | $x_{l} \geq 0$, | $i=l+1, \ldots, n, \quad 0 \leq l \leq n$ |
| Problem LSEI | $E \mathbf{x}=\mathbf{f}$ | (equations to be exactly satisfied) |
|  | $A \mathrm{x} \cong \mathrm{b}$ | (equations to be approximately satisfied, least squares sense) |
|  | $G \mathbf{x} \geq$ h | (inequality constraints that the solution must satisfy) |

In both problems the matrices $E$ and $A$ are real and of respective dimensions $m_{E}$ by $n$ and $m_{A}$ by $n$. For Problem NNLSE, the variables $x_{1}, \ldots, x_{i}$ are free to have either sign. For Problem LSEI, the (real) inequality constraint matrix $G$ is $m_{G}$ by $n$. The right-side vectors $\mathbf{f}, \mathbf{b}$, and $\mathbf{h}$ that appear in the two problem statements have, respectively, $m_{E}, m_{A}$, and $m_{G}$ components. The (unknown) solution vector $\mathbf{x}$ has $n$ components.

While Problem LSEI of eq. (2) appears to be a more general problem than Problem NNLSE of eq. (1), it really is not. In fact, there are a number of ways to

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transform Problem LSEI into one of the forms of Problem NNLSE. Three ways of doing this are discussed in [3]. The method we have implemented is described on pages 101-102. The successful implementation of an algorithm for solving Problem NNLSE is the key computational process. Nevertheless, it is important for applications such as constrained curve fitting [2] to have a subprogram that solves Problem LSEI of eq. (2) directly. We provide FORTRAN subprograms WNNLS( ) and LSEI( ) that solve the respective problems in eqs. (1) and (2).

In Section 2 we review mathematical and numerical analysis details pertinent to solving Problem LSEI. In Section 3 we review some necessary details for understanding our methods for solving Problem NNLSE. In Section 4 we summarize some features and advantages of the codes. These features include changing tolerances, scaling of data matrices, and optional computation of the covariance matrix. Section 5 presents a test subprogram CLSTP( ), which is included with the package. It solves the test problem with both subprograms. Section 6 contains installation guidelines and remarks.

## 2. SOLVING PROBLEM LSEI

In this section, we briefly review mathematical and algorithmic details needed to solve Problem LSEI of eq. (2) [3, pp. 101-102]. The overall process consists of four main parts.

Step 1 Problem LSEI is reduced to a subproblem with possibly fewer unknown variables and with all explicitly stated equality constraints removed.
Step 2 The problem resulting from step 1 is reduced to a new problem where the least squares matrix is a simple projection matrix and the right-side vector is zero.
Step 3 The problem resulting from step 2 is solved by reposing it as a dual problem. This dual problem consists of two special cases of Problem NNLSE, eq. (1).
Step 4 The solution obtained in step 3 is transformed to the solution of the original problem using translations, matrix multiplications, and the solution of triangular linear algebraic systems.

## 3. SOLVING PROBLEM NNLSE

The theoretical development for solving problem NNLSE of eq. (1) is presented in [3]. The fundamental point of this method involves a numerically stable implementation of a penalty function approach. The least squares equations are each weighted by a small parameter $\epsilon$, chosen in the subprogram WNNLS( ). The augmented and weighted least squares system of eq. (3) is then solved.

$$
\begin{align*}
{\left[\begin{array}{c}
E \\
\epsilon A
\end{array}\right] \mathbf{x} } & \equiv D\left[\begin{array}{l}
E \\
A
\end{array}\right] \mathbf{x} \cong D\left[\begin{array}{c}
\mathbf{f} \\
\mathbf{b}
\end{array}\right] \equiv\left[\begin{array}{c}
\mathbf{f} \\
\epsilon \mathbf{b}
\end{array}\right] \\
D & =\operatorname{diag} \overbrace{(1, \ldots, 1}^{m_{E}}, \overbrace{\epsilon, \ldots, \epsilon)}^{m_{A}}  \tag{3}\\
\mathbf{x} & \left.=\left[\begin{array}{l}
\mathbf{y} \\
\mathbf{w}
\end{array}\right]\right\} l
\end{aligned} \quad \begin{aligned}
& \mathbf{y} \text { unconstrained } \\
& \mathbf{w} \geq \mathbf{0}
\end{align*}
$$

Part of the theoretical development in [3] shows that solutions of the weighted problem of eq. (3) converge to solutions of Problem NNLSE (if it is consistent) as $\epsilon \rightarrow 0$. Within the subprogram WNNLS( ) eq. (3) is solved only once with a value of $\epsilon$ that is chosen to achieve full working accuracy in the solution. The value used in WNNLS( ) is defined by

$$
\begin{equation*}
\epsilon^{2}=\frac{10^{-4} \eta}{\gamma} \tag{4}
\end{equation*}
$$

where $\gamma=\left\|{ }_{A}^{E}\right\|,\left(\|\cdot\|=\right.$ subordinate matrix norm of $l_{\infty}$ vector norm), and $\eta=$ machine relative arithmetic precision.

The algorithm for solving eq. (3) with $\epsilon$ as defined in eq. (4) proceeds in two main steps. First we compute a (minimum-length) solution for the unconstrained variables in terms of the constrained variables. Solving for the unconstrained variables is primarily a triangularization operation. In the second main step of the process we solve for the constrained variables. This is an iterative process, that is, it is Algorithm NNLS of [7, Chap. 23]. Certain crucial differences in numerical tests are needed because of the penalty parameter $\epsilon$ that multiplies the least squares equations. These tests are discussed in [3].

## 4. USAGE SUGGESTIONS AND SUBPROGRAM OPTIONS

In Sections 2 and 3 we have outlined solution methods for solving Problem LSEI of eq. (2) and Problem NNLSE of eq. (1). As shown in [3], computing the solution of Problem NNLSE can be regarded as the core computation in solving constrained linear least squares problems.

The most satisfactory method from the standpoint of accuracy and stability is to introduce slack variables into the inequality constraints of Problem LSEI [3]. This problem is then solved using subprogram WNNLS( ). The results of solving a bounded variable Hilbert matrix problem summarized in [3] suggest that subprogram WNNLS( ) continues to compute acceptable solutions even as the problems become increasingly ill-conditioned.

The use of subprogram WNNLS( ) with the slack variable formulation does have a disadvantage compared to subprogram LSEI( ). For most problems, WNNLS( ) will require more computing time and storage than LSEI( ). This is due to the larger number of problem variables in the slack variable formulation. The advantage of efficiency with LSEI( ) may be countered by the simultaneous occurrence of poor conditioning and rounding errors. (This can occur with a poorly conditioned least squares problem.) Owing to the poor conditioning and rounding error, the feasible constraint region can be mapped to one that is infeasible. Instances of this are shown in the results of solving the bounded variable Hilbert matrix problem summarized in [3].

The choice between the two subprograms is a time and storage versus stability trade-off. Specifically, in the case of a poorly conditioned least squares problem, WNNLS( ) might obtain a solution when LSEI( ) cannot. As illustrated in [3], subprogram WNNLS( ) can also be used to extend the notion of solution for problems with infeasible constraints.

Occasionally, a user of subprogram LSEI( ) will need the covariance matrix of the least squares solution variables of minimum length. This is returned as an
output matrix if the user wants it. It is an unbiased estimate of the covariance matrix for the minimum-length solution of an equality constrained least squares problem with no inequalities. This is developed in [4] and [6].

When inequalities are included, certain additional mathematical problems must be considered. These have to do with the behavior of the set of inequalities chosen by the algorithm to be equalities. The question is as follows: What is the sensitivity of these equalities as the data are allowed to vary within its uncertainty? Inequalities may move from being satisfied as equalities to strict inequalities as the data are perturbed. The covariance matrix computed by LSEI( ) is based on the assumption that the set of equalities does not change when the solution is perturbed. No comprehensive theory is known to the authors for determining the matrix when the set of equalities does change. The user must keep these facts in mind when interpreting the covariance matrix for Problem LSEI with inequalities.

The remainder of this section describes parameters within LSEI( ) and WNNLS( ) which can optionally be changed by the user. These options fall into the three following groups.
(A) Computation of the covariance matrix.
(B) Column scaling of the data matrix.
(C) Redefinition of tolerances used for determining ranks of problem matrices.

Changes to any number of these parameters can be specified as the linked-list input in the array PRGOPT(*). Precise instructions for defining PRGOPT(*) are found in the usage prologues for LSEI( ) and WNNLS( ). If the user is satisfied with the nominal subprogram features, it is only necessary to set PRGOPT(1)=1.

Remarks about A: Nominally the covariance matrix is not computed by LSEI( ).

Remarks about B: Column scaling of the form $\mathbf{x}=D \mathbf{y}$ is always performed by LSEI( ) and WNNLS( ). Nominally $D$ is the identity matrix. Another option here is a choice for $D$ such that each nonzero column of the entire scaled data matrix has length one. The user can also specify an arbitrary $D$.

Remarks about $C$ : The user can change tolerances $t_{E}$ and $t_{A}$ in LSEI( ) and tolerance $t_{W}$ in WNNLS( ). The nominal values of $t_{E}, t_{A}$, and $t_{W}$ are $\eta^{1 / 2}$, where $\eta$ is the relative arithmetic precision of the machine. The parameter $t_{E}$ is used in approximating the rank of the equality constraint matrix $E$ of eq. (2). Its role is discussed near the end of [3, Sec. 1].

The parameter $t_{A}$ is used in approximating the rank of the least squares matrix that results from eliminating the equality constraints from eq. (2). It is used to compute the factor $\tau$, which is $t_{A}$ times the norm of this reduced least squares matrix. Then $\tau$ is used in Algorithm HFTI [7, Chap. 14].

The parameter $t_{W}$ is used by WNNLS( ) to compute the rank of the row-scaled least squares matrix as discussed in [3, Sec. 3.1].

## 5. REMARKS ON THE TESTING SUBPROGRAM CLSTP( )

The subprogram CLSTP (KLOG, COND, ISTAT) constructs and solves a constrained least squares problem that has a known solution and known condition
numbers [7, Chap. 9]. The problem generated is stated in eq. (2). The matrices $A$, $E$, and $G$ are computed using formulas

$$
\begin{aligned}
& A=U_{1} S_{1} V_{1}^{\mathrm{T}} \\
& E=U_{2} S_{2} V_{2}^{\mathrm{T}}
\end{aligned}
$$

and

$$
G=U_{3} S_{3} V_{3}^{\mathrm{T}}
$$

The problem dimensions are specified by using five integer parameters $k_{A}, k_{E}$, $k_{G}, k_{I}$, and $k_{n}$ to compute $m_{A}=2^{k_{A}}, m_{E}=2^{k_{E}}, m_{G}=2^{k_{G}}$, and $n=2^{k_{n}}$. The integer $m_{I}=2^{k_{I}}$ denotes the number of inequality constraints that are to be satisfied as strict inequalities. These five integers are passed to CLSTP( ) in the array KLOG $\left({ }^{*}\right)$ in the order indicated. If any of the values $k_{A}, k_{E}, k_{G}, k_{I}$, or $k_{n}$ are less than zero, the respective values $m_{A}, m_{E}, m_{G}, m_{I}$, or $m_{n}$ are set to zero. No computation is performed if $n=0$.

Arrays within CLSTP( ) currently have fixed dimensions that require $k_{A}, k_{E}$, $k_{G}, k_{I}$, and $k_{n}$ to all be less than or equal to 5 . Instructions for increasing the array dimensions are given as comments within CLSTP( ).

The matrices $U_{J}$ and $V_{J}$ are symmetric orthogonal Hadamard matrices of dimension $n=2^{k}$ generated by the recursion

$$
\begin{aligned}
& n:=1 \\
& U:=1 \\
& \text { For } \quad l=1, \ldots, k \\
& \quad U:=\left[\begin{array}{rr}
U & : \\
U & : \\
\quad n & -U
\end{array}\right] \\
& \quad n=n+n \\
& \text { End For } \\
& U:=n^{-1 / 2} U
\end{aligned}
$$

The matrices $S_{J}, J=1,2,3$, are rectangular diagonal matrices. The extreme diagonal terms are $\kappa_{l}$ and 1 , where $\kappa_{J} \equiv \operatorname{COND}(J)$. The intermediate diagonal terms are generated in the open interval ( $1, \kappa_{J}$ ) using the random number generator RAN( ). The output value of $t=$ RAN(ISEED) satisfies $0<t<1$. The intermediate diagonal terms are successively computed as $1+t\left(\kappa_{J}-1\right)$. Initially, ISEED is set to 100001 in CLSTP( ).

The $n$-vector $\hat{\mathbf{x}}=(1, \ldots, 1)^{\mathrm{T}}$ is used to generate the vectors

$$
\begin{aligned}
\mathbf{f} & =E \hat{\mathbf{x}} \\
\hat{\mathbf{b}} & =A \hat{\mathbf{x}}
\end{aligned}
$$

and

$$
\hat{\mathbf{h}}=G \hat{\mathbf{x}} .
$$

We add a vector $\tilde{\mathbf{b}}$ to $\hat{\mathbf{b}}$ that is orthogonal to the column space of $A$. This is
given by

$$
\tilde{\mathbf{b}}=U_{1}\left(0, \ldots, 0, g_{n+1}, \ldots, g_{m_{A}}\right)
$$

where

$$
g_{i}=\mathbf{R A N}(\text { ISEED }) \cdot\|\hat{\mathbf{b}}\| \cdot \sigma, \quad i=n+1, \ldots, m_{A}
$$

The value of $\sigma$ is specified by the variable ANSR in CLSTP( ). It is currently set to 0.01 . The right-side vector for the least squares equations in eq. (2) is $\mathbf{b} \equiv \hat{\mathbf{b}}$ $+\tilde{\mathbf{b}}$.

The right-side vector for the inequality constraints is constructed by making the first $m_{I}$ constraints strict inequalities. This is done by defining the right-side vector as $\mathbf{h}=\hat{\mathbf{h}}-\tilde{\mathbf{h}}$, where

$$
\begin{aligned}
\tilde{\mathbf{h}} & =\left(h_{1}, \ldots, h_{m_{I}}, 0, \ldots, 0^{\mathrm{T}}\right), \\
h_{i} & =\mathbf{R A N}(\text { ISEED }) \cdot\|\hat{\mathbf{h}}\|, \quad i=1, \ldots, m_{I}
\end{aligned}
$$

These techniques for generating problems with known solutions are similar to those discussed in [9, pp. 6-9]. One might obtain different sets of test problems on machines with differing arithmetic characteristics. Part of this is due to a different sequence of numbers generated by RAN( ).

We have found that column scaling is sometimes required for solving eqs. (1) and (2). In particular, when using 32 -bit floating-point arithmetic, problems generated by CLSTP( ) using the published test data occasionally failed to pass the tests when no column scaling was done. Thus the option array input for calls to both LSEI( ) and WNNLS( ) are set so that unit length column scaling is performed on all the tests.

After subprogram LSEI( ) has computed an approximate solution $\mathbf{x}^{\prime}$ for this particular form of eq. (2), and subprogram WNNLS( ) has solved for an approximate solution $\mathbf{x}^{\prime \prime}$ of the system

$$
\begin{aligned}
E \mathbf{x} & =\mathbf{f} \\
A \mathbf{x} & \cong \mathbf{b} \\
G \mathbf{x}-\mathbf{h} & =\mathbf{w}
\end{aligned}
$$

for the unknown ( $\left.x^{T}, w^{T}\right)^{T}$, we compute the differences $d x_{1}=x^{\prime}-\hat{\mathbf{x}}$ and $d x_{2}=$ $\mathbf{x}^{\prime \prime}-\hat{\mathbf{x}}$. A test is made on the value of $\|\mathbf{d x}\|$ to ensure that $\mathbf{x}^{\prime}$ or $\mathbf{x}^{\prime \prime}$ is as accurate as it deserves to be. The test of the subprogram has failed if the corresponding $\left\|d x_{l}\right\|$ is too large. Otherwise the test has passed and $\mathbf{x}^{\prime}$ or $\mathbf{x}^{\prime \prime}$ is an acceptable approximation of $\mathbf{x}$. With

$$
\begin{aligned}
\rho & =\|\tilde{\mathbf{b}}\| /\|\hat{\mathbf{b}}\| \\
\kappa & =\kappa_{1}=\text { condition number of } A \\
\eta & =\text { relative arithmetic precision } \\
\mu & =\max \left(m_{A}, n\right) \\
\nu & =\min \left(m_{A}, n\right) \\
\phi & =100
\end{aligned}
$$

each test has passed if and only if

$$
\frac{\left\|\mathbf{d} \mathbf{x}_{t}\right\|}{\|\hat{\mathbf{x}}\|} \leq \kappa(1+\kappa \rho) \eta[(6 \mu-3 \nu) \nu] \phi .
$$

The output value of ISTAT is set as follows:
ISTAT $=1$ means both LSEI( ) and WNNLS( ) failed.
$=2$ means WNNLS( ) passed but LSEI( ) failed.
$=3$ means LSEI( ) passed but WNNLS( ) failed.
$=4$ means both LSEI( ) and WNNLS( ) passed.
This measure for $\left\|\mathbf{d x}_{i}\right\|$ is based on combining the estimate for the norm of the matrix $H$ of the nearby problem that $\mathbf{x}^{\prime}$ solves (without constraints), $(A+H) \mathbf{x}^{\prime}$ $\cong \mathbf{b}$, [7, Chap. 13], together with the perturbation bounds of [7, Chap. 9].

It may be necessary to increase the value of $\phi$ slightly on some machines.
A short main program, CLSTST, is provided with the algorithm. Also provided are 11 data cards that are read by CLSTST from FORTRAN unit $=5$. Each pair of the first 10 cards specifies a distinct test case. The last (eleventh) card terminates the program execution.

The subprogram CLSTP( ) prints the computed values of the least squares residual vector length and the vectors dx for both WNNLS( ) and LSEI( ). Also printed in CLSTP( ) are the computed ranks of the equality constraint and reduced least squares matrices returned by LSEI( ). The arrays KLOG(I), $\mathbf{I}=$ 1 to 5 , and $\operatorname{COND}(\mathbf{I}), \mathbf{J}=1$ to 3 , and the value of ISTAT returned from CLSTP ( ) are printed by CLSTST. Printing is done on FORTRAN unit $=6$.

## 6. INSTALLATION GUIDELINES AND REMARKS

This section contains information for installing subprograms LSEI( ) and WNNLS( ).

Included in the package are seven groups of subprograms.
(1) LSEI, LSI, LPDP
(2) WNNLS, WNLSM, WNLIT
(3) HFTI, H12, DIFF from [7]
(4) SDOT, SSCAL, SASUM, SAXPY, SNRM2, SCOPY, SSWAP, ISAMAX, SROTM, SROTMG from [8]. (For double-precision usage DDOT, DSCAL, DASUM, DAXPY, DNRM2, DCOPY, DSWAP, IDAMAX, DROTM, DROTMG.)
(5) XERROR, XERRWV, XERABT, XERCLR, XERCTL, XERDMP, XERMAX, XERPRT, XERSAV, XGETF, XGETUA, XGETUN, XSETF, XSETUA, XSETUN, FDUMP, J4SAVE, S88FMT, NUMXER from [5]. (The subprogram NUMXER is included for completeness but is not used in this package.)
(6) I1MACH based on [1]
(7) CLSTST, CLSTP, RAN (test package)

All of the subprograms are written in 1966 American National Standard portable FORTRAN. The only machine-sensitive subprogram is I1MACH( ). It provides two environmental parameters required by the error-handling subprograms XERROR( ) and XERRWV( ). This will require modification of I1MACH( ) at each host site. FORTRAN DATA statements defining the values
of all the required constants are available for many machines in comments within the subprogram. The appropriate set of commented statements must be activated. If the values for your machine are not there, they should be provided in the order corresponding to the description near the beginning of IIMACH( ). Machines for which these constants are provided are Honeywell $600 / 6000$, IBM $360 / 370$, Xerox Sigma, CDC 6000/7000, PDP-10 (KA and KI processors), PDP-11 (16- and 32 -bit arithmetic), Burroughs 5700/6700/7700, UNIVAC 1100, Data General Eclipse, Harris, VAX, and CRAY. In addition, the user must open or declare the FORTRAN unit, designated in IIMACH(4), where any error messages will be written.

We strongly recommend that calls to the error-handling subprograms XERROR( ) and XERRWV( ) be left intact. If the size or complexity of the errorhandling package presents a problem on a particular machine, we suggest that the subprograms XERROR( ) and XERRWV( ) be replaced by shorter, ma-chine-sensitive versions. These replacements should, minimally, print the character string comprising the error message and the specified data values. Usage of the full error-handling package is discussed in [5].

To convert the package for double-precision usage, follow the editing instructions at the beginning of each subprogram in groups $1,2,3$, and 7 above. Use the double-precision version of the BLAS in group 4. No conversion is required for subprograms in groups 5 and 6.

## ACKNOWLEDGMENTS

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## ALGORITHM

[A part of the listing is printed here. The complete listing is available from the ACM Algorithms Distribution Service (see page 335 for order form).]

```
SUBROUTINE LSEI(W, MDW, ME, MA, MG, N, PRGOPT, X, RNORME, RNORML, LSEI 1\emptyset
* MODE, WS, IP) LSEI 2\emptyset
DIMENSION W(MDW,N+1),PRGOPT(*),X(N), LSEI 4\emptyset
WS(2*(ME+N)+K+(MG+2)*(N+7)),IP(MG+2*N+2) LSEI 5\emptyset
ABOVE, K=MAX(MA+MG,N). LSEI 6\emptyset
ABSTRACT LSEI 8\emptyset
THIS SUBPROGRAM SOLVES A LINEARLY CONSTRAINED LEAST SQUARES LSEI 100
PROBLEM WITH BOTH EQUALITY AND INEQUALITY CONSTRAINTS, AND, IF THELSEI 11\emptyset
uSER REQUESTS, ObTAINS A COvariance matrix of the solution lset 12\emptyset
PARAMETERS. LSEI 13\emptyset
LSEI 14\emptyset
Suppose there are given matrices e, a and g of respective lsei 15\emptyset
dIMENSIONS ME BY N, MA bY N AND MG BY N, AND vectors f, b AND H OflSEI 16\emptyset
ReSpective lengths me, ma and mg. this subroutine solves the lsei 17\emptyset
LINEARLY CONSTRAINED LEAST SQUARES PROBLEM LSEI 18\emptyset
LSEI 19\emptyset
EX = F, (E ME BY N) (EQUATIONS TO BE EXACTLY LSEI 2ø\emptyset
SATISFIED) LSEI 21\emptyset
AX = B, (A MA BY N) (EQUATIONS TO BE LSEI 22\emptyset
    APPROXIMATELY SATISFIED, LSEI 23\varnothing
    LEAST SQUARES SENSE) LSEI 24\emptyset
GX.GE.H,(G MG BY N) (INEQUALITY CONSTRAINTS) LSEI 25\emptyset
    LSEI 260
the InEQuALItIES gX.ge.h mean that every component of the product lSEI 27\emptyset
GX MUST BE .GE. THE CORRESPONDING COMPONENT OF H. LSEI 28\emptyset
LSEI 29\emptyset
IN CASE THE EQUALITY CONSTRAINTS CANNOT BE SATISFIED, A LSEI 3\emptyset\emptyset
GENERALIZED INVERSE SOLUTION RESIDUAL VECTOR LENGTH IS OBTAINED LSEI 31\emptyset
FOR F-EX. THIS IS tHE MINIMAL LENGTH POSSIblE FOR F-EX. LSEI 32\emptyset
LSEI 330
LSEI 34\emptyset
```



```
RaNk OF the matrix e is estimated during the computation. We call lsei 36\emptyset
this value kranke. It Is an Output parameter in IP(1) defined lsei 37\emptyset
BELOW. USING A GENERALIZED INVERSE SOLUTION OF EX=F, A REDUCED LSEI 38\emptyset
LEAST SQUARES PROBLEM WITH INEQUALITY CONSTRAINTS IS OBTAINED. LSEI 39\emptyset
THE TOLERANCES USED IN THESE TESTS FOR DETERMINING THE RANK LSEI 40\emptyset
of e and the rank of the reduced least squares problem are lsei 41\emptyset
gIVEN IN SANDIA TECH. REPT. SAND 78-129\emptyset. THEY CAN BE LSEI 42\emptyset
MODIFIED bY THE USER IF NEW VALUES ARE PROVIDED IN LSEI 43\emptyset
THE OPTION LIST OF THE ARRAY PRGOPT(*). LSEI 44\emptyset
LSEI 450
THE EDITING REQUIRED TO CONVERT THIS SUBROUTINE FROM SINGLE TO LSEI 46\emptyset
DOUBLE PRECISION INVOLVES THE FOLLOWING CHARACTER STRING CHANGES. LSEI 47\emptyset
USE AN EDITING COMMAND (CHANGE) /STRING-1/(TO)STRING-2/. LSEI 48\emptyset
(START EdITING at line WITH C++ IN COLS. 1-3.) LSEI 49\emptyset
/REAL (12 BLANKS)/DOUBLE PRECISION/,/SASUM/DASUM/,/SDOT/DDOT/, LSEI 5\emptyset\emptyset
/SNRM2/DNRM2/,/ SQRT/ DSQRT/,/ ABS/ DABS/,/AMAXI/DMAX1/,, LSEI 51\emptyset
/SCOPY/DCOPY/,/SSCAL/DSCAL/,/SAXPY/DAXPY/,/SSWAP/DSWAP/,/E\emptyset/D\emptyset/, LSEI 52\emptyset
/, DUMMY/,SNGL(DUMMY)/,/SRELPR/DRELPR/ LSEI 53\emptyset
LSEI 54\emptyset
```

C

```
WRITTEN BY R. J. HANSON AND K. H. HASKELL. FOR FURTHER MATH. LSEI 55\emptyset
AND ALGORITHMIC DETAILS SEE SANDIA LABORATORIES TECH. REPTS. LSEI 56\emptyset
SAND 77-\emptyset552, (1978), SAND 78-129\emptyset, (1979), AND LSEI 57\emptyset
MATH. PROGRAMMING, VOL. 21, (1981), P.98-118.
LSEI 58@
```

| SUBROUTINE WNNLS (W, MDW, ME, MA, N, L, PRGOPT, X, RNORM, MODE,* IWORK, WORK) | WNN | 10 |
| :---: | :---: | :---: |
|  | WNN | $2 \emptyset$ |
|  | WNN | $3 \emptyset$ |
| DIMENSION W (MDW, $\mathrm{N}+1$ ) , PRGOPT (*) , X ( N$), \mathrm{IWORK}(\mathrm{M}+\mathrm{N})$, WORK ( $\mathrm{M}+5 \times \mathrm{N}$ ) | WNN | 40 |
|  | WNN | $5 \emptyset$ |
| ABSTRACT | WNN | 60 |
|  | WNN | $7 \emptyset$ |
| THIS SUBPROGRAM SOLVES A LINEARLY CONSTRAINED LEAST SQUARES | WNN | $8 \emptyset$ |
| PROBLEM. SUPPOSE THERE ARE GIVEN MATRICES E AND A OF | WNN | $9 \emptyset$ |
| RESPECTIVE DIMENSIONS ME BY N AND MA BY N, AND VECTORS F | WNN | $10 \emptyset$ |
| AND B Of RESPECTIVE LENGTHS ME AND MA. THIS SUBROUTINESOLVES THE PROBLEM | WNN | $11 \emptyset$ |
|  | WNN | $12 \emptyset$ |
|  | WNN | $13 \emptyset$ |
| EX $=\mathrm{F}$, (EQUATIONS TO BE EXACTLY SATISFIED) | WNN | 140 |
|  | WNN | $15 \emptyset$ |
| $A X=B$, (EQUATIONS TO BE APPROXIMATELY SATISFIED, IN THE LEAST SQUARES SENSE) | WNN | $16 \emptyset$ |
|  | WNN | $17 \emptyset$ |
|  | WNN | $18 \emptyset$ |
| SUBJECT TO COMPONENTS L+1, ..., N NONNEGATIVE | WNN | 190 |
|  | WNN | 200 |
| ANY VALUES ME.GE. $\emptyset$, MA.GE. $\emptyset$ AND $\emptyset$. LE. L .LE.N ARE PERMITTED. | WNN | 210 |
|  | WNN | 220 |
| THE PROBLEM IS REPOSED AS PROBLEM WNNLS | WNN | 230 |
|  | WNN | 240 |
| $(\mathrm{WT} * \mathrm{E}) \mathrm{X}=(\mathrm{WT} * \mathrm{~F})$ | WNN | 250 |
| ( A) ( B), (LEAST SQUARES) | WNN | $26 \emptyset$ |
| SUBJECT TO COMPONENTS L+1,..., N NONNEGATIVE. | WNN | $27 \emptyset$ |
|  | WNN | $28 \emptyset$ |
| THE SUBPROGRAM CHOOSES THE HEAVY WEIGHT (OR PENALTY PARAMETER) | WT . WNN | $29 \emptyset$ |
|  | WNN | 300 |
| THE PARAMETERS FOR WNNLS ARE | WNN | 310 |
|  | WNN | $32 \emptyset$ |
| INPUT. . | WNN | 330 |
|  | WNN | $34 \emptyset$ |
| W (*,*), MDW, THE ARRAY W(*,*) IS DOUBLE SUBSCRIPTED WITH FIRST | WNN | $35 \emptyset$ |
| ME, MA, $\mathrm{N}, \mathrm{L}$ DIMENSIONING PARAMETER EQUAL TO MDW. FOR THIS | WNN | 360 |
| DISCUSSION LET US CALL M $=$ ME + MA. THEN MDW | WNN | $37 \emptyset$ |
| MUST SATISFY MDW.GE.M. THE CONDITION MDW.LT.M | WNN | $38 \emptyset$ |
| IS AN ERROR. | WNN | 390 |
|  | WNN | $4 \emptyset \emptyset$ |
| THE ARRAY $W(*, *)$ CONTAINS THE MATRICES AND VECTORS | S WNN | 410 |
|  | WNN | 420 |
| (E F) | WNN | 430 |
| (A B) | WNN | 440 |
|  | WNN | 450 |
| IN ROWS AND COLUMNS 1,..., M AND 1,..., $\mathrm{N}+1$ | WNN | 460 |
| RESPECTIVELY. COLUMNS $1, \ldots, \mathrm{~L}$ CORRESPOND TO | WNN | 470 |
| UNCONSTRAINED VARIABLES X(1), .. , X (L) . THE | WNN | 480 |
| REMAINING VARIABLES ARE CONSTRAINED TO BE | WNN | $49 \emptyset$ |
| NONNEGATIVE. THE CONDITION L.LT. $\emptyset$. OR. L.GT.N IS | WNN | $5 \emptyset \emptyset$ |
| AN ERROR. | WNN | 510 |
|  | WNN | 520 |


| C | PRGOPT(*) | THIS ARRAY IS THE OPTION VECTOR. | WNN |
| :--- | :--- | :--- | :--- |
| C | IF THE USER IS SATISFIED WITH THE NOMINAL | WNN | $54 \emptyset$ |
| C | SUBPROGRAM FEATURES SET | WNN | $55 \emptyset$ |
| C |  | PRGOPT $(1)=1$ (OR PRGOPT $(1)=1 . \emptyset)$ | WNN |
| C |  |  | WN |


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