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APPLIED STATISTICS

```
C
C
          UNPACK THE MATRIX
      CALL UNPACK(VCOV, MPLONE, LENWRK)
      RETURN
      END
Ç
      SUBROUTINE UNPACK(X, N, LENX)
0000000000
          ALGORITHH AS 139.1 APPL, STATIST, (1979) VOL.28, NO.2
          THIS SUBROUTINE EXPANDS A SYMMETRIC MATRIX STORED IN LOWER
          TRIANGULAR FORM IN THE FIRST N*(N+1)/2 POSITIONS OF X
          INTO A MATRIX USING THE FIRST NON POSITIONS
          LENX = THE LENGTH OF VECTOR X - MUST BE NOT LESS THAN NAN
      DIMENSION X(LENX)
      NSQ = N + N
      II = NSQ
      JJ = N \pm (N + 1) / 2
C
C
C
          STORE LAST ROW
      DO 10 I = 1, N
X(II) = X(JJ)
      II = II = I
      JJ = JJ = 1
   18 CONTINUE
      DO 80 1 = 2, N
Ç
Ċ
          OBTAIN UPPER PART OF MATRIX FROM PART ALREADY SHIFTED
      IJ \Rightarrow I = 1
      KK = NSQ + 1 + I
      DO 50 J = 1, IJ
      X(II) = X(KK)
      II = II = 1
      KK = KK = N
   50 CONTINUE
0000
          OUTAIN LOWER PART OF MATRIX FROM
          URIGINAL TRIANGULAR STORAGE
      IJ = N = IJ
      DO 70 J = 1, IJ
X(II) = X(JJ)
      II = II = I
      JJ = JJ =
                 1
   78 CONTINUE
   8Ø
      CONTINUE
      RETURN
      END
```

Algorithm AS 140

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Clustering the Nodes of a Directed Graph

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Keywords: Clustering; Directed graph; Maximum likelihood; transfer algorithm

LANGUAGE

ISO Fortran

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STATISTICAL ALGORITHMS

DESCRIPTION AND PURPOSE

The nodes of a directed graph are to be partitioned into clusters so that for any ordered pair of clusters, the nodes of the first cluster are nearly all linked to the nodes of the second cluster, or nearly all not linked. In this way, a summary is made of the linkages of the graph. Busacker and Saaty (1965) has a discussion of directed graphs and a variety of their applications.

The criterion chosen to evaluate the partition is the likelihood function. Consider the $N \times N$ association matrix B of the N nodes of the graph. If there are NCLUS clusters, then B may be thought of as being partitioned into $NCLUS \times NCLUS$ cells corresponding to the partition of the nodes; cell (a, b), for clusters a and b, has S(a, b) links and Z(a, b) entries. Assume that each binary entry of B is an independent Bernoulli trial with $\Pr\{B(I,J) = 1\}$ equal to P(a, b), where node I is in cluster a and node J is in cluster b. Then the maximum likelihood estimate of P(a, b) is

$$\hat{P}(a,b) = S(a,b)/Z(a,b),$$

and the overall likelihood is equal to

$$\prod_{1 \leq a,b \leq NCLUS} \hat{P}(a,b)^{S(a,b)} (1-\hat{P}(a,b))^{(Z(a,b)-S(a,b))}$$

(The diagonal elements of B are not used in the likelihood calculations.) Hartigan (1975) suggests the use of maximum likelihood in non-hierarchical clustering; the related Shannon-Wiener information measure (or approximations to it) has been used for quite some time in hierarchical clustering. See Williams and Lambert (1959) and MacNaughton-Smith (1965).

The algorithm is a "transfer" algorithm; an initial partition is produced by subroutine *INIT*, and subroutine *ALLOC* transfers each node in turn to the cluster for which the overall likelihood is maximized. Swaps of pairs of nodes between clusters, as in Banfield and Bassill (1977), are not considered. This algorithm further differs from standard transfer algorithms (for example, Banfield and Bassill) by selecting more judiciously the transfers to be tested, by handling the simultaneous clustering of the rows and columns of the association matrix, and by handling large sparse linkage matrices in list form.

Method

The association matrix B is not used in its $N \times N$ form, but in the form of a vector X. The first N elements of X are a directory, and the remaining elements are the links in the graph. The numbers of the nodes to which node I is linked are stored in X beginning at location X(I). Entries in X must be packed to the left so that the last node to which node I is linked is immediately followed in X by the list of nodes for node I+1.

Subroutine *INIT* constructs an initial partition of the nodes. If ITYPE = 0, the partition is constructed by approximating the first eigenvector of *B* (using eight iterations of the power method) and sorting the nodes so that their components in the eigenvector are in ascending order. The sorted nodes are then split into *NCLUS* initial clusters. If *ITYPE* = 1, a user supplied initial partition, specified in *CLUS*, is used.

Subroutine ALLOC transfers a node from one cluster to another if the move increases the log likelihood by more than TH, and if the second cluster is smaller than MXSIZE, a given maximum size for clusters. ALLOC makes global passes, in which all transfers are checked, and local passes, in which transfers between clusters that did not change in the previous pass are not checked. A local pass follows any pass in which a transfer was executed; a global pass follows a local pass which had no transfers. ALLOC begins with a global pass and continues until there is a global pass with no transfers, at which time a local optimum has been reached. This technique reduces computation by ignoring unlikely transfers except when testing for a local optimum. On return, the output structures of ALLOC contain the final partition in

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CLUS, the size of each cluster in SIZE, the matrix of success counts in P and the overall log likelihood in R1(1).

STRUCTURE

SUBROUTINE INIT(X, N, XLEN, NCLUS, MXCLUS, MXSIZE, ITYPE, CLUS, Y, SIZE, P, IOLD, INEW, IFAULT)

Formal parameters

X	Integer array (XLEN)	input: data vector
Ν	Integer	input: number of nodes
XLEN	Integer	input: length of X
NCLUS	Integer	input: number of clusters requested
MXCLUS	Integer	input: maximum number of clusters
MXSIZE	Integer	input: maximum size of a cluster
IT YPE	Integer	input: type of initialization
CLUS	Integer array (N)	input/
		output: initial cluster of each node
Y	Integer array (XLEN)	output: data vector (by columns of B)
SIZE	Integer array (MXCLUS)	output: initial size of each cluster
Р	Real array (MXCLUS, MXCLUS)	output: initial matrix of success counts
IOLD	Integer array (N)	workspace:
INEW	Integer array (N)	workspace:
IFAULT	Integer	output: fault indicator

Fault indicator

IFAULT = 0 no fault

- 1 NCLUS outside its range
- 2 $MXSIZE * NCLUS \leq N$
- 3 error in X directory: $X(i) \leq X(i-1)$, some $i \leq N$; $X(1) \neq N+1$; or X(N) > XLEN
- 4 reference in X to node number <1 or >N
- 5 same link listed twice in X
- 6 all-zero column of the association matrix B
- 7 illegal cluster specified in initialization
- 8 initial cluster violates size restrictions

SUBROUTINE ALLOC(X, Y, N, XLEN, NCLUS, MXCLUS, MXSIZE, TH, MXS2, CLUS, SIZE, P, R1, R2, TLOG, IOLD, INEW)

Formal parameters

These	are the same as for <i>INIT</i> except	
Y	Integer array (XLEN)	input: data vector (by columns of B)
TH	Real	input: threshold of incremental likeli- hood
MXS2	Integer	input: equal to MXSIZE squared
CLUS	Integer array (N)	input/
SIZE	Integer array (MXCLUS)	output: current cluster of each node input/
P	Real array (MXCLUS, MXCLUS)	output: current size of each cluster input/
		counts

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R 1	Real array (MXCLUS)	workspace/
		output: $R1(1)$ returns the overall log
		likelihood
R2	Real array (MXCLUS)	workspace:
TLOG	Real array (MXS2)	workspace:

AUXILIARY ALGORITHMS

ALLOC calls the real function XLIKE(P1, R1, S1, S2, S3, S4, Y1, TLOG, MXS2), which is included. XLIKE calculates the change in log likelihood between P1 successes in S1 * S2trials and P1 - Y1 * R1 successes in S3 * S4 trials.

RESTRICTIONS

1. $1 < NCLUS \leq MXCLUS; NCLUS < N.$

2. NCLUS * MXSIZE > N.

3. The X vector must be such that every row and column of the association matrix B has a non-zero element. The easiest way to assure this is to set the diagonal elements of B equal to 1; this will not affect the clusters. Faults of types 3 and 6 can indicate an all-zero row or column of B.

4. No link may be listed twice in X.

5. The algorithm does not accept missing values; that is, the information in X is taken to be a complete description of the linkages of the graph.

6. Cluster sizes must be greater than zero and less than MXSIZE.

ACCURACY

The final partition produced is a local optimum and may not be a global optimum. Also, there may be other partitions which result in the same log likelihood. Use of several initial partitions will reduce the risk of selecting a poor local optimum.

The accuracy of the change in log likelihood and overall log likelihood calculations depends on the accuracy of the real arithmetic on the particular computer in use. Each change in log likelihood calculation requires 20 * NCLUS real additions, and the overall log likelihood calculation requires $3 * NCLUS^2$ real additions.

STORAGE AND TIME

The variable storage requirement for this algorithm is less than 2XLEN+3N+ $3MXCLUS + MXCLUS^2 + MXSIZE^2 + 100$ words.

The amount of time required for convergence depends on N, XLEN, NCLUS and the configuration of the graph itself, but computation is roughly proportional to $N * NCLUS^2$. A sample graph of 71 nodes and 243 links executed in 20.6 sec for 15 clusters on an IBM 370/158.

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APPLIED STATISTICS

```
SUBROUTINE INIT(X, N, XLEN, NCLUS, MXCLUS, MXSIZE, ITYPE,
      * CLUS, Y, SIZE, P, IOLD, INEW, IFAULT)
C
C
C
C
C
C
C
C
C
C
          ALGORITHM AS 140.1 APPL, STATIST, (1979) VOL.28, NO.2
          CONSTRUCT AN INITIAL PARTITION OF THE NODES
      INTEGER XLEN, FIRST, X(XLEN), Y(XLEN), CLUS(N), SIZE(MXCLUS),
        INEW(N), IOLD(N)
      REAL P(MXCLUS, MXCLUS)
       LOGICAL FLAG
C
C
          CHECK INPUTS
Ċ
       IFAULT = 1
       IF (NCLUS LE, 1 .OR, NCLUS .GE, N .OR, NCLUS .GT. MXCLUS) RETURN
       IFAULT = 2
       IF (NCLUS * MXSIZE .LE. N) RETURN
       IFAULT = 3
       DO 1 I = 2, N
       L = I = 1
       IF (X(I) .LE. X(L)) RETURN
    1 CONTINUE
       M = N + 1
       IF (X(1) , NE, H , DR, X(N) , GT. XLEN) RETURN
       IFAULT = 4
       DO 2 I = M, XLEN
       IF (X(I) _LE. Ø .OR. X(I) .GT. N) RETURN
    2 CONTINUE
       IFAULT = 5
      00 5 I = 1, N
      FIRST = X(I)
      L = I + 1
      LAST = X(L) = 1
       IF (I .EQ. N) LAST = XLEN
      IF (FIRST , EQ, LAST) GOTO 5
JLAST = LAST = 1
      DO 4 J = FIRST, JLAST
       JTEST = X(J)
      KFIRST = J + 1
DO 3 K = KFIRST, LAST
       IF (JTEST .EQ. X(K)) RETURN
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
C
C
C
C
C
          CONSTRUCT Y VECTOR. THE Y VECTOR HOLDS THE ASSOCIATION
          MATRIX BY COLUMNS RATHER THAN BY ROWS AS X DOES.
      DO 6 I = 1, N
       INEW(I) = Ø
       Y(I) = N + 1
    6 CONTINUE
       Y(H) = Ø
      DO 7 I = 1, N
      FIRST = X(I)
      LAST = X(I + 1) = 1

IF (I _ EQ, N) LAST = XLEN

D0 7 J = FIRST, LAST
      KFIRST = X(J) + 1
      DO 7 K = KFIRST, N
      Y(K) = Y(K) + 1
    7 CONTINUE
      DO 8 I = 1, N
      FIRST = X(I)
      LAST = X(I + 1) = 1
IF (I EQ, N) LAST = XLEN
      DO 8 J = FIRST, LAST
      ITEMP = X(J)
      L = Y(ITEMP) + INEW(ITEMP)
      Y(L) = I
      INEW(ITEMP) = INEW(ITEMP) + 1
```

```
8 CONTINUE
        IFAULT = 6
        DO 9 I = 2, N
     IF (Y(I) LE, Y(I = 1)) RETURN
9 CONTINUE
        IF (Y(1) .NE. M .OR. Y(N) .GT, XLEN) RETURN
IF (ITYPE .EQ, 1) GOTO 33
IFAULT = 0
C
C
C
C
           APPROXIMATE FIRST EIGENVECTOR
        DO 11 I = 1, N
    11 IOLD(I) = 1
       DO 13 ITER = 1,
DO 12 I = 1, N
                           - 8
        LAST = X(I + 1) = 1
       IF (I EG N) LAST = XLEN
DO 12 J = FIRST, LAST
ITEMP = X(J)
        INEW(I) = INEW(I) + IOLD(ITEMP)
    12 CONTINUE
        DO 13 I = 1, N
        IOLD(I) = INEW(I)
    13 CONTINUE
Ç
Ç
           SORT BY FIRST EIGENVECTOR
Ĉ
        DO 14 I = 1, N
    14 INEW(I) = I
        DO 16 I = 1, N
       FLAG = TRUC,
DO 15 J = 2, N
        L = J - 1
        ITEMP = INEW(L)
       M = INEW(J)
       IF (IOLD(M) ,GE, IOLD(ITEMP)) GOTO 15
       FLAG = FALSE
INEW(J) = INEW(L)
        INEW(L) = M
   15 CONTINUE
        IF (FLAG) GOTO 17
   16 CONTINUE
C
C
C
           PARTITION INTO INITIAL CLUSTERS
   17 KSTART = N / NCLUS
       DO 21 I = 1, NCLUS
   21 SIZE(I) = KSTART
       ILAST = MOD(N, NCLUS)
IF (ILAST EQ. 0) GOTO 31
DO 22 I = 1, ILAST
   22 \text{ SIZE(I)} = \text{SIZE(I)} + 1
   31 J = 1
       DO 32 I = 1, NCLUS
       KLAST = SIZE(I)
       DO 32 K = 1, KLAST
       ITEMP = INEW(J)
       CLUS(ITEMP) = I
       J = J + 1
   32 CONTINUE
       GOTO 40
   33 DO 34 I = 1, NCLUS
   34 \ \text{SIZE}(I) = 0
       IFAULT = 7
       DO 35 I = 1, N
       J = CLUS(I)
       IF (J LE, 0 OR, J GT, NCLUS) RETURN
Size(j) = Size(j) + 1
   35 CONTINUE
       IFAULT =
       DO 36 I = 1, NCLUS
       IF (SIZE(I) LE. Ø .OR. SIZE(I) .GT. MXSIZE) RETURN
```

```
36 CONTINUE
       IFAULT = Ø
Ç
Ç
          SET UP P MATRIX, SUCCESS COUNTS
Ĉ
   40 DO 41 I = 1, NCLUS
      DO 41 J = 1, NCLUS
   41 P(I, J) = 0.0
       DO 42 I = 1, N
       FIRST = X(I)
      LAST = X(I + 1) = 1
IF (I EG. N) LAST = XLEN
DO 42 J = FIRST, LAST
       IF (X(J) EQ, 1) GOTO 42
ITEMP = X(J)
       ITEMP = CLUS(ITEMP)
       ITEMP2 = CLUS(I)
       P(ITEMP2, ITEMP) = P(ITEMP2, ITEMP) + 1.0
   42 CONTINUE
       RETURN
       END
Ç
       SUBROUTINE ALLOC(X, Y, N, XLEN, NCLUS, MXCLUS, MXSIZE,
      * TH, MXS2, CLUS, SIZE, P, R1, R2, TLOG, IOLD, INEW)
C
C
          ALGORITHM AS 140.2 APPL, STATIST, (1979) VOL.28, NO.2
00000
          FROM AN INITIAL PARTITION OF THE NODES OF A GRAPH,
          REALLOCATE NODES TO CLUSTERS TO FIND A LOCALLY
          MAXIMUM LIKELIHOOD PARTITION
      INTEGER XLEN, FIRST, X(XLEN), Y(XLEN), CLUS(N),
SIZE(MXCLUS), IOLD(N), INEW(N)
REAL P(MXCLUS, MXCLUS), TLOG(MXS2), R1(MXCLUS), R2(MXCLUS)
       LOGICAL GLOBAL
ç
          INITIALIZE TLOG, INEW, IOLD, PASS,
C
       DO 1 I = 1, MXS2
     1 TLOG(I) = FLOAT(I) * ALOG(FLOAT(I))
    2 DO 3 I = 1, NCLUS
       INEW(I) = 0
       IOLO(I) = 1
    3 CONTINUE
       GLOBAL = .TRUE.
С
C
C
C
C
C
C
          MOVE A NODE TO A NEW CLUSTER IF THE MOVE INCREASES
          THE LIKELIHOOD.
          ONLY CHECK MOVES IF ONE OF THE CLUSTERS HAS IOLD = 1.
    4 DO 59 ITER = 1, N
       NBEST = CLUS(ITER)
       BTEST = TH
ç
          SET UP ARRAY OF ASSOCIATIONS (R) FOR THIS NODE
č
       DO 10 I = 1, NCLUS
       R1(I) = 0.0
       R2(I) = 0.0
    10 CONTINUE
       FIRST = X(ITER)
       L = ITER + 1
       LAST = X(L) - 1
       IF (ITER ,EQ, N) LAST = XLEN
DO 11 I = FIRST, LAST
       IF (X(I) .EQ, ITER) GOTO 11
       ITEMP = X(I)
       ITEMP = CLUS(ITEMP)
       R1(ITEMP) = R1(ITEMP) + 1.0
    11 CONTINUE
       FIRST = Y(ITER)
       LAST = Y(L) = 1
```

```
IF (ITER .EQ. N) LAST = XLEN
       DO 12 I = FIRST, LAST
       IF (Y(I) .EQ, ITER) GOTO 12
ITEMP = Y(I)
        ITEMP = CLUS(ITEMP)
       R2(ITEMP) = R2(ITEMP) + 1.0
   12 CONTINUE
C
ç
           CHECK EACH CLUSTER FOR AN INCREASE IN LIKELIHOOD
       L = CLUS(ITER)
       DO 49 M = 1, NCLUS
      IF (L .CO. M .OR. SIZE(M) .GE, MXSIZE .OR.
* IOLD(L) + IOLD(M) .EQ. 0) GOTO 49
       TEST = 0,0
       DO 20 J = 1, NCLUS
       IF (J _EQ, L _OR, J _EQ, M) GOTO 20
IF (P(L, J) _GT, Ø,0) TEST = TEST + XLIKE(P(L, J), R1(J), SIZE(L),
       SIZE(J), SIZE(L) = 1, SIZE(J), 1,0, TLOG, MXS2)
IF (P(M, J) GT. 0,0 GR, R1(J) GT. 0,0) TEST = TEST +
XLIKE(P(M, J), R1(J), SIZE(M), SIZE(J), SIZE(M) + 1, SIZE(J),
         -1.0, TLOG, MXS2)
       IF (P(J, L) GT, 0,0) TEST = TEST + XLIKE(P(J, L), R2(J), SIZE(L),
SIZE(J), SIZE(L) = 1, SIZE(J), 1.0, TLOG, MXS2)
       IF (P(J, M),GT, 0,0,0R, R2(J),GT, 0,0) TEST = TEST +
xLIKE(P(J, M), R2(J), SIZE(M), SIZE(J), SIZE(M) + 1, SIZE(J),
      .
         -1.0, TLOG, MXS2)
   20 CONTINUE
       TEST = TEST + XLIKE(P(L, L), R1(L) + R2(L), SIZE(L) = 1, SIZE(L),

SIZE(L) = 1, SIZE(L) = 2, 1.0, TLOG, MXS2) +

XLIKE(P(L, M), R1(M) = R2(L), SIZE(L), SIZE(M), SIZE(L) = 1,
          SIZE(M) + 1, 1,0, TLOG, MXS2) +
          XLIKE(P(M, L), H2(M) = RI(L) , SIZE(L), SIZE(M), SIZE(L) = 1.
      *
          SIZE(M) + 1, -1,0, TLUG, MXS2) +
          XLIKE(P(M, M), R1(M) + R2(M),
                                                  SIZE(M) = 1, SIZE(M),
          SIZE(M) + 1, SIZE(M), -1, A, TLOG, MXS2)
        IF (TEST LE, BTEST) GOTO 49
        BTEST . TEST
       NBEST # M
    49 CONTINUE
C
C
           MOVE TO BEST CLUSTER
C
        IF (NBEST _EQ, L) GOTO 59
        M . NBEST
        DO 50 II = 1, NCLUS
        P(L, II) = P(L, II) = R1(II)
        P(M, 1I) = P(M, II) + R1(II)
        P(II, L) = P(II, L) = R2(II)
        P(II, N) = P(II, M) + R2(II)
   50 CONTINUE
        SIZE(L) = SIZE(L) = 1
        SIZE(M) = SIZE(M) + 1
        CLUS(ITER) = NBEST
        INEW(L) = 1
        INEW(M) = 1
   59 CONTINUE
С
C
           CHECK FOR OPTIMUM, WERE THERE ANY MOVES THIS PASS.
С
       DO 60 I = 1, NCLUS
        IF (INEW(I) GT. 0) GOTO 62
   60 CONTINUE
¢
č
           NO MOVES, IF A GLOBAL CHECK, FINISH,
IF A LOCAL CHECK, MAKE À GLOBAL CHECK,
C
       IF (GLOBAL) GOTO 70
       GOTO 2
C
           SOME MOVES, RESET IOLD, INEW, MAKE A LOCAL CHECK,
```

```
62 GLOBAL = FALSE
DO 63 I = 1, NCLUS
      IOLD(I) = INEW(I)
       INEW(I) = 0
   63 CUNTINUE
      GOTU 4
C
C
C
          COMPUTE OVERALL LOG LIKELIHOOD
   70 R1(1) = 0.0
      DO 72 I = 1, NCLUS
      R1(1) = R1(1) + XLIKE(0,0, P(I, I), I, I, SIZE(I) = 1,
        SIZE(1), -1,0, TLOG, MXS2)
      DO 71 J = 1, NCLUS
      IF (I .NE, J) R1(1) = R1(1) + XLIKE(0,0, P(I, J),
        I, I, SIZE(I), SIZE(J), -1,0, TLOG, MXS2)
   71 CONTINUE
   72 CONTINUE
      RETURN
       END
Ç
       REAL FUNCTION XLIKE(P1, R1, S1, S2, S3, S4, Y1, TLOG, MXS2)
000000
          ALGURITHM AS 140.3 APPL, STATIST, (1979) VOL.28, NO.2
          EVALUATE THE CHANGE IN LOG LIKELIHOOD BETWEEN P SUCCESSES IN
          SI * S2 TRIALS AND P1 . Y1 * R1 SUCCESSES IN S3 * S4 TRIALS,
       INTEGER S1, S2, S3, S4, P, R, X, Z
       REAL TLUG(MXS2)
       XLIKE = 0.0
       P = P1
       Z = S1 + S2
       R = Z - P
       IF (R .NE, M .AND, P .NE, 0) XLIKE = TLOG(Z) - TLOG(P) - TLOG(R)
X = P) - YI + R1
       Z = S3 + S4
       R = Z = X
       IF (R .NE, Ø .AND, X .NF, Ø)
XLIKE = XLIKE + TLOG(X) + TLOG(R) + TLOG(Z)
       RETURN
       END
```

Algorithm AS 141

Inversion of a Symmetric Matrix in Regression Models

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LANGUAGE

ISO Fortran

INTRODUCTION

In a regression model Y = Xb, b is estimated by $(X'X)^{-1}X'Y$. To obtain the regression without a particular variable and thence a partial F value for that variable, $(W'W)^{-1}W'Y$ may be used where W is obtained from X by deleting the column in X corresponding to the variable.

The Fortran subroutine SINV computes $(W'W)^{-1}$ directly from $(X'X)^{-1}$, achieving a significant gain in time compared to the inversion of (W'W). It is largely based on Algorithm