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APPLIED STATISTICS

```
C CHNPACK THE MATRIX 
    DIMENSION X(LENX)
        NSO =N*N
        II = NSQ
        JJ=N*(N+1)/2
C
    STORE LAST ROW
        DO 10I = 1, N
        X(II) = x(JJ)
        II= II - !
        JJ = JJ - 1
    10
    DO 801 = 2, N
    OETAIN UPPER PART OF MATRIX FROM PART ALREADY SHIFTED
        IJ=1-1
        KK = NSQ + 1 I I
        DO 50 J = 1, IJ
        X(II) = X(KK)
        II=II=!
        KK = KK - N
        50 CONTINUE
    OHTAIN LOWEF PART OF MATRIX FROM
        URIGINAL TRIANGULAR STORAGE
        IJ = N . IJ
        DO 70 J = 1. IJ
        x(II) = x(JJ)
        II=1I*!
        JJ= JJ=1
70 CONTINUE
80 CONTINUE
    RETURN
    END
```


## Algorithm AS 140

## Clustering the Nodes of a Directed Graph

By Gary W. Oehlert $\dagger$<br>Yale University

Keywords: CLUSTERING; DIRECTED GRAPH; MAXIMUM LIKELIHOOD; TRANSFER ALGORITHM
Language

## ISO Fortran

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## 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 $N C L U S$ clusters, then $B$ may be thought of as being partitioned into NCLUS $\times N C L U S$ 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 $\operatorname{Pr}\{B(I, J)=1\}$ 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

$$
\prod_{1 \leqslant a, b \leqslant N C L U S} \hat{P}(a, b)^{S(a, b)}(1-\hat{P}(a, b))^{(Z(a, b)-S(a, b))}
$$

(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 ShannonWiener 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 $A L L O C$ 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 $\mathbf{X}$. The first $N$ elements of $\mathbf{X}$ 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 $\mathbf{X}$ beginning at location $\mathbf{X}(I)$. Entries in $\mathbf{X}$ must be packed to the left so that the last node to which node $I$ is linked is immediately followed in $\mathbf{X}$ 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 $N C L U S$ initial clusters. If $I T Y P E=1$, a user supplied initial partition, specified in $C L U S$, is used.

Subroutine $A L L O C$ transfers a node from one cluster to another if the move increases the $\log$ likelihood by more than $T H$, and if the second cluster is smaller than $M X S I Z E$, a given maximum size for clusters. $A L L O C$ 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 $A L L O C$ contain the final partition in

CLUS, the size of each cluster in $S I Z E$, 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 ( $X 2 E N$ ) | input: data vector |
| $N$ | 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 |
| M ${ }^{\text {PSILE }}$ | Integer | input: maximum size of a cluster |
| ITYPE | Integer | input: type of initialization |
| CLUS | Integer array ( $N$ ) | input/ |
| $Y$ | Integer array (XLEN) | output: initial cluster of each node <br> output: data vector (by columns of $B$ ) |
| SIZE | Integer array ( $M X C L U S$ ) | output: initial size of each cluster |
| $P$ | 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 |  |  |
| $I F A U L T=0$ no fault |  |  |
| 1 NCLUS outside its range |  |  |
| $2 M X S I Z E * N C L U S \leqslant N$ |  |  |
| 3 error in $X$ directory: $X(i) \leqslant X(i-1)$, some $i \leqslant N ; X(1) \neq N+1$; or $X(N)>X L E N$ |  |  |
| 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 ( $, Y, N, X L E N, ~ N C L U S, ~ M X C L U S, ~ M X S I Z E, ~ T H, ~ M X S 2, ~ C L U S, ~$ SIZE, P, R1, R2, TLOG, IOLD, INEW) |  |  |
| Formal parameters |  |  |
| These are the same as for INIT except |  |  |
| $Y$ | Integer array ( $X 2 E N$ ) | input: data vector (by columns of $B$ ) |
| TH | Real | input: threshold of incremental likelihood |
| MXS2 | Integer | input: equal to $M X S I Z E$ squared |
| CLUS | Integer array ( $N$ ) | input/ |
| SIZE | Integer array (MXCLUS) | output: current cluster of each node input/ |
| $\boldsymbol{P}$ | Real array (MXCLUS, MXCLUS) | output: current size of each cluster input/ <br> output: current matrix of success counts |

R1 Real array (MXCLUS)

R2 Real array ( $M X C L U S$ )
TLOG
Real array (MXS2)
workspace/
output: $R 1$ (1) returns the overall $\log$ likelihood
workspace: workspace:

## Auxiliary Algorithms

$A L L O C$ calls the real function $X L I K E(P 1, R 1, S 1, S 2, S 3, S 4, Y 1, T L O G, M X S 2)$, which is included. $X L I K E$ calculates the change in log likelihood between $P 1$ successes in $S 1 * S 2$ trials and $P 1-Y 1 * R 1$ successes in $S 3 * S 4$ trials.

## Restrictions

1. $1<N C L U S \leqslant M X C L U S ; N C L U S<N$.
2. $N C L U S * M X S I Z E>N$.
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 $20 * N C L U S$ real additions, and the overall log likelihood calculation requires $3 * N C L U S^{2}$ real additions.

## Storage and Time

The variable storage requirement for this algorithm is less than $2 X L E N+3 N+$ $3 M X C L U S+M X C L U S^{2}+M X S I Z E^{2}+100$ words.

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

## Acknowledgement

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```
        SUBROUTINE INITCX, N, XLEN, NCLUS, MXCLUS, MXSIZE, ITYPE,
        * CLUS, Y, SIZE, P, IOLD, INEW, IFAULT)
            ALGORITHM AS $40.I 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),
    * INEN(N), IOLD(N)
    REAL P(MXCLUS, MXCLUS)
    LOGICAL FLAC
        CMECK INPUTS
        IFAULT = 1
        IF (NCLUS &LE, 1,OR, NCLUS .GE,N .OR.NCLUS .GT. MXCLUS) RETURN
        IFAULTE2
        IF (NCLUS * HXSIZE .LE.N) RETURN
        IFAULT = 3
        DO 1 I =2,N
        L=L-1
        IF (X(I) .LE: X(L)) RETURN
        l CONTINUE
        M=N+1
        IF (X(1) NE,M ORE X(N) ,GT, XLEN) RETURN
        IFAULT = 4
        DO 2I= M, XLEN
        IF (X(I) -LE: OOR& X(I) &GT.N) RETURN
    2 CONTINUE
        IFAULT =5
        OO S I = 1,N
        FIRST = X(I)
        L = I + !
        LAST = X(L) - 1
        IF (I ,EQ.N) LAST = XLFN
        IF (FIRST,EQ, LAST) COTO 5
        JLAST = LAST - }
        DO 4 J = FIRST, JLAST
        JTEST = X(J)
        KFIRST = J +1
        DO 3 K = KFIRST, LAST
        IF (JTEST E&, X(K)) RETURN
    3 CONTINUE
    4 CONTINUE
    5 CONTINUE
            CONSTRUCT Y VECTOR. THE Y VECTOR HOLDS THE ASSOCIATION
            MATRIX BY COLUMNS RATHER IHAN BY ROWS AS X DOES.
    DO 6 I M 1,N
    INEW(I)=0
    Y(I) =N+1
    6 CONTINUE
    Y(M) = a
    DO }7\mathrm{ I = 1,N
    FIRST = X(I)
    LAST = X(I + 1) m 1
    IF (I EO.N) LAST: XLEN
    00 7 J = FIRST, LAST
    KFIRST = X(J) +1
    DO }7\mathrm{ K = KFIRST, N
    Y(K) = Y(K) + 1
7 CONTINUE
    DO 8 I = 1, N
    FIRST = X(I)
    WAST = X(I + 1) - 1
    IF (I .EG.N) LAST % XLEN
    DO & J = FIRST, LAST
    ITEMP = X(J)
    L = Y(ITEMP) + INEW(ITEMP)
    Y(L) =I
    INEW(ITEMP) = INEW(ITEMP) & &
```

```
        8 CONTINUE
            IFAULT = 6
            DO 9 I = 2,N
    IF (Y(I) ,WE: Y(I - 1)J RETURN
9 GONTINUE
    IF (Y(l),NE,M,OR, Y(N) GT, XLEN) RETURN
    IF (ITYPE,EEQ, &) GOTO 33
    IFAULT = 0
C
    11 IOLD(I)=!
    DO 13 ITER = 1. 
    DO 12 I = l, N
    LAST = X(I + 1) - 1
    IF (I ,EN, N) LAST = XLEN
    DO 12 J =FIRST, LAST
    ITEMP = X(J)
    INEW(I) = INEW(I) & IOLD(ITEMP)
    12 CONTINUE
    DO 13I = 1, N
    IOLU(I) = INEW(I)
    13 GONTINUE
C
C
    17 KSTART = N / NCLUS
    DO 2! I = 1, NCLUS
    21 SIZE(I) = KSTART
    ILAST = MOD(N: NCLUS)
    IF (ILAST EQ, D) GOTO 3&
    DO 22 I = L. ILAST
    22 SIZE(I) = SIZE(I) + {
    31 J = 1
    DO 32 I = 1, NCLUS
    KLAST = SIZE(I)
    DO 32 K = 1. KLAST
    ITEMP = INEW(J)
    CLUS(ITEMP) - I
    J = J + l
    32 CONTINUE
    GOTO 40
    33 DO 34 I = 1, NClUS
    34 SIZE(I) = 0
    IFAULT = 7
    DO 35I = 1, N
    J = CLUS(I)
    IF%(J LLE:OUOR&J,GT. NCLUS) RETURN
    35 CONTINUE
    IFAULT =8
    DO 36 I = 1, NCLUS
    IF (SIZE(I) GE, OOR, SIZE(I) .GT, MXSIZE) RETURN
```

```
    36 CONTINUE
    IFAULT |
C
    48 DO 41 I = 1, NCLUS
    DO 4! J = & NCLUS
    41P(I,J)=0.0
    DO 42 I = 1,N
    FIRST = X(I)
    LAST = X(I + 1) = 1
    IF (I EQ. N) LAST = XLEN
    DO 42 J = FIRST: LAST
    IF (X(J) EQ, I) GOTO 42
    ITEMP = X(J)
    ITEMP = CLUS(ITEMP)
    ITEMPR = CLUS(I)
    P(ITEMP2, ITEMP) =P(ITEMP2, ITEMP) + 1.0
    42 CONTINUE
    RETURN
    END
C
C
    SUBROUTINE ALLOC(X, Y, N% XLEN, NCLUS, MXCLUS, MXSIZE,
    * TH, MXS2, CLUS, SIZE, P, R\, R2, TLOG, IOLD, INEW)
        ALGORITHM AS 140.2 APPL. STATIST. (1979) VOL,28, NO,2
        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), IOLO(N), INEW(N)
        REAL P(MXCLUS,'MXCLUS),' TLOG(MXS2), R1(MXCLUS), R2(MXCLUS)
        LOGICAL GLOBAL
            INITIALIZE TLOG, INEW, IOLD, PASS.
    DO 1 I = 1, MXS2
    1 TLOG(I) = FLOAT(I) * ALOG(FLOAT(I))
    2 DOSI = 1, NCLUS
        INEW(I) = 0
        IOLU(I) = 1
        3 CONTINUE
            GLOBAL = .TRUE:
                    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
            SET UP ARRAY OF ASSUCIATIONS (R) FOR THIS NODE
    DO 10 I = 1, NCLUS
    R1(I)=0,0
    R2(I) = 0,0
io continue
    FIRST = X(ITER)
    L = ITER + 1
    LAST = X(L) - 1
    IF (ITER ,EQ,N) LAST = XLEN
    DD il I = FIRST, LAST
    IF (X(I) .EQ. ITER) GOTO 11
    ITEMP = X(I)
    ITEMP = CLUS(ITEMP)
    R1(ITEMP) = R\(ITEMP) + 100
11 CONTINUE
    FIRST = Y(ITER)
    LAST = Y(L) - I
```

```
        IF (ITER ,EQ,N) LAST = XLEN
        DO 12 I = FIRST, LAST
        IF (Y(I),EO, ITER) COTO 12
        ITEMP = Y(I)
        ITEMP = CLUS(ITEMP)
        R2(ITEMP) = R2(ITEMP) + 1,0
    12 CONTINUE
            CHECK EACH CLUSTER FOR AN INCREASE IN LIKELIHOOD
        L = CLUS(ITER)
        DO 49 M = 1, NCLUS
        IF (L, [O,M OR, SIZE(M),GE, MXSIZE,OR.
        * IOLU(L) + IOLD(M) EEQ. D) GOTO 49
            TEST = 0&口
            DO 20 J = 1, NClus
            IF (J,EQ, L OR, J,EE. M) GOTO 20
            IF (P(L, J),GT, 0,0) TEST F TEST + XLIKE(P(L, J), RI(J), SIZE(L),
        * SIZE(J), SIZE(L) - 1, SIZE(J), 1,0, TLOG, MXS2S
            IF (P(M, J) &GT, O,N ,OR, RI(J) GGT, O,O) TEST E TEST +
            * XLIKE(P(M,J), RI(J), SIZE(M), SIZE(J), SIZE(M) + 1, SIZE(J).
            * -1.0, TLOG, MXS2)
            IF (P(J,L),CT. D,(U) TEST = TEST + XLIKE(P(J,L), R2(J), SIZE(L),
            * SIZE(J), SIZE(L) - 1, SIZE(J), 1,0, TLOG, MXS2)
            LF (P(J,M) &GT, O&, OR, R2(J),GT, O, Ø) TEST = TEST +
            * XLIKE(P(J,M), RZ(J), SIZE(M), SIZE(J), SIZE(M) + d, SIZE(J),
    * -1.0, TLOG, MXS2J
2b CONTINUE
            TEST = TEST + XLIKE(P(L, L), RI(L) + R2(L), SIZE(L) - 1, SIZE(L),
        * SIZE(L) - 1, SIZE(L) - 2, 1.0, TLOG, MXS2) +
        * XLIKE(P(L,M), RI(M) - RZ(L) , SIZE(L), SIZE(M), SIZE(L) - 1,
        * SIZ[(M) + 1, 1, D, TLOG, MXS2) +
        * XLIKE(P(N, L), NZ(M) - RL(L), SIZE(L), SIZE(M), SIZE(L. - 1.
        * SIZE(M) + 1, m1.0, TLOG, MXS2) +
        * XLIKE(P(M,M), RI(M) + R2(M) , SIZE(M) - 1, SIZE(M),
        * SIZE(M) + l, SIZE(M), m1, A, TLOG, MXS2)
            IF (TEST LEE. BTEST) GOTO 49
            BTEST : TEST
            NBEST -M
    49 CONTINUE
            MOVE TO BEST CLUSTER
            IF (NBEST .E.G, L) GOTO 59
            M NBEST
            DO 50 II = 1, NCLUS
            P(L, II) = P(L, II) * KI(II)
            P(M, 1I) = P(M,II) + RI(II)
            P(II,L) = P(II,L) R2(II)
            P(II, N) = P(II, M) + R2(II)
    50 COINIINUE
            SIZE(L)=SIZE(L) - 1
            SIZE(M) = SIZE(M) +1
            CLUS(ITER) = NBEST
            INEW(L) = 1
            INEW(M) = 1
    69 CONTINUE
            CHECK FUK OPTIMUM, WERE THERE ANY MOVES THIS PASS,
    DO 60 I = 1, NCLUS
    IF (INEW(I) GT, O) COTO 62
    GA CONTINUE
            NO MOVES, IF A GLOBAL CHECK, FINISH.
            IF A LOCAL CHECK, MAKE A GLOBAL CHECK.
        IF (GLOBAL) GOTO 70
        GOTO 2
            SOME MOVES, RESET IOLD, INEW, MAKE A LOCAL CHECK.
```

```
    62 GLOBAL = .FALSE.
        DO 63I = 1, NCLUS
        IULU(I) = INEW(I)
        INEW(I) = B
    63 CUNTINUE
        gOTO 4
C
            COMPUTE OVERALL LOG LIKELIHOOD
    70 RI(1) = 0.0
        DO }72\mathrm{ I = 1, NCLUS
        KI(I)=RI(I) + XLIKECO,O,P(I, I), I, I, SIZE(I) - &o
        * SIZE(I), -1,A, TLOG, MXS2)
            DO 71 J =1, NCLUS
            IF (I,NE,J) RI(I) = RI(I) + XLIKE(0,0, P(I, J),
        * I, I, SIZE(I), SIZE(J), -1,0, TLOG, MXS2)
    7) CONTINUE
    72 continue
        RETURN
        END
C
    REAL FUNCTION XLIKE(P1, R1, S1, S2, S3, S4, Y1, TLOG, MXS2)
のnのnのn
            ALGORITHM AS &4U,3 APPL, STATIST. (1979) VOL.28, NO,2
            EVALUATE THE CHANGE IN LOG LIKELIHOOD BETWEEN P SUCCESSES IN
            SI * S2 TRIALS AND PI - YI * RI SUCCESSES IN S3 * S4 TRIALS:
    INTEGER S1, S2, S3, S4, P, R, X, Z
    HEAL TLUG(MXS2)
    XLIKE = A,B
    P= P1
    Z=S1 * S2
    K=L-P
    IF (K,NE,N,AND,P ,NE, D) XLIKE= TLOG(Z) - TLOG(P) = TLOG(R)
    X=PI - Yl * RI
    Z = S3 * S4
    R=2-x
    IF (K,NE, ,AND, X,NT, B)
    * XLIKE = XLIKE + TLOG(X) + TLOG(R) - TLOG(Z)
        RETURN
        ENO
```


## Algorithm AS 14I

Inversion of a Symmetric Matrix in Regression Models

By Philippe Kent<br>Department of Mathematics，Ecole Polytechnique Fédérale，Lausanne，Switzerland

## Language

ISO Fortran

## Introduction

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

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

