SOFTWARE FOR ESTIMATING SPARSE JACOBIAN MATRICES

by

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Printed in the United States of America
Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

NTIS price codes
Printed copy: A04
Microfiche copy: A01
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July 1982
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ABSTRACT

In many nonlinear problems it is necessary to estimate the Jacobian matrix of a nonlinear mapping $F$. In large scale problems the Jacobian of $F$ is usually sparse, and then estimation by differences is attractive because the number of differences can be small compared to the dimension of the problem. For example, if the Jacobian matrix is banded then the number of differences needed to estimate the Jacobian matrix is, at most, the width of the band. In this paper we describe a set of subroutines whose purpose is to estimate the Jacobian matrix of a mapping $F$ with the least possible number of function evaluations.
Software for Estimating Sparse Jacobian Matrices

Thomas F. Coleman and Jorge J. Moré
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1. Introduction.

In many nonlinear problems it is necessary to estimate the Jacobian matrix of a mapping \( F : \mathbb{R}^n \to \mathbb{R}^m \). In large scale problems the Jacobian \( F'(x) \) is usually sparse, and then estimation by differences is attractive because the number of differences can be small compared to the dimension of the problem. For example, if the Jacobian matrix is banded then the number of differences needed to estimate the Jacobian matrix is, at most, the width of the band. In this paper we describe a set of subroutines whose purpose is to estimate the Jacobian matrix of a mapping \( F : \mathbb{R}^n \to \mathbb{R}^m \) with the least possible number of function evaluations.

The problem of estimating a sparse Jacobian matrix can be phrased in the following terms: Given a sparse \( m \) by \( n \) matrix \( A \), obtain vectors \( d_1, d_2, \ldots, d_p \) such that \( Ad_1, Ad_2, \ldots, Ad_p \) determine \( A \) uniquely. In this formulation \( A \) is associated with the Jacobian matrix \( F'(x) \) and the product \( Ad \) is associated with an estimate of \( F'(x)d \). Typically, the estimate of \( F'(x)d \) is obtained by the forward difference

\[
F(x+d) - F(x) = F'(x)d + o(\|d\|),
\]

or the central difference

\[
\frac{1}{h}[F(x+d) - F(x-d)] = F'(x)d + o(\|d\|^{\frac{3}{2}})
\]

approximations. Thus each evaluation of \( Ad \) requires at least one function evaluation.

Our algorithms for determining a matrix \( A \) are based on the observation of Curtis, Powell, and Reid [1974] that a group of columns can be determined with an evaluation of \( Ad \) if no two columns in this group have a nonzero in the same row position. To establish this claim, let \( a_1, \ldots, a_n \) be the columns of \( A \), and let \( \{ a_j : a_j \in C \} \) be a group of columns such that no two columns in this group have a nonzero in the same row position. If \( d \in \mathbb{R}^n \) is a vector with components \( \delta_j \neq 0 \) if...
\(a_j\) belongs to \(C\) and \(\delta_j = 0\) otherwise, then

\[
Ad = \sum_{j \in C} \delta_j a_j.
\]

and since no two columns in \(C\) have a nonzero in the same row position, for each nonzero \(a_j\) with \(j \in C\) we have

\[
(Ad)_i = \delta_j a_{ij}.
\]

In view of this observation, it is possible to determine an \(m\) by \(n\) matrix \(A\) if we partition the columns of \(A\) into groups \(C_1, \ldots, C_p\) so that each column belongs to one and only one group, and so that no two columns in a group have a nonzero in the same row position. A partition of the columns of \(A\) with this property is consistent with the determination of \(A\).

In the CPR algorithm as proposed by Curtis, Powell, and Reid [1974], the groups \(C_1, \ldots, C_p\) are formed one at a time by scanning the columns in the order \(a_1, a_2, \ldots, a_n\), and by including a column in the current group if it has not been included in a previous group, and if it does not have a nonzero in the same row position as another column already in the group. By looking at the problem from a graph theory point of view, Coleman and More [1981] showed that it is possible to considerably improve the CPR algorithm by scanning the columns in a carefully selected order. Various orderings were considered and analyzed by Coleman and More [1981]; one of our purposes here is to describe the implementation of the resulting algorithms.

Many users will only be interested in subroutines DSM and FDJS. These are the interface routines for the package, and with these two subroutines it is quite easy to estimate the Jacobian matrix of a mapping \(F: \mathbb{R}^n \to \mathbb{R}^m\) with a minimal or nearly minimal number of function evaluations. An example illustrating the uses of DSM and FDJS appears in Section 4.

Given the sparsity pattern of an \(m\) by \(n\) matrix \(A\), subroutine DSM determines an optimal or nearly optimal consistent partition of the columns of \(A\). The consistent partition is specified by an array \(ngrp\) of length \(n\) by setting \(ngrp(jcal)\) to the group number of column \(jcal\). Subroutine DSM is an interface routine for the ordering algorithms and is quite easy to use; additional details can be found in Section 2.

Given a consistent partition of the columns of the Jacobian matrix, subroutine FDJS determines an approximation to those columns in a given group of the partition. The entire Jacobian matrix is determined by calling FDJS for each group in the partition. Subroutine FDJS stores the Jacobian matrix with a column-oriented definition of the sparsity pattern. If the user is storing the Jacobian matrix with a different data structure it is necessary to modify FDJS, or to provide an interface between the two data structures. For this reason the
coding of FDJS is described in Section 3.

An example illustrating the uses of subroutines DSM and FDJS is provided in Section 4. This example also serves as a test program for our package. In Section 5 we provide an overview of the subroutines included in the package and a description of the transition from the data structure used by DSM to the data structure used by the algorithms called by DSM. Implementation details and an analysis of the running time of the algorithms used by DSM appear in Section 6. It is only in this section that we need a modest amount of graph theory.

Section 7 contains some of the numerical results that we have obtained with subroutine DSM. These results were obtained with the sparsity patterns of Everstine [1979] and show that on practical problems DSM and FDJS can estimate the Jacobian matrix of a mapping \( F : \mathbb{R}^n \to \mathbb{R}^m \) with a minimal or nearly minimal number of function evaluations. All computations were done on a VAX 11/780.

2. Subroutine DSM.

Given the sparsity pattern of an \( m \times n \) matrix \( A \), subroutine DSM determines an optimal or nearly optimal consistent partition of the columns of \( A \).

The user specifies a definition of the sparsity pattern of \( A \) by providing the ordered pairs \((i,j)\) for which \( a_{ij} \neq 0\):

\[
(2.1) \quad (\text{indrow}(k),\text{indcol}(k)), \quad k = 1,2, \ldots, npairs.
\]

These pairs can be provided in any order. Moreover, duplicate pairs are allowed so that \( npairs \) need not agree with the number of nonzeros in \( A \).

On output DSM defines a consistent partition of the columns of \( A \) via the integer array \( ngrp \) by setting \( ngrp(jcol) \) to the group number of column \( jcol \). In addition, the variable \( mingroup \) provides a lower bound on the number of groups possible in a consistent partition, and the variable \( maxgrp \) is the number of groups in the partition obtained by DSM. On output DSM also transforms the specification of the sparsity pattern (2.1) provided by \( \text{indrow} \) and \( \text{indcol} \) into an alternative specification which is more appropriate for the the algorithms used by DSM. This alternative specification is explained at the end of this section.

A lower bound on the number of groups in a consistent partition is \( p_{\max} \), where \( p_{\max} \) is the maximum number of nonzero elements in any row of \( A \). Usually \( mingroup \) is set to \( p_{\max} \), but on some problems \( mingroup \) may exceed \( p_{\max} \). For example, if

\[
A = \begin{bmatrix}
  x & x \\
  x & x & x \\
  x & x
\end{bmatrix}
\]

then \( mingroup \) is set to 3. In practice DSM needs, at worst, one or two more
groups than the bound specified by \( \text{mingrp} \). For many problems \( \text{maxgrp} \) agrees with \( \text{mingrp} \) and then DSM is optimal.

Execution times for subroutine DSM are quite satisfactory since the number of operations required by one call is proportional to

\[
(2.2) \quad \sum_{i=1}^{m} p_i^2.
\]

where \( p_i \) is the number of nonzeros in the \( i \)-th row of \( A \). This bound is appropriate because many sparse matrix computations require at least \((2.2)\) operations. For example, the number of operations needed to compute \( A^T A \) is at least a constant multiple of \((2.2)\).

The claim that \((2.2)\) is a measure of the running time of DSM assumes that \( n_{\text{pairs}}, m, \) and \( n \) are not more than a constant times \((2.2)\). This is certainly the case in any non-trivial situation since \((2.2)\) is not less than the number of nonzero elements of \( A \).

An impression of the overhead required by DSM can be obtained by comparing DSM with a subroutine for computing the sparse LU factorization of a matrix. We used the factorization subroutine F01BRF from the NAG library because it is an excellent program. For test problems we used the 30 sparsity patterns in the Everstine [1979] collection with the nonzero entries of the matrix being uniformly distributed random numbers in \((0,1)\). On these problems DSM was always faster than the factorization subroutine. Indeed, on twelve of the problems (in particular, on the 7 problems with \( n > 878 \)) DSM was at least 10 times faster than the factorization subroutine. The storage requirements of DSM also compare very favorably because the factorization subroutine requires an unspecified amount of storage to handle the fill-in of the factorization in addition to the storage required for the matrix and the sparsity pattern. Finally, note that in a typical nonlinear problem DSM is only called once whereas the factorization subroutine is usually called many times.

Implementation of DSM so that the execution time is proportional to \((2.2)\) requires an appropriate data structure. The ordered pairs \((i,j)\) for which \( a_{ij} \neq 0 \) is a convenient data structure for the user, but DSM requires a different data structure. The algorithms called by DSM require both "column-oriented" and "row-oriented" definitions of the sparsity pattern. The arrays \( \text{indrow} \) and \( \text{ipntr} \) provide a column-oriented definition of the sparsity pattern if the nonzero elements of the \( j \)-th column are

\[
\text{indrow}(k), \quad k = \text{ipntr}(j), \ldots , \text{ipntr}(j+1)-1.
\]

The arrays \( \text{indcol} \) and \( \text{ipntr} \) provide a row-oriented definition of the sparsity pattern if the nonzero elements of the \( i \)-th row are
Given the ordered pairs (2.1) for which \( a_y \neq 0 \), subroutine DSM generates column-oriented and row-oriented definitions of the sparsity pattern. The transition from (2.1) is not difficult and is described in more detail in Section 5.

3. Subroutine FDJS.

Given a consistent partition of the columns of the Jacobian matrix, subroutine FDJS determines an approximation to those columns in a given group of the partition.

An approximation to the columns of the Jacobian matrix in group \( \text{numgrp} \) can be obtained by specifying a difference parameter array \( d \) with \( d(jcol) \) nonzero if and only if \( jcol \) is a column in group \( \text{numgrp} \), and an approximation to \( F'(x)d \) in the array \( \text{fjacd} \). The approximation to the columns of the Jacobian matrix in group \( \text{numgrp} \) are stored in the array \( \text{fjac} \). Subroutine FDJS stores the Jacobian matrix in an array \( \text{fjac} \) with a column-oriented definition of the sparsity pattern; that is, the nonzero elements of the \( j \)-th column of the Jacobian matrix are stored in positions

\[
\text{fjac}(k), \ k = \text{ipntr}(j), \ldots, \text{ipntr}(j+1)-1.
\]

If the user is storing the Jacobian matrix with a different data structure it is then necessary to modify FDJS or to provide an interface between the two data structures.

If the consistent partition is specified by an array \( \text{ngrp} \) by setting \( \text{ngrp}(jcol) \) to the group number of column \( jcol \), then the user can define the difference parameter array \( d \) with the section of code in Program 3.1.

\[
\begin{align*}
do & 10 jcol = 1, n \nonumber \
d(jcol) = \text{zero} \qquad & \text{if } (\text{ngrp}(jcol) \neq \text{numgrp}) \
d(jcol) = \eta(jcol) \quad & 10 \text{ continue} 
\end{align*}
\]

Program 3.1

The array \( \eta \) contains the difference parameters used to estimate the Jacobian matrix. The user must provide suitable values for this array. The user must also provide an estimate for \( F'(x)d \) in an array \( \text{fjacd} \). For example, the estimate

\[
F(x + d) - F(x)
\]

corresponds to the forward difference formula, and the estimate

\[
\frac{1}{2}[F(x + d) - F(x - d)]
\]

corresponds to the central difference formula.
Given \( d \) and \( fjacd \), it is then possible to determine all the elements in the columns of the Jacobian matrix in group \( numgrp \). The method for storing this information depends on the data structure used to store the Jacobian matrix; if the Jacobian matrix is stored with a column-oriented definition of the sparsity pattern then the section of code in Program 3.2 can be used.

```fortran
  do 30 jcol = 1, n
    if (ngrp(jcol) .ne. numgrp) go to 20
    jpl = jpntr(jcol)
    jpu = jpntr(jcol+1) - 1
    if (jpu .lt. jpl) go to 20
    do 10 jp = jpl, jpu
      ir = indrow(jp)
      fjac(jp) = fjacd(ir)/d(jcol)
  10 continue
  20 continue
  30 continue
```

Program 3.2

This code stores in the array \( fjac \) an approximation to the columns of the Jacobian matrix \( F'(x) \) which are in group \( numgrp \). To estimate the whole Jacobian it is necessary to execute Programs 3.1 and 3.2 for \( numgrp \) set to 1, 2, \ldots, \( maxgrp \). An example of the use of FDJS can be found in Section 4.

4. Example.

The uses of subroutines DSM and FDJS can be illustrated by considering the problem of approximating the Jacobian matrix \( F'(x) \) of a mapping \( F: \mathbb{R}^n \rightarrow \mathbb{R}^n \) such that \( F'(x) \) has a sparsity pattern of the form

\[
(4.1) \quad \begin{pmatrix}
  T_1 & D_3 \\
  D_1 & T_2 & D_3 \\
  D_2 & D_4 & B
\end{pmatrix}
\]

where the \( T \)'s have tridiagonal patterns, the \( D \)'s have diagonal patterns, and \( B \) is of lower bidiagonal form. This is a simplified form of the neutron kinetics problem described by Carver and MacEwen [1981].

A consistent partition of the columns of (4.1) can be determined with a call to DSM:

```fortran
  call dsm(n,n,nnz,indrow,indcol,ngrp,maxgrp,mingrp, \\
           info,jpntr,jpntr,iwa,liwa,bwa)
```

We are mainly interested in the first seven parameters of the calling sequence. The parameters \( nnz \), \( indrow \), and \( indcol \) define the sparsity pattern of (4.1). These parameters can be determined with the section of code in Program 4.1, where it is assumed that each of the submatrices in (4.1) is of order \( t \) so that
\( n = 3l \), and \( \text{nnz} \) denotes the number of nonzero elements in (4.1).

\[
l = n/3
\]
\[
\text{nnz} = 0
\]
\[
do 60 \ j = 1, n
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
\text{if} (j \ .eq. l \ .or. j \ .eq. 2l \ .or. j \ .eq. 3l) \text{ go to 10}
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j + 1
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
10 \text{ continue}
\]
\[
\text{if} (j \ .eq. 1 \ .or. j \ .eq. l+1 \ .or. j \ .gt. 2l) \text{ go to 20}
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j - 1
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
20 \text{ continue}
\]
\[
\text{if} (j \ .gt. 2l) \text{ go to 30}
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j + l
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
30 \text{ continue}
\]
\[
\text{if} (j \ .le. l) \text{ go to 40}
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j - l
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
40 \text{ continue}
\]
\[
\text{if} (j \ .gt. l) \text{ go to 50}
\]
\[
\text{nnz} = \text{nnz} + 1
\]
\[
\text{indrow} (\text{nnz}) = j + 2l
\]
\[
\text{indcol} (\text{nnz}) = j
\]
\[
50 \text{ continue}
\]
\[
60 \text{ continue}
\]

Program 4.1

Table 4.1 provides the output values of \( \text{mingrp} \) and \( \text{maxgrp} \) produced by DSM. These results show that DSM requires 6 groups to determine a matrix of the form (4.1) for each of the tested dimensions.

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \text{nnz} )</th>
<th>( \text{mingrp} )</th>
<th>( \text{maxgrp} )</th>
<th>time</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1295</td>
<td>5</td>
<td>6</td>
<td>1.28</td>
</tr>
<tr>
<td>600</td>
<td>2595</td>
<td>5</td>
<td>6</td>
<td>2.75</td>
</tr>
<tr>
<td>900</td>
<td>3895</td>
<td>5</td>
<td>6</td>
<td>3.80</td>
</tr>
<tr>
<td>1200</td>
<td>5195</td>
<td>5</td>
<td>6</td>
<td>4.93</td>
</tr>
</tbody>
</table>

Table 4.1. Output from DSM for the Neutron Kinetics Problem.

Also note that \( \text{maxgrp} \) does not agree with \( \text{mingrp} \). In some cases it is not possible to determine a matrix \( A \) with \( \text{mingrp} \) groups, but for (4.1) this is indeed the case. This can be shown by noting that a consistent partition of the columns of (4.1) is obtained if column \( j \) is assigned to group \( ngrp(j) \) where
This example shows that for regular structures like (4.1) it is sometimes possible to improve on DSM. Finally, note that the execution time grows linearly with $n$. This is to be expected since it is proportional to (2.2).

The use of FDJS can be illustrated by considering the mapping $F: \mathbb{R}^n \rightarrow \mathbb{R}^n$ with components $f_i: \mathbb{R}^n \rightarrow \mathbb{R}$ defined by

\[(4.2) \quad f_i(x) = \varphi(\xi_i + \sum_{k \in S_i} \xi_k), \quad \varphi(\xi) = (((1 + \xi) + 1), \]

where $\xi_k$ is the $k$-th component of $x$, and the set $S_i$ represents the sparsity pattern of the $i$-th row of the matrix (4.1). This is a simple function, but it serves quite well to illustrate the use of FDJS.

The subroutine in Program 4.2 evaluates $F$ at $x$ and returns $F(x)$ in the array $fvec$. In this program we make use of the fact that DSM returns in $\text{indcol}$ and $\text{ipntr}$ a row-oriented definition of the sparsity pattern.

```
subroutine fcn(n,x,indcol,ipntr,fvec)
  integer n
  integer indcol(1),ipntr(1)
  real z(n),fvec(n)
  C
  Function subroutine for testing FDJS.
  C
  integer i,ip,ipl,ipu,k
  real sum
  do 20 i = 1, n
    sum = 0.0
    ip = ipntr(i)
    ipu = ipntr(i+1) - 1
    do 10 ip = ip, ipu
      k = indcol(ip)
      sum = sum + z(k)
  10 continue
  sum = sum + z(i)
  fvec(i) = sum*(1.0 + sum) + 1.0
  20 continue
return
end
```

Program 4.2

We can now use FDJS to obtain an approximation to the Jacobian matrix of $F$. The code in Program 4.3 stores the approximation in the array $fjac$. The difference parameters used in this code are only for illustrative purposes.
call fcn(n,x,indcol,ipntr,fvec)
do 30 numgrp = 1, maxgrp
   do 10 j = 1, n
      d(j) = 0.0
      if (ngrp(j) .eq. numgrp) d(j) = 0.001
      xd(j) = x(j) + d(j)
   continue
   call fcn(n,xd,indcol,ipntr,fjacd)
do 20 i = 1, n
   fjacd(i) = fjacd(i) - fvec(i)
   continue
20 call fdjs(n,indrow,jpntr,ngrp,numgrp,d,fjacd,fjac)
30 continue

Program 4.3


We have already described the interface subroutines DSM and FDJS in our package. The purpose of this section is to provide a brief overview of the remainder of the package.

All of our algorithms for determining a consistent partition of the columns of an m by n matrix A use the sequential algorithm with some ordering of the columns of A. A consistent partition is obtained by first determining an ordering of the columns and then calling the sequential algorithm to obtain the consistent partition. Subroutine SEQ implements the sequential algorithm and the subroutines DEGR, IDO, and SLO determine an ordering of the columns of A. In the remaining sections we shall describe these subroutines in detail.

Subroutine DSM obtains a consistent partition by calling the sequential algorithm with the ordering subroutines in the order SLO, IDO, and DEGR. All three ordering subroutines are used in an attempt to produce optimal or near optimal results in all cases. If any of the orderings leads to a consistent partition with mingrp groups then DSM terminates at that point; otherwise DSM returns the best result obtained.

The transition from the data structure (2.1) to the column-oriented and row-oriented definitions of the sparsity pattern is accomplished by subroutines SRTDAT and SETR. Because this transition is not difficult, we describe these subroutines briefly.

Subroutine SRTDAT permutes indrow and indcol so that indcol is in non-decreasing order, and determines jpntr so that indrow and jpntr provide a column-oriented definition of the sparsity pattern. This is done by first determining the number of nonzeroes in the columns of A and setting pointers to the start of the columns in indrow. The sorting is accomplished by examining each component of indcol, and if the current component is not in position then it is placed in position and the displaced component is made the current component.
The execution time for SRTDAT is proportional to the number of input pairs in (2.1) so that if there are no duplicates then the execution time is proportional to the number of nonzeroes in $A$. After execution of SRTDAT it is easy to eliminate any duplicates in the input pairs (2.1), so we now assume that this has been done.

Given a column-oriented definition of the sparsity pattern of a matrix $A$, subroutine SETR determines a row-oriented definition of the sparsity pattern. This is done by first determining the number of nonzeroes in the rows of $A$, then setting pointers to the start of the rows in $indcol$, and finally filling $indcol$. It is straightforward to show that the execution time for SETR is proportional to the number of nonzeroes in $A$.

For ease of reference, we next provide a brief description of the purposes of the subroutines in our package for estimating sparse Jacobian matrices. With the exception of NUMSRT all of the subroutines have been mentioned earlier; NUMSRT is just a simple bucket sort.

Subroutine DEGR: Given the sparsity pattern of an $m$ by $n$ matrix $A$, this subroutine determines the degree sequence for the intersection graph of the columns of $A$.

Subroutine DSM: This subroutine determines an optimal or near-optimal consistent partition of the columns of a sparse $m$ by $n$ matrix $A$.

Subroutine FDJS: Given a consistent partition of the columns of an $m$ by $n$ Jacobian matrix into groups, this subroutine computes approximations to those columns in a given group.

Subroutine IDO: Given the sparsity pattern of an $m$ by $n$ matrix $A$, this subroutine determines the incidence degree ordering of the columns of $A$.

Subroutine NUMSRT: Given a sequence of integers, this subroutine groups together those indices with the same sequence value and, optionally, sorts the sequence into either ascending or descending order.

Subroutine SEQ: Given the sparsity pattern of an $m$ by $n$ matrix $A$, this subroutine determines a consistent partition of the columns of $A$ by a sequential algorithm.
Subroutine SETR: Given a column-oriented definition of the sparsity pattern of an \( m \times n \) matrix \( A \), this subroutine determines a row-oriented definition of the sparsity pattern of \( A \).

Subroutine SLO: Given the sparsity pattern of an \( m \times n \) matrix \( A \), this subroutine determines the smallest-last ordering of the columns of \( A \).

Subroutine SRTDAT: Given the non-zero elements of an \( n \times n \) matrix \( A \) in arbitrary order as specified by their row and column indices, this subroutine permutes these elements so that their column indices are in non-decreasing order.

6. Implementation Details.

The sequential algorithm and the ordering algorithms used by subroutine DSM have been described by Coleman and Moré [1981]. Implementation of these algorithms is not straightforward, and thus we now describe the implementation of these algorithms and, in particular, show that these implementations execute in time proportional to (2.2)

The sequential algorithm and the ordering algorithms can be described best with the help of some graph theory terminology. A graph \( G \) is an ordered pair \((V,E)\) where \( V \) is a finite and non-empty set of vertices and the edges \( E \) are unordered pairs of distinct vertices. The vertices \( u \) and \( v \) are adjacent if \((u,v)\) is an edge with endpoints \( u \) and \( v \). The degree of a vertex \( v \) is the number \( \deg(v) \) of edges with \( v \) as an endpoint.

Given an ordering \( v_1,v_2,\ldots,v_n \) of the vertices of a graph \( G \), we can use a sequential algorithm to partition the vertices of \( G \) into groups such that the vertices in a given group are not adjacent. At the \( k \)-th stage of the sequential algorithm the groups \( ngrp(v_1),\ldots,ngrp(v_{k-1}) \) have been assigned, and \( ngrp(v_k) \) is set to the smallest positive integer such that \( ngrp(v_k) \neq ngrp(v_j) \) if \((v_k,v_j)\) is an edge of \( G \) for some \( 1 \leq j < k \).

We are interested in the application of these concepts to a special class of graphs. Given an \( m \times n \) matrix \( A \) with columns \( a_1,a_2,\ldots,a_n \), we define a graph \( G(A) \) with vertices \( a_1,a_2,\ldots,a_n \) and edge \((a_i,a_j)\) if and only if \( i \neq j \) and columns \( i \) and \( j \) have a nonzero in the same row position. In graph theory terminology \( G(A) \) is the intersection graph of the columns of the matrix \( A \). It should now be clear that the sequential algorithm on \( G(A) \) generates a consistent partition of the columns of \( A \), and that the purpose of an ordering is to minimize the number of groups required by the sequential algorithm.

The array \( ngrp \) defines a coloring of \( G \) in the sense that \( ngrp(u) \neq ngrp(v) \).
If $u$ and $v$ are adjacent. Thus the sequential algorithm can be viewed as a graph coloring algorithm. This is the point of view adopted by Coleman and Moré [1981]; in this paper we de-emphasize the graph coloring viewpoint and instead prefer to work in terms of consistent partitions since this concept is closer to the software. On the other hand, the graph coloring viewpoint is important because the ordering algorithms only make sense when viewed as graph coloring algorithms.

An ordering $v_1, v_2, \ldots, v_n$ of the vertices of a graph $G$ is a largest-first ordering if $\{\deg(v_j)\}$ is non-increasing. The description of the other two ordering algorithms require additional graph theory terminology: Given a graph $G = (V,E)$ and a non-empty subset $W$ of $V$, the subgraph $G[W]$ induced by $W$ has vertex set $W$ and edge set

$\{(u,v) : (u,v) \in E \text{ and } u,v \in W\}$.

In the smallest-last ordering the $k$-th vertex $v_k$ is determined after $v_{k+1}, \ldots, v_n$ have been selected by choosing $v_k$ so that its degree in the subgraph induced by

$V - \{v_{k+1}, \ldots, v_n\}$

is minimal. In the incidence-degree ordering $v_k$ is determined after $v_1, \ldots, v_{k-1}$ have been selected by choosing $v_k$ so that its degree in the subgraph induced by $\{v_1, \ldots, v_k\}$ is maximal. The incidence degree of $v_k$ is the degree of $v_k$ in this subgraph.

The first two algorithms are well-known in the graph coloring literature, but the incidence degree ordering was introduced by Coleman and Moré [1981]. For a general graph $G$ these algorithms can be implemented to run in time proportional to $|V| + |E|$ provided we are given the adjacency lists for the graph, that is, arrays $nptr(\cdot)$ and $nghbr(\cdot)$ such that the vertices adjacent to the $j$-th vertex are

$nghbr(k), k = nptr(j), \ldots, nptr(j+1)-1$.

See, for example, Matula and Beck [1981]. However, the adjacency lists for $G(A)$ may require storage of order $n^2$ even if $A$ is sparse, so this data structure is not appropriate. Our ordering algorithms use the column-oriented and the row-oriented definitions of the sparsity pattern of $A$ and thus require only $2 \tau$ words of storage where $\tau$ is the number of nonzero elements of $A$.

We now describe the ordering algorithms and the sequential algorithm. We only attempt to cover the important details and not a complete description of the algorithms. The description of certain tasks is done in Fortran 77. For ease of portability, however, the package is written in Fortran 66.
6.1. Largest-First Ordering.

The purpose of subroutine DEGR is to obtain the degree sequence for \( G(A) \) and thus the largest-first ordering is determined by JEGR.

Program 6.1 determines an array \( \text{adj} \) such that \( \text{adj}(1), \ldots, \text{adj}(\text{deg}) \) are the columns adjacent to column \( j \) and \( \text{deg} \) is the degree of column \( j \). The array \( \text{mark} \) is used to mark column \( j \) and those columns adjacent to column \( j \).

\[
\text{mark}(j) = \text{true}.
\]
\[
\text{deg} = 0
\]
\[
do 20 \text{jp} = \text{ipntr}(j), \text{ipntr}(j+1)-1
\]
\[
i = \text{indrow}(\text{jp})
\]
\[
do 10 \text{ip} = \text{ipntr}(i), \text{ipntr}(i+1)-1
\]
\[
\text{adjcol} = \text{indcol}(\text{ip})
\]
\[
\text{if (not. mark(adjcol)) then}
\]
\[
\text{deg} = \text{deg} + 1
\]
\[
\text{adj(deg)} = \text{adjcol}
\]
\[
\text{mark(adjcol)} = \text{true}.
\]
\[
\text{end if}
\]
\[
10 \ \text{continue}
\]
\[
20 \ \text{continue}
\]

Program 6.1

After the degree of column \( j \) is determined Program 6.2 un-marks the columns adjacent to column \( j \) and also unmarks column \( j \).

\[
dc 10 \ \text{l} = 1, \text{deg}
\]
\[
\text{mark(adj(l))} = \text{false}.
\]
\[
10 \ \text{continue}
\]
\[
\text{mark}(j) = \text{false}.
\]

Program 6.2

If we execute Programs 6.1 and 6.2 for \( j = 1, 2, \ldots, n \) then the degrees of \( G(A) \) are obtained. The following algorithm uses the array \( \text{ngrp} \) to store the degree sequence of \( G(A) \) by setting \( \text{ndeg}(j) \) to the degree of column \( j \).

Algorithm. Degrees of \( G(A) \):

For \( j = 1, 2, \ldots, n \):

- a) Find all columns adjacent to column \( j \) with Program 6.1.
- b) Un-mark column \( j \).
- c) Un-mark the columns adjacent to column \( j \).
- d) Let \( \text{ndeg}(j) = \text{deg} \).

The running time of this algorithm can be analyzed by noting that the number of operations needed to execute Programs 6.1 and 6.2 is proportional to

\[
(6.1) \quad \sum_{a_j = 0}^{\text{deg}(a_j)}
\]
where \( \rho_i \) is the number of nonzero elements in the \( i \)-th row. The total amount of work needed to execute the programs for \( j = 1, 2, \ldots, n \) is thus proportional to

\[
\sum_{j=1}^{n} \left( \sum_{i=1}^{l} \rho_i \right) + \sum_{j=1}^{n} \deg(a_j).
\]

Since

\[
\sum_{j=1}^{n} \left( \sum_{i=1}^{l} \rho_i \right) = \sum_{i=1}^{l} \rho_i^2, \quad \sum_{j=1}^{n} \deg(a_j) \leq \sum_{i=1}^{l} \rho_i^2,
\]

we have shown that the time needed to execute DEGR is proportional to (2.2).

6.2. Smallest-Last and Incidence Degree Orderings.

The implementations of the smallest-last and incidence degree orderings are very similar. In the smallest-last ordering the column chosen at the \( k \)-th stage has minimal degree in the graph induced by the un-ordered columns, while in the incidence degree ordering the chosen column has maximal incidence degree among the un-ordered columns. From this description it is clear that we need a data structure which permits the easy updating of the two types of degrees. A doubly-linked list is a standard structure which satisfies this requirement.

We can implement a doubly-linked list with the three arrays \texttt{head}, \texttt{prev}, and \texttt{next}. Each un-ordered column \( j \) is in a list of columns with the same degree. The first column in the list of columns with degree \( \text{deg} \) is \( \text{head}(\text{deg}) \) unless \( \text{head}(\text{deg}) = 0 \). In this case there are no columns in the \( \text{deg} \) list. The column before \( j \) in the degree list of column \( j \) is \( \text{prev}(j) \) unless \( \text{prev}(j) = 0 \). In this case \( j \) is the first column in the degree list. The column after \( j \) in the degree list of column \( j \) is \( \text{next}(j) \) unless \( \text{next}(j) = 0 \). In this case \( j \) is the last column in the degree list.

In the above description the term degree may refer either to the degree in the graph induced by the un-ordered columns or to the incidence degree for an un-ordered column. This permits us to discuss the smallest-last and incidence degree orderings at the same time. In the sequel we shall refer to these degrees as the degrees for the un-ordered columns.

It is easy to update the degree lists for the un-ordered columns. For example, if \texttt{numdeg} is the degree of column \( j \) then Program 6.3 deletes column \( j \) from the \texttt{numdeg} list and inserts it into the \texttt{numdeg + 1} list.

We now have all the ingredients necessary to implement the smallest-last and incidence degree orderings.
Delete column $j$ from the numdeg list.

\[
\begin{align*}
&\text{if (prev}(j) \text{.eq. 0) head(numdeg) = next}(j) \\
&\text{if (prev}(j) \text{.gt. 0) next(prev}(j)) = \text{next}(j) \\
&\text{if (next}(j) \text{.gt. 0) prev(next}(j)) = \text{prev}(j)
\end{align*}
\]

Add column $j$ to the numdeg + 1 list.

\[
\begin{align*}
&\text{prev}(j) = 0 \\
&\text{next}(j) = \text{head(numdeg+1)} \\
&\text{if (head(numdeg+1) .gt. 0) prev(head(numdeg+1)) = } j \\
&\text{head(numdeg+1) = } j
\end{align*}
\]

Program 6.3

**Algorithm. Smallest-last ordering.**

For $k = n, n-1, \ldots, 1$

a) Choose a column $j$ of minimal degree and let $\text{list}(k) = j$.

b) Delete column $j$ from the list of columns of minimal degree.

c) Find all un-marked columns adjacent to column $j$ with Program 6.1.

d) Update the degree lists for the un-ordered columns.

e) Un-mark the columns adjacent to column $j$.

In this algorithm we must not un-mark column $j$. Thus, in step e the un-marked columns are precisely those columns which have not been assigned a place in the ordering. The incidence degree ordering is quite similar to the smallest-last ordering. The only difference is that it is now necessary to update the incidence degrees of the graph induced by the un-ordered columns.

**Algorithm. Incidence degree ordering.**

For $k = 1, 2, \ldots, n$

a) Choose a column $j$ of maximal incidence degree and let $\text{list}(k) = j$.

b) Delete column $j$ from the list of columns of maximal incidence degree.

c) Find all un-marked columns adjacent to column $j$ with Program 6.1.

d) Update the incidence degree lists for the un-ordered columns.

e) Un-mark the columns adjacent to column $j$.

In both ordering algorithms it is necessary to keep track of the degrees for the un-ordered columns. An array $\text{list}$ can be used for this purpose provided we modify step a in both algorithms so that $\text{list}(j) = k$. Thus $\text{list}(j)$ is the degree of the $j$-th column if $j$ is an un-ordered column, while if $j$ is ordered then $\text{list}(j)$ is the position of column $j$ in the order. If the array $\text{list}$ is inverted at the end of the algorithm then $\text{list}(k)$ is the $k$-th column in the ordering.
The argument used to analyze the running time of the largest-first ordering also applies to the smallest-last and incidence degree ordering because the number of operations needed to order column \( j \) is proportional to \((6.1)\). Thus both the smallest-last and incidence degree orderings execute in time proportional to \((2.2)\).

The implementation of the incidence degree ordering in subroutine IDO has a feature that is not present in the above algorithm. This additional feature can be motivated by noting that the ordering produced by IDO is arbitrary at certain stages. In particular, the choice of the first column is arbitrary because initially all columns have zero incidence degree. Also note that if \( G(A) \) is disconnected then the choice of the first column in each connected component is also arbitrary because the maximal incidence degree is zero at the start of the ordering process for each component. For these reasons IDO attempts to choose a column of maximal degree among the columns of maximal incidence. This is done by searching the first

\[
(6.2) \quad \frac{1}{n} \sum_{i=1}^{m} \rho_{i}^{2}
\]

elements in the list of columns of maximal incidence degree and choosing a column with the largest degree. Note that if the whole list of columns of maximal incidence is searched then IDO executes in time proportional to \(n^2\) on certain problems, but that if the length of the search is bounded by \((6.2)\) then IDO runs in time proportional to \((2.2)\). On the other hand, by limiting the length of the search we may fail to find a column of largest degree. This last objection is handled by initially sorting the list of columns of maximal incidence degree in decreasing order according to their degrees. If this is done then the first element in the list of columns of maximal incidence has the largest degree whenever the maximal incidence is zero (recall that this happens at the start of the ordering process for each connected component); if the maximal incidence is greater than zero then the list of columns of maximal incidence is usually small, so \((6.2)\) is not a severe restriction on the length of the search.

In the version of the incidence degree ordering used by Coleman and Moré [1981] the chosen column had the least number of nonzero elements among the columns of maximal incidence. This choice is often quite effective. For example, this choice produces optimal results in the neutron kinetics problem of Section 4. The version of the incidence degree ordering used in IDO, however, usually leads to slightly better results for DSM.

A by-product of the smallest-last and incidence degree orderings is the lower bound \( \min grp \) on the number of groups needed by any consistent partition of the columns of \( A \). This lower bound is obtained by determining a set of columns that are mutually adjacent in \( G(A) \), in graph theory terminology such a
set is a clique of $G(A)$. The orderings can be used to determine a clique by noting that if the $k$-th column in either ordering has degree $k - 1$ then $G(A)$ has a clique of size $k$. Note that this property is shared by the smallest-last and incidence degree orderings, but not by the largest-first ordering. It is also possible to determine the size of a clique in $G(A)$ by computing $\rho_{\text{max}}$ where $\rho_{\text{max}}$ is the maximum number of nonzero elements in any row of $A$. This observation is based on the fact that if columns $j_1, \ldots, j_k$ have a nonzero in a given row then these columns form a clique in $G(A)$. Subroutine DSM sets $m\text{ingrp}$ to the size of the largest clique found by one of the techniques discussed above.

6.3. The Sequential Algorithm.

In the sequential algorithm the order of the columns is specified by the array $\text{list}$ by letting $\text{list}(k)$ be the $k$-th vertex in the ordering. On output from the sequential algorithm the array $n\text{grp}$ specifies a consistent partition of the columns of $A$ by setting $n\text{grp}(j)$ to the group number of the $j$-th column.

Algorithm. Sequential algorithm.

For $k = 1, 2, \ldots, n$

a) Find all columns adjacent to column $j = \text{list}(k)$ with Program 6.1.

b) Un-mark the columns adjacent to column $\text{list}(k)$.

c) Mark all the groups of the columns adjacent to column $\text{list}(k)$.

d) Let $n\text{grp}(\text{list}(k))$ be the smallest un-marked group.

e) Un-mark the groups.

The running time of this algorithm is proportional to (2.2) because the number of operations needed to determine the group of column $\text{list}(k)$ is proportional to (6.1). It is possible to improve the running time of this algorithm by noting that we can mark the groups of columns adjacent to column $\text{list}(k)$ as we determine the adjacent columns. Thus, in the subroutine SEQ steps a, b, and c are replaced by a section of code which marks the group number of columns which are adjacent to column $\text{list}(k)$.

7. Numerical Results.

In Section 2 we have already discussed the overhead required by DSM. and have shown that the requirements of DSM are quite modest. In this section we present evidence which shows that on practical problems DSM usually requires, at worst, one or two groups more than the bound specified by $m\text{ingrp}$.

Table 7.1 shows the results of using DSM on the 30 sparsity patterns of the Everstine [1979] collection. These are symmetric patterns for matrices of order $n$ with $n$ ranging from 59 to 2880. In addition to the order $n$ of the matrix, Table 7.1 contains the number $nnz$ of nonzeroes in the matrix, and the output values
for \texttt{mingrp} and \texttt{maxgrp}. Note that on 19 of the problems \texttt{maxgrp} agrees with \texttt{mingrp} and therefore DSM is optimal on these problems. DSM may still be optimal on the other problems because \texttt{mingrp} is always set to the size of a clique in $G(A)$, and it is possible for the largest clique in $G(A)$ to be less than the number of groups in an optimal consistent partition of the columns of $A$. For example, if $A$ is a lower bidiagonal matrix of order $n$ with a non-zero in the $(1,n)$ position then the largest clique of $G(A)$ has size 2 but a consistent partition of the columns of $A$ needs at least 3 groups if $n$ is odd and $n \geq 3$.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$n$ & \texttt{nnz} & \texttt{mingrp} & \texttt{maxgrp} \\
\hline
59 & 267 & 6 & 6 \\
66 & 320 & 6 & 6 \\
72 & 222 & 5 & 5 \\
87 & 541 & 13 & 13 \\
162 & 1182 & 9 & 10 \\
193 & 3493 & 30 & 30 \\
198 & 1392 & 12 & 12 \\
209 & 1743 & 17 & 17 \\
221 & 1629 & 12 & 12 \\
234 & 834 & 10 & 10 \\
245 & 1461 & 13 & 13 \\
307 & 2523 & 9 & 11 \\
310 & 2448 & 11 & 11 \\
346 & 3226 & 19 & 20 \\
361 & 2953 & 9 & 10 \\
419 & 3563 & 14 & 15 \\
492 & 3156 & 11 & 11 \\
503 & 6027 & 25 & 25 \\
512 & 3502 & 15 & 16 \\
592 & 5104 & 15 & 15 \\
607 & 5131 & 14 & 16 \\
758 & 5994 & 11 & 11 \\
869 & 7285 & 15 & 15 \\
878 & 7448 & 10 & 11 \\
918 & 7384 & 13 & 14 \\
992 & 16744 & 18 & 18 \\
1005 & 8621 & 27 & 27 \\
1007 & 8575 & 10 & 11 \\
1242 & 10426 & 12 & 14 \\
2680 & 25026 & 19 & 19 \\
\hline
\end{tabular}
\caption{Output from DSM for Naval Problems.}
\end{table}

\textbf{Acknowledgment.} The codes described in this paper have benefited considerably from Burt Garbow's contribution; we are very grateful for his help.
8. References.


Matula, D. W. and Beck, L. L. [1981]. Smallest-last ordering and clustering and graph coloring algorithms, Report 8104, Department of Computer Science and Engineering, Southern Methodist University, Dallas, Texas.
This appendix contains the listings for the test program and for the package for estimating sparse Jacobian matrices. We first list the test program and then list DSM and (in alphabetical order) the subroutines called by DSM: DEGR, IDO, NUMSRT, SEQ, SETR, SLO, SRTDAT. The last subroutine listed is FDJS. Note that this is a single precision subroutine; to obtain a double precision version it is only necessary to replace the single precision declaration by a double precision declaration.
************
This is a test program for subroutines dsm and fdjs.
The test data represents a neutron kinetics problem.

************
integer i,info,ipl,iplu,jipl,jplu,jpu,k,l,liwa,*
    mazgrp, maxrow, mingroup, minrow, n, nnz, numgrp, nwrit
integer indcol(6000), indrow(6000), ipntr(1201), jpntr(1201), *
    ngrp(1200), liwa(7200)
logical bua(1200)
real dsm, errij, errmax, fjact, sum
real d(1200), fjac(6000), fjacd(1200), fvec(1200), x(1200), xd(1200)

Logical output unit is assumed to be number 6.

data nwrit /6/
liwa = 7200

Test for dsm and fdjs.

write (nwrit,1000)
do 150 n = 300, 1200, 300
    write (nwrit,2000)

Definition of sparsity pattern.

l = n/3
nnz = 0

    do 60 j = 1, n
      nnz = nnz + 1
      indrow(nnz) = j
      indcol(nnz) = j
      if (j .eq. l or. j .eq. 2*l or. j .eq. 3*l) go to 10
      nnz = nnz + 1
      indrow(nnz) = j + 1
      indcol(nnz) = j
      continue
10    if (j .eq. l + 1 or. j .eq. l+1 or. j .gt. 2*l) go to 20
      nnz = nnz + 1
      indrow(nnz) = j - 1
      indcol(nnz) = j
      continue
20    if (j .gt. 2*l) go to 30
      nnz = nnz + 1
      indrow(nnz) = j + l
      indcol(nnz) = j
      continue
30    if (j .le. l) go to 40
      nnz = nnz + 1
      indrow(nnz) = j - l
      indcol(nnz) = j
      continue
40
IF (J .GT. L) GO TO 50
NNZ = NNZ + 1
INDROW(NNZ) = J + 24
INDCOL(NNZ) = J
50 CONTINUE
60 CONTINUE

CALL DSM.

CALL DSM(N, N, NNZ, INDROW, INDCOL, NGRP, MAXGRP, MINGRP,
       INFO, IPNTR, JPNTR, IWA, TIWA, BWA)
IF (INFO .LE. 0) WRITE (NWRITE, 4000) INFO

STATISTICS FOR THE MATRIX.

MAXROW = 0
MINROW = N
DO 70 I = 1, N
   MAXROW = MAX0(MAXROW, IPNTR(I+1) - IPNTR(I))
   MINROW = MIN0(MINROW, IPNTR(I+1) - IPNTR(I))
70 CONTINUE
DNSM = FLOAT(100*NNZ)/FLOAT(N**2)
WRITE (NWRITE, 3000) N, NNZ, DNSM, MINROW, MAXROW, MAXGRP, MINGRP

TEST FOR FDJS.

DO 80 J = 1, N
   Z(J) = FLOAT(J)/FLOAT(N)
80 CONTINUE
CALL Fcn(N, Z, INDCOL, IPNTR, FVEC)

APPROXIMATE THE JACOBIAN MATRIX.

DO 110 NUMGRP = 1, MAXGRP
   DO 90 J = 1, N
      D(J) = 0.0
      IF (NGRP(J) .EQ. NUMGRP) D(J) = 0.001
      XD(J) = X(J) + D(J)
90 CONTINUE
CALL Fcn(N, XD, INDCOL, IPNTR, FJACD)
DO 100 I = 1, N
   FJACD(I) = FJACD(I) - Func(I)
100 CONTINUE
CALL FDJS(N, INDROW, JPNTR, NGRP, NUMGRP, D, FJACD, FJAC)
110 CONTINUE

TEST THE APPROXIMATION TO THE JACOBIAN.

ERRMAX = 0.0
DO 140 J = 1, N
   JPL = JPNTR(J)
   JPU = JPNTR(J+1) - 1
   DO 130 JP = JPL, JPU
      T = INDROW(JP)
130 CONTINUE
140 CONTINUE
sum = 0.0
ipl = indptr(i)
ipu = indptr(i+1) - 1
do 120 ip = ipl, ipu
   k = indcol(ip)
   sum = sum + x(k)
   continue
120
   sum = sum + x(i)
fjact = 1.0 + 2.0*sum
if (i .eq. j) fjact = 2.0*fjact
errij = fjact(jp) - fjact
if (fjact .gt. 0.0) errij = errij/fjact
errmax = amax1(errmax,errij)
130
   continue
140
   continue
write (6,5000) errmax
150
   continue
stop

Format statements.

1000 format(//' Tests for dsm and fdjs - Neutron Kinetics Problem' //
   ' Statistics generated '//
   '  n - number of columns '/
   '  nnz - number of non-zero elements '/
   '  dnsm - matrix density (percentage) '/
   '  minrow - minimum number of non-zeros in any row '/
   '  maxrow - maximum number of non-zeros in any row '/)
2000 format (// 3x, 'n', 6x, 'nnz', 5x, 'dnsm', 5x,
   ' minrow', 4x, 'maxrow', 4x, 'mingrp', 4x, 'maxgrp' //)
3000 format (2(i5,3x),f6.2, 4x, 4(i5, 5x))
4000 format (//' *** mistake in input data, info is ***',i6)
5000 format (//' largest relative error of approximation is ',e10.2)
end
subroutine fcn(n,x,indcol,ipntr,fvec)
integer n
integer indcol(1),ipntr(1)
real x(n),fvec(n)

Function subroutine for testing fdjs.

integer i,ip,ipl,ipu,k
real sum
do 20 i = 1, n
    sum = 0.0
    ipl = ipntr(i)
    ipu = ipntr(i+1) - 1
    do 10 ip = ipl, ipu
        k = indcol(ip)
        sum = sum + x(k)
    10 continue
    sum = sum + x(i)
    fvec(i) = sum*(1.0 + sum) + 1.0
20 continue
return

Last card of subroutine fcn.

end
**subroutine dsm**

> The purpose of dsm is to determine an optimal or near-optimal consistent partition of the columns of a sparse
> \( m \) by \( n \) matrix \( A \).

The sparsity pattern of the matrix \( A \) is specified by the arrays \( \text{indrow} \) and \( \text{indcol} \). On input the indices for the non-zero elements of \( A \) are

\[
\text{indrow}(k), \text{indcol}(k), \quad k = 1, 2, \ldots, \text{npairs}.
\]

The \((\text{indrow}, \text{indcol})\) pairs may be specified in any order. Duplicate input pairs are permitted, but the subroutine eliminates them.

The subroutine partitions the columns of \( A \) into groups such that columns in the same group do not have a non-zero in the same row position. A partition of the columns of \( A \) with this property is consistent with the direct determination of \( A \).

The subroutine statement is

**subroutine dsm**

where

- \( m \) is a positive integer input variable set to the number of rows of \( A \).
- \( n \) is a positive integer input variable set to the number of columns of \( A \).
- \( \text{npairs} \) is a positive integer input variable set to the number of \((\text{indrow}, \text{indcol})\) pairs used to describe the sparsity pattern of \( A \).
- \( \text{indrow} \) is an integer array of length \( \text{npairs} \). On input \( \text{indrow} \) must contain the row indices of the non-zero elements of \( A \). On output \( \text{indrow} \) is permuted so that the corresponding column indices are in non-decreasing order. The column indices can be recovered from the array \( \text{jptntr} \).
- \( \text{indcol} \) is an integer array of length \( \text{npairs} \). On input \( \text{indcol} \)
must contain the column indices of the non-zero elements of A. On output indcol is permuted so that the corresponding row indices are in non-decreasing order. The row indices can be recovered from the array ipntr.

ngrp is an integer output array of length n which specifies the partition of the columns of A. Column jcol belongs to group ngrp(jcol).

maxgrp is an integer output variable which specifies the number of groups in the partition of the columns of A.

mingrp is an integer output variable which specifies a lower bound for the number of groups in any consistent partition of the columns of A.

info is an integer output variable set as follows. For normal termination info = 1. If m, n, or npairs is not positive or liwa is less than max(m,6*n), then info = 0. If the k-th element of indrow is not an integer between 1 and m or the k-th element of indcol is not an integer between 1 and n, then info = -k.

ipntr is an integer output array of length m + 1 which specifies the locations of the column indices in indcol. The column indices for row i are

\[\text{indcol}(k), \ k = \text{ipntr}(i),...\text{ipntr}(i+1)-1.\]

Note that ipntr(m+1)-1 is then the number of non-zero elements of the matrix A.

jpntr is an integer output array of length n + 1 which specifies the locations of the row indices in indrow. The row indices for column j are

\[\text{indrow}(k), \ k = \text{jpntr}(j),...\text{jpntr}(j+1)-1.\]

Note that jpntr(n+1)-1 is then the number of non-zero elements of the matrix A.

iwa is an integer work array of length liwa.

tiwa is a positive integer input variable not less than max(m,6*n).

bwa is a logical work array of length n.

Subprograms called

MINPACK-supplied ... degr,ido,numrsrt,seq,setr,slo,srtdat

FORTRAN-supplied ... max0
Check the input data.

```fortran
info = 0
if (m .lt. 1 .or. n .lt. 1 .or. npairs .lt. 1 .or.
  * liwa .lt. max0(m,5*n)) go to 130
  do 10 k = 1, npairs
    info = -k
    if (indrow(k) .lt. 1 .or. indrow(k) .gt. m .or.
      * indcol(k) .lt. 1 .or. indcol(k) .gt. n) go to 130
  10 continue
  info = 1
```

Sort the data structure by columns.

```fortran
call srtdat(n,npairs,indrow,indcol,jpntr,iwa(1))
```

Compress the data and determine the number of non-zero elements of A.

```fortran
do 20 i = 1, m
  iwa(i) = 0
20 continue
nnz = 0
do 70 j = 1, n
  jpl = jpntr(j)
  jpu = jpntr(j+1) - 1
  jpntr(j) = nnz + 1
  if (jpu .lt. jpl) go to 60
  do 40 jp = jpl, jpu
    ir = indrow(jp)
    if (iwa(ir) .ne. 0) go to 30
    nnz = nnz + 1
    indrow(nnz) = ir
    iwa(ir) = 1
30 continue
40 continue
  jpl = jpntr(j)
  do 50 jp = jpl, nnz
    ir = indrow(jp)
    iwa(ir) = 0
50 continue
60 continue
70 continue
  jpntr(n+1) = nnz + 1
```

Extend the data structure to rows.

```fortran
call setr(m,n,indrow,jpn.tr,indcol,jpntr,iwa(1))
```
Determine a lower bound for the number of groups.

\[
\text{mingrp} = 0 \\
do 80 \text{i} = 1, m \\
\quad \text{mingrp} = \max(\text{mingrp}, \text{ipntr(i+1)-ipntr(i)}) \\
80 \text{continue}
\]

Determine the degree sequence for the intersection graph of the columns of A.

call degr(n, indrow, jpntr, indcol, ipntr, iwa(5*n+1), iwa(n+1), bwa)

Color the intersection graph of the columns of A with the smallest-last (SL) ordering.

call slo(n, indrow, jpntr, indcol, ipntr, iwa(5*n+1), iwa(n+1), iwa(3*n+1), bwa)
call seq(n, indrow, jpntr, indcol, ipntr, iwa(4*n+1), ngrp, maxgrp, 
* iwa(n+1), bwa)
\text{mingrp} = \max(\text{mingrp}, \text{maxclq})
\text{if (maxgrp .eq. mingrp) go to 130}

Color the intersection graph of the columns of A with the incidence-degree (ID) ordering.

call ido(m, n, indrow, jpntr, indcol, ipntr, iwa(5*n+1), iwa(n+1), 
* maxclq, iwa(1), iwa(n+1), iwa(3*n+1), bwa)
call seq(n, indrow, jpntr, indcol, ipntr, iwa(4*n+1), iwa(1), ngrp, maxgrp, 
* iwa(n+1), bwa)
\text{mingrp} = \max(\text{mingrp}, \text{maxclq})
\text{if (numgrp .ge. maxgrp) go to 100}
\text{maxgrp} = \text{numgrp}
do 90 \text{j} = 1, n \\
\quad \text{ngrp(j)} = \text{iwa(j)}
90 \text{continue}
\text{if (maxgrp .eq. mingrp) go to 130}
100 \text{continue}

Color the intersection graph of the columns of A with the largest-first (LF) ordering.

call numsrt(n, n-1, iwa(5*n+1), -1, iwa(4*n+1), iwa(2*n+1), iwa(n+1))
call seq(n, indrow, jpntr, indcol, ipntr, iwa(4*n+1), iwa(1), ngrp, 
* iwa(n+1), bwa)
\text{if (numgrp .ge. maxgrp) go to 120}
\text{maxgrp} = \text{numgrp}
do 110 \text{j} = 1, n \\
\quad \text{ngrp(j)} = \text{iwa(j)}
110 \text{continue}
120 \text{continue}

Exit from program.
130 continue
   return

* Last card of subroutine dsm.

* end
subroutine degr(n,indrow,jpntr,indcol,ipntr,ndeg,iwa,bwa)
  integer n
  integer indrow(1),jpntr(1),indcol(1),ipntr(1),ndeg(n),iwa(n)
  logical bwa(n)
*********

subroutine degr

Given the sparsity pattern of an m by n matrix A, this subroutine determines
the degree sequence for the intersection graph of the columns of A.

In graph-theory terminology, the intersection graph of the columns
of A is the loopless graph G with vertices a(j), j = 1, 2,..., n, where a(j)
is the j-th column of A and with edge (a(i),a(j)) if and only if columns i and j
have a non-zero in the same row position.

Note that the value of m is not needed by degr and is therefore not present
in the subroutine statement.

The subroutine statement is

  subroutine degr(n,indrow,jpntr,indcol,ipntr,ndeg,iwa,bwa)

where

  n is a positive integer input variable set to the number of columns of A.

  indrow is an integer input array which contains the row indices for the
  non-zeroes in the matrix A.

  jpntr is an integer input array of length n + 1 which specifies the
  locations of the row indices in indrow.

    indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

    Note that jpntr(n+1)-1 is then the number of non-zero elements of the
    matrix A.

  indcol is an integer input array which contains the column indices
  for the non-zeroes in the matrix A.

  ipntr is an integer input array of length m + 1 which specifies
  the locations of the column indices in indcol.

    indcol(k), k = ipntr(i),...,ipntr(i+1)-1.

    Note that ipntr(m+1)-1 is then the number of non-zero elements of the
    matrix A.
ndege is an integer output array of length n which
specifies the degree sequence. The degree of the
j-th column of A is ndeg(j).

iwa is an integer work array of length n.

bwa is a logical work array of length n.

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**********
integer deg,ic,ip,ipl,ipu,ir,jcol,jp,jpl,jpu

Initialization block.

do 10 jpl = 1, n
    ndeg(jp) = 0
    bwa(jp) = .false.
10 continue

Compute the degree sequence by determining the contributions
to the degrees from the current(jcol) column and further
columns which have not yet been considered.

if (n .lt. 2) go to 90
do 80 jcol = 2, n
    bwa(jcol) = .true.
    deg = 0
80 continue

Determine all positions (ir,jcol) which correspond
to non-zeroes in the matrix.

jpl = jpntr(jcol)
jpu = jpntr(jcol+1) - 1
if (jpu .lt. jpl) go to 50
do 40 jp = jpl, jpu
    ir = indrow(jp)
40 continue

For each row ir, determine all positions (ir,ic)
which correspond to non-zeroes in the matrix.

ipl = ipntr(ir)
ipu = ipntr(ir+1) - 1
do 30 ip = ipl, ipu
    ic = indcol(ip)
30 continue

Array bwa marks columns which have contributed to
the degree count of column jcol. Update the degree
counts of these columns. Array iwa records the
marked columns.

if (bwa(ic)) go to 20
bwa(ic) = .true.
\[ ndeg(ic) = ndeg(ic) + 1 \]
\[ \text{deg} = \text{deg} + 1 \]
\[ \text{iwa}(\text{deg}) = ic \]
20     continue
30     continue
40     continue
50     continue

Un-mark the columns recorded by \text{iwa} and finalize the degree count of column \text{jcol.}

if (\text{deg} .lt. 1) go to 70
do 60 \text{jp} = 1, \text{deg}
   ic = \text{iwa}(\text{jp})
   \text{bwa}(ic) = .false.
60     continue
   \text{ndeg(jcol)} = \text{ndeg(jcol)} + \text{deg}
70     continue
80     continue
90 continue
return

Last card of subroutine degr.

end
subroutine ido(m,n,indrow,jpntr,jpnptr,indcol,ipntr,ndeg,list,
  + maxclq,twa1,twa2,twa3,twa4,bwa)
  
  integer m,n,maxclq
  integer indrow(1),jpntr(1),indcol(1),ipntr(1),ndeg(n),list(n),
  *  twa1(n),twa2(n),twa3(n),twa4(n)
  logical bwa(n)

C***********
C
C subroutine ido
C
given the sparsity pattern of an m by n matrix A, this
C subroutine determines an incidence-degree ordering of the
C columns of A.
C
The incidence-degree ordering is defined for the loopless
C graph G with vertices a(j), j = 1,2,...,n where a(j) is the
C j-th column of A and with edge (a(i),a(j)) if and only if
C columns i and j have a non-zero in the same row position.
C
At each stage of ido, a column of maximal incidence is
C chosen and ordered. If jcol is an un-ordered column, then
C the incidence of jcol is the number of ordered columns
C adjacent to jcol in the graph G. Among all the columns of
C maximal incidence, ido chooses a column of maximal degree.
C
The subroutine statement is
C
  subroutine ido(m,n,indrow,jpntr,jpnptr,indcol,ipntr,ndeg,list,
  + maxclq,twa1,twa2,twa3,twa4,bwa)

where

  m is a positive integer input variable set to the number
  of rows of A.

  n is a positive integer input variable set to the number
  of columns of A.

  indrow is an integer input array which contains the row
  indices for the non-zeroes in the matrix A.

  jpntr is an integer input array of length n + 1 which
  specifies the locations of the row indices in indrow.
  The row indices for column j are
  indrow(k), k = jpntr(j)....jpntr(j+1)-1.

  Note that jpntr(n+1)-1 is then the number of non-zero
  elements of the matrix A.

  indcol is an integer input array which contains the
  column indices for the non-zeroes in the matrix A.

  ipntr is an integer input array of length m + 1 which
  specifies the locations of the column indices in indcol.
specifies the locations of the column indices in indcol.
The column indices for row i are

\[ \text{indcol}(k), k = \text{ipntr}(i), \ldots, \text{ipntr}(i+1)-1. \]

Note that \( \text{ipntr}(m+1)-1 \) is then the number of non-zero
elements of the matrix \( A \).

ndeg is an integer input array of length \( n \) which specifies
the degree sequence. The degree of the \( j \)-th column
of \( A \) is \( \text{ndeg}(j) \).

tlist is an integer output array of length \( n \) which specifies
the incidence-degree ordering of the columns of \( A \). The \( j \)-th
column in this order is \( \text{list}(j) \).

mazcLq is an integer output variable set to the size
of the largest clique found during the ordering.

iwa1,iwa2,iwa3, and iwa4 are integer work arrays of length \( n \).

bwa is a logical work array of length \( n \).

Subprograms called

MINPACK-supplied ... numsrt

FORTRAN-supplied ... maxO

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Sort the degree sequence.

call numsrt(n,n-1,ndeg,-1,iwa1,iwa4,iwa3)

Initialization block.

Create a doubly-linked list to access the incidences of the
columns. The pointers for the linked list are as follows.

Each un-ordered column \( jcol \) is in a list (the incidence list)
of columns with the same incidence.

\( \text{iwa1}(\text{numinc}+1) \) is the first column in the \text{numinc} list
unless \( \text{iwa1}(\text{numinc}+1) = 0 \). In this case there are
no columns in the \text{numinc} list.

\( \text{iwa2}(\text{jcol}) \) is the column before \( jcol \) in the incidence list
unless \( \text{iwa2}(\text{jcol}) = 0 \). In this case \( jcol \) is the first
column in this incidence list.

iwa3(jcol) is the column after jcol in the incidence list unless iwa3(jcol) = 0. In this case jcol is the last column in this incidence list.

If jcol is an un-ordered column, then list(jcol) is the incidence of jcol in the graph. If jcol is an ordered column, then list(jcol) is the incidence-degree order of column jcol.

maxinc = 0
do 10 jp = 1, n
    list(jp) = 0
    bwa(jp) = .false.
    iwa1(jp) = 0
    l = iwa4(jp)
    if (jp.ne. 1) iwa2(l) = iwa4(jp-1)
    if (jp.ne. n) iwa3(l) = iwa4(jp+1)
10  continue
iwa1(1) = iwa4(1)
l = iwa4(1)
iwa2(1) = 0
l = iwa4(n)
iwa3(l) = 0

Determine the maximal search length for the list of columns of maximal incidence.

maxist = 0
do 20 ir = 1, m
    maxist = maxist + (ipntr(ir+1) - ipntr(ir))**2
20  continue
maxist = maxist/n
maxclq = 1

Beginning of iteration loop.

do 140 numord = 1, n

Choose a column jcol of maximal degree among the columns of maximal incidence.

jp = iwa1(maxinc+1)
numlst = 1
numwgt = -1
30  continue
    if (ndeg(jp) .le. numwgt) go to 40
    numwgt = ndeg(jp)
    jcol = jp
40  continue
jp = iwa3(jp)
numlst = numlst + 1
if (jp.gt. 0 .and. numlst .le. maxlst) go to 30
list(jcol) = numord
Delete column jcol from the list of columns of maximal incidence.

\[
l = iwa2(jcol)
\]

if \(l \leq 0\) \(iwa1(\text{maxinc}+1) = iwa3(jcol)\)
if \(l > 0\) \(iwa3(l) = iwa3(jcol)\)
\(l = iwa3(jcol)\)
if \(l > 0\) \(iwa2(l) = iwa2(jcol)\)

Update the size of the largest clique found during the ordering.

\[
\text{if (mazinc = 0)} \ ncomp = 0
\text{ncomp = ncomp + 1}
\text{if (mazinc + 1 \geq ncomp)} \ \text{maxclq} = \text{max0}(\text{maxclq}, \text{ncomp})
\]

Update the maximal incidence count.

50 continue
\[
\text{if (iwa1(\text{maxinc}+1) > 0)} \ \text{go to 60}
\]
\[
\text{mazinc} = \text{mazinc} - 1
\text{if (mazinc \leq 0)} \ \text{go to 50}
\]
60 continue

Find all columns adjacent to column jcol.
\[
bwa(jcol) = \text{true}.
\]
\[
deg = 0
\]

Determine all positions (ir,jcol) which correspond to non-zeroes in the matrix.
\[
jpl = \text{jpntr}(jcol)
\]
\[
jpu = \text{jpntr}(jcol+1) - 1
\text{if (jpu < jpl) go to 100}
\text{do 90 ip = jpl, jpu}
\]
\[
\text{itr} = \text{indrow}(ip)
\]

For each row ir, determine all positions (ir,ic) which correspond to non-zeroes in the matrix.
\[
\text{ipl = ipntr(ir)}
\]
\[
\text{ipu = ipntr(ir+1) - 1}
\text{do 80 ip = ipl, ipu}
\]
\[
\text{ic = indcol(ip)}
\]

Array bwa marks columns which are adjacent to column jcol. Array iwa4 records the marked columns.
\[
\text{if (bwa(ic)) go to 70}
\]
\[
bwa(ic) = \text{true}.
\]
\[
deg = deg + 1
\]
\[
iwa4(deg) = ic
\]
Update the pointers to the incidence lists.

if (deg .lt. 1) go to 130
    do 120 jp = 1, deg
        ic = iwa4(jp)
        if (list(ic) .gt. 0) go to 110
        numinc = -list(ic) + 1
        list(ic) = -numinc
        maxinc = max0(maxinc,numinc)
    
    Delete column ic from the numinc-1 list.
    
    l = iwa2(ic)
    if (l .eq. 0) iwa1(numinc) = iwa3(ic)
    if (l .gt. 0) iwa3(l) = iwa3(ic)
    l = iwa3(ic)
    if (l .gt. 0) iwa2(l) = iwa2(ic)
    
    Add column ic to the numinc list.
    
    head = iwa1(numinc+1)
    iwa1(numinc+1) = ic
    iwa2(ic) = 0
    iwa3(ic) = head
    if (head .gt. 0) iwa2(head) = ic
    continue
    
Un-mark column ic in the array bwa.
    
    bwa(ic) = .false.
    continue
    
End of iteration loop.
    
Invert the array list.
    
    do 150 jcol = 1, n
        numord = list(jcol)
        iwa1(numord) = jcol
    continue
    
    do 160 jp = 1, n
        list(jp) = iwa1(jp)
    continue
    
return
Last card of subroutine ido.
end
subroutine nurnsrt (nnmax, num, mode, index, last, next)
integer n, nnmax, mode
integer num(n), index(n), last(1), next(n)

************

subroutine nurnsrt

Given a sequence of integers, this subroutine groups
together those indices with the same sequence value
and, optionally, sorts the sequence into either
ascending or descending order.

The sequence of integers is defined by the array num,
and it is assumed that the integers are each from the set
0,1,...,nnmax. On output the indices k such that num(k) = l
for any l = 0,1,...,nnmax can be obtained from the arrays
last and next as follows.

\[ k = \text{last}(l+1) \]
\[ \text{while (} k \neq 0 \text{) } k = \text{next}(k) \]

Optionally, the subroutine produces an array index so that
the sequence num(index(i)), i = 1,2,...,n is sorted.

The subroutine statement is

subroutine nurnsrt (nnmax, num, mode, index, last, next)

where

n is a positive integer input variable.

nnmax is a positive integer input variable.

num is an input array of length n which contains the
sequence of integers to be grouped and sorted. It
is assumed that the integers are each from the set
0,1,...,nnmax.

mode is an integer input variable. The sequence num is
sorted in ascending order if mode is positive and in
descending order if mode is negative. If mode is 0,
no sorting is done.

index is an integer output array of length n set so
that the sequence

num(index(i)), i = 1,2,...,n

is sorted according to the setting of mode. If mode
is 0, index is not referenced.

last is an integer output array of length nnmax + 1. The
index of num for the last occurrence of l is last(l+1)
for any \( l = 0, 1, \ldots, \text{nnmax} \) unless \( \text{last}(l+1) = 0 \). In this case \( l \) does not appear in \( \text{num} \).

next is an integer output array of length \( n \). If \( \text{num}(k) = l \), then the index of \( \text{num} \) for the previous occurrence of \( l \) is \( \text{next}(k) \) for any \( l = 0, 1, \ldots, \text{nnmax} \) unless \( \text{next}(k) = 0 \). In this case there is no previous occurrence of \( l \) in \( \text{num} \).

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***********

integer \( i, j, jp, k, l, \text{nnzxp1}, \text{nnzxp2} \)

Determine the arrays next and last.

\[
\text{nnzxp1} = \text{nnmax} + 1 \\
do \text{10} \quad i = 1, \text{nnzxp1} \\
\text{last}(i) = 0 \\
\text{10} \quad \text{continue}
\]

\[
do \text{20} \quad k = 1, n \\
i = \text{num}(k) \\
\text{next}(k) = \text{last}(l+1) \\
\text{last}(l+1) = k \\
\text{20} \quad \text{continue}
\]

if \( \text{mode} \cdot \text{eq} \cdot 0 \) go to 60

Store the pointers to the sorted array in index.

\[
i = 1 \\
\text{nnzxp2} = \text{nnzxp1} + 1 \\
do \text{50} \quad j = 1, \text{nnzxp1} \\
\text{fp} = j \\
\text{if} \ (\text{mode} \cdot \text{lt} \cdot 0) \ 	ext{fp} = \text{nnzxp2} \cdot j \\
k = \text{last}(\text{fp}) \\
\text{30} \quad \text{continue}
\]

\[
\text{if} \ (k \cdot \text{eq} \cdot 0) \ 	ext{go to 40} \\
\text{index}(k) = k \\
i = i + 1 \\
k = \text{next}(k) \\
\text{go to 30}
\]

\[
\text{40} \quad \text{continue}
\]

\[
\text{50} \quad \text{continue}
\]

\[
\text{60} \quad \text{continue}
\]

return

Last card of subroutine \text{nmsrt}.

end
subroutine seq(n,indrow,jpntr,indcol,ipntr,list,ngrp,mazgrp, iwa,bwa)
  * integer n,mazgrp
  integer indrow(1),jpntr(1),indcol(1),ipntr(1),list(n),ngrp(n).
  * iwa(n)
  logical bwa(n)

*********

subroutine seq

Given the sparsity pattern of an m by n matrix A, this subroutine determines a consistent partition of the columns of A by a sequential algorithm.

A consistent partition is defined in terms of the loopless graph G with vertices a(j), j = 1,2,...,n where a(j) is the j-th column of A and with edge (a(i),a(j)) if and only if columns i and j have a non-zero in the same row position.

A partition of the columns of A into groups is consistent if the columns in any group are not adjacent in the graph G. In graph-theory terminology, a consistent partition of the columns of A corresponds to a coloring of the graph G.

The subroutine examines the columns in the order specified by the array list, and assigns the current column to the group with the smallest possible number.

Note that the value of m is not needed by seq and is therefore not present in the subroutine statement.

The subroutine statement is

subroutine seq(n,indrow,jpntr,indcol,ipntr,list,ngrp,mazgrp, iwa,bwa)

where

n is a positive integer input variable set to the number of columns of A.

indrow is an integer input array which contains the row indices for the non-zeroes in the matrix A.

jpntr is an integer input array of length n + 1 which specifies the locations of the row indices in indrow.

The row indices for column j are

indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

Note that jpntr(n+1)-1 is then the number of non-zero elements of the matrix A.

indcol is an integer input array which contains the
Column indices for the non-zeroes in the matrix A.

`ipntr` is an integer input array of length `n + 1` which specifies the locations of the column indices in `idxcol`. The column indices for row `i` are

\[ \text{idxcol}(k), \ k = \text{ipntr}(i), \ldots, \text{ipntr}(i+1)-1. \]

Note that `ipntr(m+1)` is then the number of non-zero elements of the matrix `A`.

`list` is an integer input array of length `n` which specifies the order to be used by the sequential algorithm. The `j`-th column in this order is `list(j)`.

`ngrp` is an integer output array of length `n` which specifies the partition of the columns of `A`. Column `jcol` belongs to group `ngrp[jcol]`.

`maxgrp` is an integer output variable which specifies the number of groups in the partition of the columns of `A`.

`iwa` is an integer work array of length `n`.

`bwa` is a logical work array of length `n`.

---

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*****

```fortran
integer deg,ic,ip,ipl,ipuir,jJcol,jp,jpl,jpu,I,numgrp
```

Initialization block.

```
maxgrp = 0
do 10 fp = 1, n
    ngrp(fp) = n.
    bwa(fp) = .false.
 10 continue
bwa(n) = .true.
```

Beginning of iteration loop.

```
do 100 j = 1, n
    jcol = list(j)
```

Find all columns adjacent to column `jcol`.

```
deg = 0
```

Determine all positions in `jcol` which correspond to non-zeroes in the matrix.

```
jpl = jpntr(jcol)
```
\[ jpu = jpntr(jcol+1) - 1 \]

If \( jpu \leq jpl \) go to 50

\[ \text{do 40 } jp = jpl, jpu \]

\[ \text{ir} = \text{indrow}(jp) \]

For each row \( \text{ir} \), determine all positions \( \text{ir,ic} \) which correspond to non-zeroes in the matrix.

\[ \text{ipl} = jpntr(ir) \]

\[ \text{ipu} = jpntr(ir+1) - 1 \]

\[ \text{do 30 } ip = ipl, ipu \]

\[ \text{ic} = \text{indcol}(ip) \]

\[ l = \text{ngrp}(ic) \]

Array \( bwa \) marks the group numbers of the columns which are adjacent to column \( jcol \).

Array \( iwa \) records the marked group numbers.

\[ \text{if (bwa(l)) go to 20} \]

\[ \text{bwa(l)} = \text{.true.} \]

\[ \text{deg} = \text{deg} + 1 \]

\[ \text{iwa(deg)} = l \]

20 continue

30 continue

40 continue

50 continue

Assign the smallest un-marked group number to \( jcol \).

\[ \text{do 60 } jp = 1, n \]

\[ \text{numgrp} = jp \]

\[ \text{if (not. bwa(jp)) go to 70} \]

60 continue

70 continue

\[ \text{ngrp}(jcol) = \text{numgrp} \]

\[ \text{maxgrp} = \text{max0(maxgrp,numgrp)} \]

Un-mark the group numbers.

\[ \text{if (deg .lt. 1) go to 90} \]

\[ \text{do 80 } jp = 1, \text{deg} \]

\[ l = \text{iwa(jp)} \]

\[ \text{bwa(l)} = \text{.false.} \]

80 continue

90 continue

100 continue

End of iteration loop.

return

Last card of subroutine seq.

end
subroutine setr(m,n,indrow,jpntr,indcol,ipntr,iwa)
integer m,n
integer indrow(1),jpntr(1),indcol(1),ipntr(1),iwa(m)
*********

subroutine setr

Given a column-oriented definition of the sparsity pattern
of an m by n matrix A, this subroutine determines a
row-oriented definition of the sparsity pattern of A.

On input the column-oriented definition is specified by
the arrays indrow and jpntr. On output the row-oriented
definition is specified by the arrays indcol and ipntr.

The subroutine statement is

subroutine setr(m,n,indrow,jpntr,indcol,ipntr,iwa)

where

m is a positive integer input variable set to the number
of rows of A.

n is a positive integer input variable set to the number
of columns of A.

indrow is an integer input array which contains the row
indices for the non-zeroes in the matrix A.

jpntr is an integer input array of length n + 1 which
specifies the locations of the row indices in indrow.
The row indices for column j are

indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

Note that jpntr(n+1)-1 is then the number of non-zero
elements of the matrix A.

indcol is an integer output array which contains the
column indices for the non-zeroes in the matrix A.

ipntr is an integer output array of length m + 1 which
specifies the locations of the column indices in indcol.
The column indices for row i are

indcol(k), k = ipntr(i),...,ipntr(i+1)-1.

Note that ipntr(1) is set to 1 and that ipntr(m+1)-1 is
then the number of non-zero elements of the matrix A.

iwa is an integer work array of length m.

Determine the number of non-zeroes in the rows.

\[
\text{do } 10 \text{ ir } = 1, m \\
\quad \text{iwa(ir)} = 0 \\
10 \text{ continue} \\
\text{nnz } = \text{jpntr}(n+1) - 1 \\
\text{do } 20 \text{ jp } = 1, \text{nnz} \\
\quad \text{ir} = \text{indrow(jp)} \\
\quad \text{iwa(ir)} = \text{iwa(ir)} + 1 \\
20 \text{ continue} \\
\]

Set pointers to the start of the rows in indcol.

\[
\text{ipntr}(1) = 1 \\
\text{do } 30 \text{ ir } = 1, m \\
\quad \text{ipntr(ir+1)} = \text{ipntr(ir)} + \text{iwa(ir)} \\
\quad \text{iwa(ir)} = \text{ipntr(ir)} \\
30 \text{ continue} \\
\]

Fill indcol.

\[
\text{do } 60 \text{jcol } = 1, n \\
\quad \text{jpl } = \text{jpntr(jcol)} \\
\quad \text{jpu } = \text{jpntr(jcol+1)} - 1 \\
\quad \text{if (jpu .lt. jpl)} \text{ go to } 50 \\
\quad \text{do } 40 \text{ jp } = \text{jpl}, \text{jpu} \\
\quad \quad \text{ir} = \text{indrow(jp)} \\
\quad \quad \text{l } = \text{iwa(ir)} \\
\quad \quad \text{indcol(l)} = \text{jcol} \\
\quad \quad \text{iwa(ir)} = \text{iwa(ir)} + 1 \\
40 \text{ continue} \\
50 \text{ continue} \\
60 \text{ continue} \\
\text{return} \\
\]

Last card of subroutine setr.
subroutine slo(n,indrow,jpntr,indcol,ipntr,ndeg,list,
  * maxclq,iwa1,iwa2,iwa3,iwa4,bwa)
integer n,maxclq
integer indrow(1),jpntr(1),indcol(1),ipntr(1),ndeg(n),
  * list(n),iwa1(n),iwa2(n),iwa3(n),iwa4(n)
logical bwa(n)
*************

subroutine slo

Given the sparsity pattern of an m by n matrix A, this subroutine determines the smallest-last ordering of the columns of A.

The smallest-last ordering is defined for the loopless graph G with vertices a(j), j = 1,2,...,n where a(j) is the j-th column of A and with edge (a(i),a(j)) if and only if columns i and j have a non-zero in the same row position.

The smallest-last ordering is determined recursively by letting list(k), k = n,...,1 be a column with least degree in the subgraph spanned by the un-ordered columns.

Note that the value of m is not needed by slo and is therefore not present in the subroutine statement.

The subroutine statement is

subroutine slo(n,indrow,jpntr,indcol,ipntr,ndeg,list,
  maxclq,iwa1,iwa2,iwa3,iwa4,bwa)

where

n is a positive integer input variable set to the number of columns of A.

indrow is an integer input array which contains the row indices for the non-zeroes in the matrix A.

jpntr is an integer input array of length n + 1 which specifies the locations of the row indices in indrow. The row indices for column j are

indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

Note that jpntr(n+1)-1 is then the number of non-zero elements of the matrix A.

indcol is an integer input array which contains the column indices for the non-zeroes in the matrix A.

ipntr is an integer input array of length m + 1 which specifies the locations of the column indices in indcol. The column indices for row i are
\textit{indcol}(k), k = \textit{ipntr}(i), \ldots, \textit{ipntr}(i+1)-1.

Note that \textit{ipntr}(m+1)-1 is then the number of non-zero elements of the matrix \( A \).

\textit{ndeg} is an integer input array of length \( n \) which specifies the degree sequence. The degree of the \( j \)-th column of \( A \) is \( \textit{ndeg}(j) \).

\textit{list} is an integer output array of length \( n \) which specifies the smallest-last ordering of the columns of \( A \). The \( j \)-th column in this order is \( \text{list}(j) \).

\textit{maxclq} is an integer output variable set to the size of the largest clique found during the ordering.

\textit{iwa1}, \textit{iwa2}, \textit{iwa3}, and \textit{iwa4} are integer work arrays of length \( n \).

\textit{bwa} is a logical work array of length \( n \).

\textbf{Subprograms called}

\textit{FORTRAN-supplied} ... \textit{minO}

\textit{Argonne National Laboratory, MINPACK Project, June 1982.}
\textit{Thomas F. Coleman, Burton S. Garbow, Jorge J. More}

*********
\textit{integer} \textit{deghead,icipiplipu,irjcol,jpjpljpu},
\textit{*}
\textit{l,mindeg,numdeg,numord}

\textbf{Initialization block.}

\textit{mindeg} = \( n \)
\textbf{do} 10 \textit{jp} = 1, \( n \)
\textit{iwa1}(\textit{jp}) = 0
\textit{bwa}(\textit{jp}) = .false.
\textit{list}(\textit{jp}) = \textit{ndeg}(\textit{jp})
\textit{mindeg} = minO(\textit{mindeg},\textit{ndeg}(\textit{jp}))
\textbf{10} \textbf{continue}

Create a doubly-linked list to access the degrees of the columns. The pointers for the linked list are as follows.

Each un-ordered column \( jcol \) is in a list (the degree list) of columns with the same degree.

\textit{iwa1}(\textit{numdeg}+1) is the first column in the \textit{numdeg} list unless \textit{iwa1}(\textit{numdeg}+1) = 0. In this case there are no columns in the \textit{numdeg} list.

\textit{iwa2}(\textit{jcol}) is the column before \( jcol \) in the degree list unless \textit{iwa2}(\textit{jcol}) = 0. In this case \( jcol \) is the first
column in this degree list.

tiwa3(jcol) is the column after jcol in the degree list
unless tiwa3(jcol) = 0. In this case jcol is the last
column in this degree list.

If jcol is an un-ordered column, then list(jcol) is the
degree of jcol in the graph induced by the un-ordered
columns. If jcol is an ordered column, then list(jcol)
is the smallest-last order of column jcol.

do 20 jp = 1, n
  numdeg = ndeg(jp)
  head = iwa1(numdeg+1)
  iwa1(numdeg+1) = jp
  iwa2(jp) = 0
  iwa3(jp) = head
  if (head .gt. 0) iwa2(head) = jp
20  continue
maxclq = 0
numord = n

Beginning of iteration loop.

30 continue

Mark the size of the largest clique
found during the ordering.

if (mindeg + 1 .eq. numord and maxclq .eq. 0)
  maxclq = numord

Choose a column jcol of minimal degree mindeg.

40 continue
  jcol = iwa1(mindeg+1)
  if (jcol .gt. 0) go to 50
  mindeg = mindeg + 1
  go to 40
50  continue
list(jcol) = numord
numord = numord - 1

Termination test.

if (numord .eq. 0) go to 120

Delete column jcol from the mindeg list.

l = iwa3(jcol)
iwa1(mindeg+1) = l
if (l .gt. 0) iwa2(l) = 0

Find all columns adjacent to column jcol.
bwa(jcol) = .true.

deg = 0

Determine all positions (ir,jcol) which correspond to non-zeroes in the matrix.

jpl = jpmtr(jcol)
jpu = jpmtr(jcol+1) - 1
if (jpu .lt. jpl) go to 90
do 80 jp = jpl, jpu
   tr = indrow(jp)

For each row ir, determine all positions (ir,ic) which correspond to non-zeroes in the matrix.

tpl = ipntr(ir)
tpu = ipntr(ir+1) - 1
do 70 ip = ipl, ipu
   ic = indcol(ip)

Array bwa marks columns which are adjacent to column jcol. Array iwa4 records the marked columns.

if (bwa(ic)) go to 60
   bwa(ic) = .true.
deg = deg + 1
   iwa4(deg) = ic
60 continue
70 continue
80 continue
90 continue

Update the pointers to the current degree lists.

if (deg .lt. 1) go to 110
do 100 jp = 1, deg
   ic = iwa4(jp)
   numdeg = list(ic)
   list(ic) = list(ic) - 1
   mindeg = min0(mindeg, list(ic))

Delete column ic from the numdeg list.

l = iwa2(ic)
if (l .eq. 0) iwa1(numdeg+1) = iwa3(ic)
if (l .gt. 0) iwa3(l) = iwa3(ic)
l = iwa3(ic)
if (l .gt. 0) iwa2(l) = iwa2(ic)

Add column ic to the numdeg-1 list.

head = iwa1(numdeg)
twa1(numdeg) = ic
iwa2(ic) = 0
iwa3(ic) = head
if (head gt. 0) iwa2(head) = ic

c Un-mark column ic in the array bwa.
c
bwa(ic) = .false.
100 continue
110 continue
c End of iteration loop.
c
go to 30
120 continue
c Invert the array list.
c
do 130 jcol = 1, n
   numord = list(jcol)
   iwa1(numord) = jcol
130 continue
do 140 jp = 1, n
   list(jp) = iwa1(jp)
140 continue
return
c Last card of subroutine slo.
c
c end
**subroutine srtdat**

```fortran
integer n,nnz
integer indrow(nnz),indcol(nnz),jpntr(1),iwa(n)
```

Given the non-zero elements of an m by n matrix A in arbitrary order as specified by their row and column indices, this subroutine permutes these elements so that their column indices are in non-decreasing order.

**On input** it is assumed that the elements are specified in

indrow(k),indcol(k), k = 1,...,nnz.

**On output** the elements are permuted so that indcol is in non-decreasing order. In addition, the array jpntr is set so that the row indices for column j are

indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

Note that the value of m is not needed by srtdat and is therefore not present in the subroutine statement.

The subroutine statement is

```fortran
subroutine srtdat(n,nnz,indrow,indcol,jpntr,iwa)
```

where

- **n** is a positive integer input variable set to the number of columns of A.
- **nnz** is a positive integer input variable set to the number of non-zero elements of A.
- **indrow** is an integer array of length nnz. On input indrow must contain the row indices of the non-zero elements of A. On output indrow is permuted so that the corresponding column indices of indcol are in non-decreasing order.
- **indcol** is an integer array of length nnz. On input indcol must contain the column indices of the non-zero elements of A. On output indcol is permuted so that these indices are in non-decreasing order.
- **jpntr** is an integer output array of length n + 1 which specifies the locations of the row indices in the output indrow. The row indices for column j are

indrow(k), k = jpntr(j),...,jpntr(j+1)-1.

Note that jpntr(1) is set to 1 and that jpntr(n+1)-1
is then \(nnz\).

\(iwa\) is an integer work array of length \(n\).

**Subprograms called**

FORTRAN-supplied ... \(\text{max0}\)

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*********

integer \(i,j,k,l\)

Determine the number of non-zeros in the columns.

\[
do \ 10 \ j = 1, \ n  
\quad iwa(j) = 0  
10 \ continue  
\]

\[
do \ 20 \ k = 1, \ nnz  
\quad j = \text{indcol}(k)  
\quad iwa(j) = iwa(j) + 1  
20 \ continue  
\]

Set pointers to the start of the columns in \(\text{indrow}\).

\[
jpntr(1) = 1  
\]

\[
do \ 30 \ j = 1, \ n  
\quad jpntr(j+1) = jpntr(j) + iwa(j)  
\quad iwa(j) = jpntr(j)  
30 \ continue  
\]

\(k = 1\)

Begin in-place sort.

\[
40 \ continue  
\quad j = \text{indcol}(k)  
\quad \text{if} \ (k \ \text{lt.} \ jpntr(j) \ \text{or.} \ k \ \text{ge.} \ jpntr(j+1)) \ \text{go to 50}  
\]

Current element is in position. Now examine the next element or the first un-sorted element in the \(j\)-th group.

\[
k = \text{max0}(k+1,iwa(j))  
\quad \text{go to 60}  
50 \ continue  
\]

Current element is not in position. Place element in position and make the displaced element the current element.

\[
l = iwa(j)  
\quad iwa(j) = iwa(j) + 1  
\quad i = \text{indrow}(k)  
\]
indrow(k) = indrow(l)
indcol(k) = indcol(l)
indrow(l) = i
indcol(l) = j

continue
   if (k .le. nnz) go to 40
   return

Last card of subroutine srtdat.

end
subroutine fdjs(n,indrow,jpntr,ngrp,numgrp,d,fjacd,fjac)
   integer n,numgrp
   integer indrow(1),jpntr(1),ngrp(n)
   real d(n),fjacd(1),fjac(1)
**********

subroutine fdjs

Given a consistent partition of the columns of an m by n Jacobian matrix into groups, this subroutine computes approximations to those columns in a given group.

A partition is consistent if the columns in any group do not have a non-zero in the same row position.

Approximations to the columns of the Jacobian matrix in a given group can be obtained by specifying a difference parameter array d with d(jcol) non-zero if and only if jcol is a column in the group, and an approximation to jac*d where jac denotes the Jacobian matrix of a mapping F.

d can be defined with the following segment of code.

   do 10 jcol = 1, n
      d(jcol) = 0.0
      if (ngrp(jcol) .eq. numgrp) d(jcol) = eta(jcol)
   10 continue

In the above code numgrp is the given group number, ngrp(jcol) is the group number of column jcol, and eta(jcol) is the difference parameter used to approximate column jcol of the Jacobian matrix.
Suitable values for the array eta must be provided.

As mentioned above, an approximation to jac*d must also be provided. For example, the approximation

   F(x+d) - F(x)

 corresponds to the forward difference formula at x.

Note that the value of m is not needed by fdjs and is therefore not present in the subroutine statement.

The subroutine statement is

   subroutine fdjs(n,indrow,jpntr,ngrp,numgrp,d,fjacd,fjac)
   where

   n is a positive integer input variable set to the number of columns of the Jacobian matrix.
   indrow is an integer input array which contains the row
indices for the non-zeroes in the Jacobian matrix.

jpntr is an integer input array of length n + 1 which specifies the locations of the row indices in indrow. The row indices for column j are

$$\text{indrow}(k), k = \text{jpntr}(j), ..., \text{jpntr}(j+1)-1.$$ 

Note that jpntr(n+1)-1 is then the number of non-zero elements of the Jacobian matrix.

ngrp is an integer input array of length n which specifies the partition of the columns of the Jacobian matrix. Column jcol belongs to group ngrp(jcol).

numgrp is a positive integer input variable set to a group number in the partition. The columns of the Jacobian matrix in this group are to be estimated on this call.

d is an input array of length n which contains the difference parameter vector for the estimate of the Jacobian matrix columns in group numgrp.

fjacd is an input array of length m which contains an approximation to the difference vector jac*d, where jac denotes the Jacobian matrix.

fjac is an output array of length nnz, where nnz is the number of its non-zero elements. At each call of fdjs, fjac is updated to include the non-zero elements of the Jacobian matrix for those columns in group numgrp. fjac should not be altered between successive calls to fdjs.

---

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*************
integer ir, jcol, jpl, jpu

do 30 jcol = 1, n
   if (ngrp(jcol) ne. numgrp) go to 20
   jpl = jpntr(jcol)
   jpu = jpntr(jcol+1) - 1
   if (jpu .lt. jpl) go to 20
   do 10 jpl = jpl, jpu
       ir = indrow(jp)
       fjac(jp) = fjacd(ir)/d(jcol)
   10 continue
20 continue
30 continue
  return

C
C  Last card of subroutine fdjs.
C  end