A Test Matrix Collection for Non-Hermitian Eigenvalue Problems*
(Release 1.0)

Zhaojun Bai[†] and David Day[‡] and James Demmel[§] and Jack Dongarra[¶]

October 6, 1996

1 Introduction

The primary purpose of this collection is to provide a testbed for the development of numerical algorithms for solving nonsymmetric eigenvalue problems. In addition, as with many other existing collections of test matrices, our goal includes providing an easy access to "practical" eigenproblems for researchers, educators and students in the community who are interested in the origins of large scale nonsymmetric eigenvalue problems, and in the development and testing of numerical algorithms for solving challenging non-Hermitian eigenvalue problems in real applications.

In this document, we describe the mechanism for obtaining a copy of the matrices and for using the collection. All test matrices currently included in the collection are documented in Appendices.

2 Organziation of the collection

There are four directories in the collection:

- `document/` contains the postscript file of this report and the postrscript files of pictures included in the docuement.
- `utility/` contains the utility routines in FORTRAN, C and Matlab M-files for basic manilpulations and computations of the matrices included in this collection, such as read or write a sparse matrix in the HB format, matrix-vector multiplication etc.
- `data/` contains the data files of test matrices which are presented in the standard Harwell-Beoing format.

*This work was supported in part by NSF grant ASC-9313958 and in part by DOE grant DE-FG03-94ER25219.

[†]Department of Mathematics, University of Kentucky, Lexington, KY 40506.

[‡]MS 1110, Sandia National Laboratories PO Box 5800, Albuquerque, NM 87185.

[§]Computer Science Division and Mathematics Department, University of California, Berkeley, CA 94720.

[¶]Department of Computer Science, University of Tennessee, Knoxville, TN 37996 and Mathematical Sciences Section, Oak Ridge National Laboratory, Oak Ridge, TN 37831.

- `matsrc/` contains the test matrices which are presented in the matrix-vector product format or in the subroutine format.

3 How to obtain the collection

The entire collection (document, software and data) is available through direct electronic transfer on the `MatrixMarket`, a web resource for test matrix collections. The URL of the MatrrixMarket is `http://math.nist.gov/MatrixMarket`.

4 Matrix Formats and Usage

There are three formats in which to represent the sparse matrices in the collection, namely the standard Harwell-Boeing (HB) sparse matrix format, the matrix-vector multiplication format, and the subroutine format.

4.1 HB Sparse compressed column format

The matrices stored in data files are stored in sparse column format (i.e., standard Harwell-Boeing format).[1] Utility routines `dreadm.f` and `dprtmt.f` can be used for reading or writing a real sparse matrix in this format in FORTRAN. `zreadm.f` and `zprtmt.f` are complex versions. `dreadhb.c` is the C version. Matlab M-files `dm2hb.m` and `zm2hb.m` can be used to write a real and complex sparse matrices in MATLAB to the HB format, respectively.

The following is a brief summary of the compressed column storage scheme. For more details, see the User's Guide for the Harwell-Boeing Sparse Matrix Collection.

In any sparse matrix format only the non-zero entries of a matrix are stored. An entry is specified by its row index, column index, and value. In sparse column format a single integer array and a single floating point array are used to store the row indices and the values, respectively, for all columns. The data for each column are stored in consecutive locations, the columns are stored in order, and there is no space between columns. An other integer array points to the first entry in each column.

The sparse matrix A of order n and with nnz non-zero entries is represented by a floating point array $a(1:nnz)$ that stores the values, an integer array $ia(1:nnz)$ that stores the row indices, and an integer array $ja(1:n+1)$ with the property that $ja(k+1)-1$ points to the last element in column k.

4.2 Matrix-vector multiplication format

Some of test matrices in this collection are presented in a different format than the standard Harwell-Boeing format. Instead of storing the matrix in a data file, the matrix is represented as a subroutine that computes the matrix-vector multiplications AX and/or A^TX for a given X, where X is a single vector or a block vector (matrix). These matrices are of variable size, and often depend on parameters that influence the eigenvalues.

[1] I. S. Duff, R. G. Grimes and J. G. Lewis, User's Guide for the Harwell-Boeing Sparse Matrix Collection (Release I), CERFACS, TR/PA/92/86, Oct. 1992. It is available via anonymous ftp: orion.cerfacs.fr, cd pub/harwell_boeing.

4.3 Subroutine format

In subroutine format the user generates a matrix of specified order (and parameter values if applicable) represented in compressed column or compressed row format. The matrix is stored in two integer arrays and one real array. Routines for performing matrix-vector products etc. are available in the utilities directory of the collection.

5 Acknoledgement and contributing to the collection

This work is in fact a compilation of efforts of many people. Their names will be acknowledged with the asscoiated matrices in the collection. We will keep updating the collection as new test problems become available. At a proper time, we plan to record performance data of different numerical methods and chanllenges associated with these test problems.

Your comments and contributions are welcomed. Please contact Bai by sending electronic mail to bai@ms.uky.edu or by writing to: Department of Mathematics, University of Kentucky, Lexington, KY 40506, USA.

Appendix A: Matrices in Standard HB Sparse Matrix Format

Appendix B: Matrices in Matrix-Vector Product Format

Appendix C: Matrices in Subroutine Format

Appendix D: List of Utility Routines

Appendix A

Matrices in Standard HB Sparse Matrix Format

Discipline	Matrix Keys
computational fluid dynamics	AF23560 TUB100, TUB1000 RDB200, RDB450, RDB1250, RDB2048, RDB200L, RDB450L, RDB800L, RDB1250L, RDB2048L, RDB3200L OLM100, OLM500, OLM1000, OLM2000, OLM5000
electrical engineering	BFW62A, BFW62B, BFW398A, BFW398B, BFW782A, BFW782B, DWA512, DWB512, DW2048, DW8192, DWG961A, DWG961B QH768, QH882, QH1484
quantum chemistry	QC324, QC2534
material science	CRYG2500, CRYG10000
plasma physics	MHD416A, MHD416B, MHD1280A, MHD1280B MHD3200A, MHD3200B, MHD4800B, MHD4800B
computer science	LOP163
robotic control	RBS480A, RBS480B
unknown	CK104, CK400, CK656

The following data files are also available, but the corresponding matrices are described in Appendices B and C.

Discipline	Matrix Keys
computational fluid dynamics	BWM200, BWM2000, CDDE1, CDDE2, CDDE3, CDDE4, CDDE5, CDDE6, PDE225, PDE900, PDE2961.
Aeroelasticity	TOLS90, TOLS340, TOLS1090, TOLS2000, TOLS4000.
computational mathematics	ODEP400A, ODEP400B.
Markov chain modeling	RW136, RW496, RW5151.

Title: Transient Stability Analysis of Navier-Stokes Solver

Source: A. Mahajan, NASA Lewis Research Center

Discipline: Computational fluid dynamics

Further details: This test matrix is from transient stability analysis of Navier-Stokes solvers. The order of the test matrix is 23560. The eigenvalues and eigenvectors are associated with small perturbation analysis of a finite difference representation of the Navier-Stokes equations for flows over airfoils. Such eigensystem information is central to stability analysis of Navier-Stokes solvers, for determining the modal bahavior of fluid in a fluid-structure interaction problem and for development of reduced order models based on variational principles for Navier-Stokes solvers. A repensentative eigenvalue constellation is reported in the following reference, where the Lanczos procedure with no rebiorthogonalization is used. The number of Lanczos iteration performed required for convergence was between 1000 to 1200 for convergence.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
AF23560	23560	484256	real

References:

A. Mahajan, E. H. Dowell, and D. Bliss. Eigenvalue calculation procedure for an Euler/Navier-Stokes solver with applications to flows over airfoils. *J. of Comput. Phy.*, 97:398–413, 1991.

Title: Bounded Finline Dielectric Waveguide

Source: B. Shultz and S. Gedney, Unviersity of Kentucky

Discipline: Electrical engineering

Further details: Millimeter wave technology has been applied in radar, communication, radiometry and instruments. The finline waveguide is an example of a bounded waveguide which operates extremely well in the millimeter wave spectrum. This generalized eigenvalue problem

$$Ax = \lambda Bx$$

studied in [Shultz] arises in the finite element analysis of the Maxwell's equation (see [Fernandez and Lu] and [Jin]) for finding the propagating modes and magentic field profiles of a rectangular waveguide filled with dielectric and PEC structures. The eigenvalues and corresponding eigenvectors of interest are the ones with positive real parts, which correspond to the propagation modes of a waveguide. The matrix A is non-symmetric and B is symmetric positive definite. Though real data is collected here, in applications, complex matrices may be involved.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
BFW62A	62	450	real
BFW62B	62	342	real
BFW398A	398	3678	real
BFW398B	398	2910	real
BFW782A	782	7514	real
BFW782B	782	5982	real

References:

B. Shultz, Bounded Waveguide Eigenmodes, Finite Element Method Solution, Masters Thesis, Department of Electrical Engineering, Unviersity of Kentucky, 1994.

F. A. Fernandez and Y. Lu, Variational finite element analysis of dielectric waveguide with non spurious solutions, Electron. Letter., 26(25):2125–2126, 1990.

J. Jin, The Finite Element Method in Electromagnetics, John Wiley & Sons, Inc., New York, 1993.

Title: Chuck Matrices

Source: J. Cullum, IBM T. J. Watson Research Center

Discipline: unknown

Further details: According to the reference, this set of test matrices is supplied by Chuck Siewert of North Carolina State. The application background of these matrices is not clear. The objective is to compute those eigenvalues with magnitudes greater than 1. The matrices have several multiple eigenvalues and clustered. The eigenvalues occur in clusters of order 4; each cluster consists of two pairs of very nearly multiple eigenvalues.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
CK104	104	992	real
CK400	400	2860	real
CK656	656	3884	real

References:

J. Cullum and R. A. Willoughby, A Practical Procedure for Computing Eigenvalues of Large Sparse Nonsymmetric Matrices, In Large Scale Eigenvalue Problem, J. Cullum and R. A. Willoughby eds. Elsevier Science Pub. North-Holland, 1986.

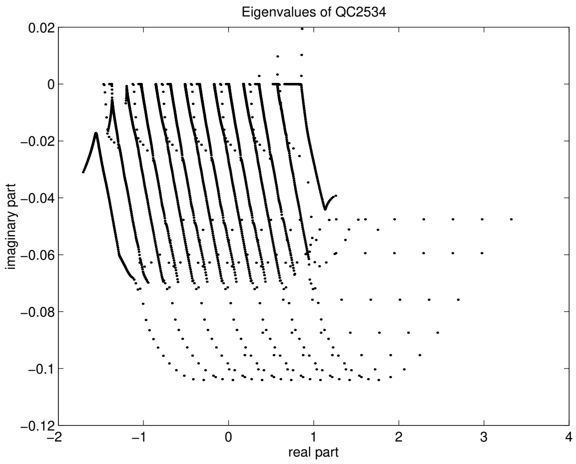
Title: Model H_2^+ in an Electromagnetic Field

Source: S. I. Chu, Unviersity of Kansas

Discipline: Quantum chemistry

Further details: The physical problem is to determine the laser-induced molecular resonance states of H_2^+ in an electro-magnetic field. The complex-scaling technique applied to the self-adjoint Hamiltonian from quantum mechanics yields a complex symmetric eigenvalue problem $Ax = \lambda x$. To determine the stability of the state, Floquet exponents are computed by the standard Fourier-grid method.

The computational task is to determine the eigenvalues nearest to or above the real axis. The figure displays the eigenvalues computed by the QR algorithm for the matrix QC2534.



Data files:

Filename/Key	Order	Number of nonzeros	Data type
QC324	324	26730	complex
QC2534	2534	463360	complex

References:

S.I. Chu, Complex quasivibrational energy formalism for intense-field multiphoton and above-threshold dissociation: complex-scaling Fourier-grid Hamiltonian method, Journal of Chemical Physics, Vol.94, No. 12, 7901–7909, 1991.

Title: DIffusion Model Study for Crystal Growth Simulation

Source: C. Yang, Rice University

Discipline: Material Science

Further details This is a large nonsymmetric standard eigenvalue problem that arises from the stability analysis of a crystal growth problem. To determine the stability of the interfacial crystallization of a piece of solid crystal solidifying into some undercooled melt, solutions of the following equations are sought.

$$\begin{aligned} \frac{1}{\eta^2+\xi^2}\left[\frac{\partial^2 U}{\partial \xi^2}+\frac{\partial^2 U}{\partial \eta^2}+2P\left(\eta\frac{\partial U}{\partial \eta}-\xi\frac{\partial U}{\partial \xi}\right)\right] &= \lambda U, \\ \frac{-1}{1+\xi^2}\left[\frac{\partial U}{\partial \eta}+4P^2N+2P(N+\xi\frac{\partial N}{\partial \xi})\right] &= \lambda N, \\ U = 2PN \quad \text{at } \eta = 1. \end{aligned}$$

Zero Dirichlet boundary condition is imposed at infinity. The variable U in the above equations represents the temperature perturbation of the liquid, and N describes the interface perturbation in a transformed (parabolic) coordinate system. The constant P is the Peclet number. The second equation is satisfied only at the interface $\eta = 1$. Eigenvalues with largest real parts are of interest. They indicate the growth or decay of the initial disturbance at the solid-liquid interface. A change of variable is used to map the partial differential equation from an infinite domain to a finite box $[0, 1] \times [1, 2]$. The matrix eigenvalue problem follows from discretization using the standard second order finite difference formulae. The Peclet number used here is $P = 0.05$.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
CRYG2500	2500	12349	real
CRYG10000	10000	49699	real

References:

C. Yang, D. C. Sorensen, D. I. Meiron and B. Wedeman, Numerical Computation of the Linear Stability of the Diffusion Model for Crystal Growth Simulation, Technical Report, TR96-04, Department of Comp & Applied Mathematics, Rice University, 1996.

Title: Square Dielectric Waveguide

Source: H. Dong, Unviersity of Minnesota

Discipline: Electrical engineering

Further details: Dielectric channel waveguide problems arise in many integrated circuit applications. Finite difference discretization of the governing Helmholtz equation for the magnetic field H,

$$\begin{aligned} \nabla^2 H_x + k^2 n^2(x,y) H_x &= \beta^2 H_x, \\ \nabla^2 H_y + k^2 n^2(x,y) H_y &= \beta^2 H_y, \end{aligned}$$

leads to the nonsymmetric eigenvalue problem of the form

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix} = \beta^2 \begin{pmatrix} B_{11} & \\ & B_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix}$$

where C_{11} and C_{22} are five- or tri-diagonal matrices, C_{12} and C_{21} are (tri-) diagonal matrices, and B_{11} and B_{22} are nonsingular diagonal matrices. This generalized eigenvalue problem is reduced to a standard eigenvalue problem $Ax = x\lambda$, where $A = B^{-1}C$, since B is diagonal.

The computational task is to determine the right most eigenvalues and their corresponding eigenvectors. In some cases, there are eigenvalues with negative real part several orders of magnitude larger than the desired eigenvalues with positive real part. This problem presents a challenge to existing numerical methods.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
DWA512	512	2480	real
DWB512	512	2500	real
DW2048	2048	10114	real
DW8192	8192	41746	real

Note that DWA512 and DWB512 are the matrices of same order which correspond to different parameter values.

References:

H. Dong, A. Chronopoulos, J. Zou and A. Gopinath, Vectorial integrated finite-difference analysis of dielectric waveguides, private communication, 1993

A. Galick, T. Kerhoven and U. Ravaioli, Iterative solution of the eigenvalue problem for a dielectric waveguid, IEEE Trans. Microwave Theory Tech. vol. MTT-40, pp.699–705, 1992.

Title: Dispersive Waveguide Structures

Source: S. Gedney and U. D. Navsariwala, Unviersity of Kentucky

Discipline: Electrical engineering

Further details: This is a complex symmetric eigenvalue problem $Ax = \lambda Bx$, where both A and B are complex and symmetric, but not Hermitian. Moreover, the matrices A and B are of the forms

$$\begin{pmatrix} A_{11} & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix},$$

respectively. In the work of Tan and Pan, it is shown that the eigenvalue problem is derived from using the edge element method to solve the waveguide problem of conductors with finite conductivity and cross section in a lossy dielectric media. The matrix size can easily reach a few thousands.

The subblock matrix A_{11} is 705 by 705, and banded. The computational task is to find the eigenvalues with the smallest positive real parts.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
DWG961A	961	3405	complex
DWG961B	961	10591	complex

References:

J. Tan and G. Pan, A new edge element analysis of dispersive waveguiding structures, IEEE trans. on microwave theory and tech. Vol.43, No.11, pp.2600–2607, Nov. 1995.

S. Gedney and U. D. Navsariwala, personal communication, 1996

Title: Alfven Spectra in Magnetohydrodynamics

Source: A. Booten[2] M. N. Kooper, H. A. van der Vorst, S. Poedts and J. P. Goedbloed, University of Utrecht, the Netherlands.

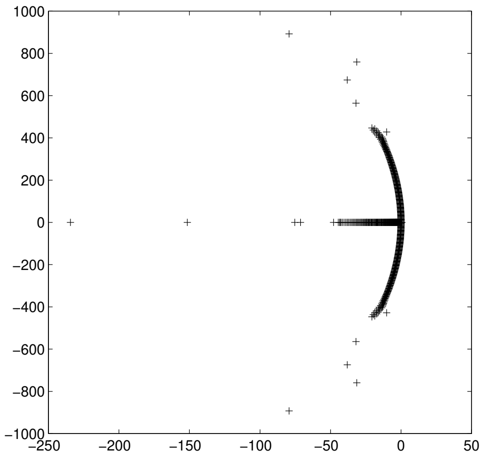
Discipline: Plasma Physics

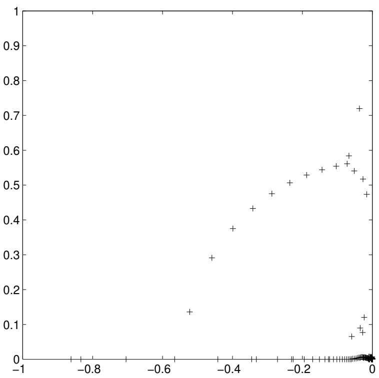
Further details Large nonsymmetric generalized matrix eigenvalue problems ($Ax = \lambda Bx$) arise in the modal analysis of dissipative magnetohydrodynamics (MHD). The MHD system combines Maxwell's and fluid flow equations. The physical objective of these MHD systems is to derive nuclear energy from the fusion of light nuclei. The plasmas generated exhibit both the characteristics of an ordinary fluid and special features caused by the magnetic field. The study of linearised motion in MHD has contributed significantly to the understanding of resistive and nonadiabatic MHD plasma phenomena such as plasma stability, wave propagation and heating.

The MHD equations are solved by applying a Galerkin finite elment method, which leads to the generalized eigenvalue problem. The spectrum ranges over several orders of magnitude (see figures below) corresponding to the time scales of different aspects of nuclear fusion reactions. Details are given in the literature.

Kerner reports difficulties in numerically computing the eigenvalues of the Alfeven wave operator. The spectrum of this operator consists of three branches. More precisely, it is reported that the eigenvalues at the intersection of the branches are problematic.

The left figure below displays the spectrum of the 1280×1280 MHD matrix computed by the QR algorithm. The right figure focuses on the intersection of the three branches (Alfven spectra).





[2]The test matrix data was made available to us by Dr. Albert Booten, less than a month before his unexpected death by heart failure during a sports event in November 12, 1995. Albert was an able young scientist and a very friendly person and we will miss him very much.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
MHD416A	416	8562	real
MHD416B	416	2312	real
MHD1280A	1280	47906	complex
MHD1280B	1280	22778	complex
MHD3200A	3200	68026	real
MHD3200B	3200	18316	real
MHD4800A	4800	102252	real
MHD4800B	4800	27520	real

References:

W. Kerner, Large-scale complex eigenvalue problem, J. of Comp. Phy. 85:1–85, 1989.

J. Cullum, W. Kerner and R. Willoughby, A generalized nonsymmetric Lanczos procedure, Comp. Phys. Comm., 53:19–48, 1989

M.N. Kooper, H.A. van der Vorst, S. Poedts, and J.P. Goedbloed, Application of the implicitly updated Arnoldi methods with a complex shift and invert strategy in MHD, *Journal of Comp. Phys.*, **118**, 320-328, 1995.

J. G. L. Booten, P. M. Meijer, H. J. J. te Riele and H. A. van der Vorst, Parallel Arnoldi method for the construction of a Krylov subspace basis: an application in magnetohydrodynamics. In Proceedings of International Conference and Exhibition on High-Performance Computing and Networking, Munich, Germany, April, 1994. Vol.II: Networking and Tools, W. Gentzsch and U. Harms, eds., Lecture Notes in Computer Science 797, Springer-Verlag, Berlin, 1994.

Z. Bai, D. Day and Q. Ye, ABLE: an adaptive block Lanczos method for non-Hermitian eigenvalue problems, Research Report 95-04, Department of Mathematics, University of Kentucky, May 1995 (revised version, Feb. 1996).

Title: Quebec Hydroelectric Power System
Key: QH882

Source: Deo Ndereyimana, Quebec, Canada

Discipline: Power systems simulations

Further details: This set of matrices is from the application of the Hydro-Quebec power systems' small-signal model. In the application, one wants to compute all eigenvalues $a + ib$ in a box of the complex plane. Specifically, $a_{\min} < a < a_{\max}$ and in general, $a_{\min} = -300$ and $a_{\max} = 300$. $b_{\min} < b < b_{\max}$ and in general, $b_{\min} = 0$ and $b_{\max} = 2 \times 60\pi$. Note that the matrices are highly unbalanced.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
QH768	768	2934	real
QH882	882	3354	real
QH1484	1484	6110	real

References:

Deo Ndereyimana, personal communication, 1994

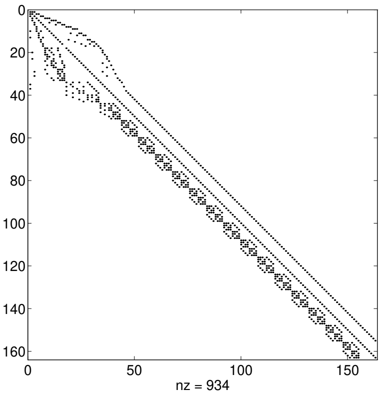
Title: LOPSI Stochastic Test Matrix

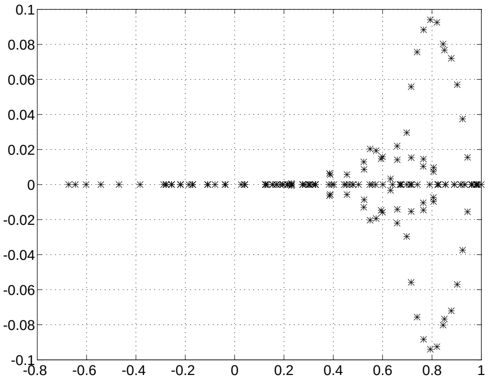
Source: W. J. Stewart, North Carolina State University and A. Jennings, Queen's University, Belfast, North Ireland.

Discipline: Analysis and evaluation of computer systems

Further details: This stochastic matrix is derived from the application of Markov modeling techniques to the analysis and evaluation of computer systems. The matrix is a 163 by 163 stochastic matrix with 935 nonzero entries. The object is to compute a few dominant eigenvalues and their corresponding eigenvectors.

The following left figure shows the sparsity structure of the 163 by 163 stochastic matrix, and the right figure shows the eigenvalue distribution.





Data files:

Filename/Key	Order	Number of nonzeros	Data type
LOP163	163	936	real

We note that the number of nonzero entries in our count is 936, however, the recorded count shown in the paper of Stewart and Jennings is 1207. The 15 dominant eigenvalues computed from the resulting matrix agree, however, with the results in the paper of Stewart and Jennings.

References:

W. J. Stewart, A comparison of numerical techniques in Markov modeling, Comm. ACM 21(2):144–152,1978.

W. J. Stewart and A. Jennings, A simultaneous iteration algorithm for real matrices, ACM Trans. Math. Soft. 7:184–198, 1981.

I. S. Duff and J. A. Scott, Computing selected eigenvalues of sparse unsymmetric matrices using subspace iteration, ACM TOMS 19:137–159, 1993.

Title: Forward Kinematics for the Stewart platform of Robotics

Source: H. Ren, University of California at Berkeley

Discipline: Robotic Control

Further details: The Stewart platform, also called left hand, is a *parallel manipulator* with six prismatic joints connecting two rigid bodies, or platforms. The base platform is considered fixed while the top platform, or end-effector, is moving in 3-dimensional space, controlled by the lenghts of joints. Parallel robots are especially useful when high stiffness and position precision are predominant requirements. The platform has one degree of freedom per joint; the position and orientation of the top platform is specified by six parameters, namely three for the orientation and three for the position in 3D space. The forward kinematics assumes that the leg lengths are known and the displacement of the top platform is to be found. The algrbraic problem reduces to the solution of a well-constrained system of polynomial equations. By using (sparse) resultant method, solving the system of polynomial equations reduces to solving the generalized eigenproblem $Ax = \lambda Bx$. The computational task is to compute the real eigenvalues and the corresponding eigenvectors (most of the eigenvalues are complex). Though the given model problem is of order 480, eigenvalue problems with thousands of unknowns commonly arise in this field.

It is requested to compute the real eigenvalues and the corresponding eigenvectors, although most of the eigenvalues are complex. It is desired to solve such matrix eigenvalue problem of order a few thousands.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
RBS480A	480	17088	real
RBS480B	480	17088	real

References:

D. Manocha and J. Canny, MultiPolynomial Resultant Algorithms, Computer Science Division Report, University of California, Berkeley, 1993

I. Emiris, Sparse Elimination and Applications in Kinematics, Ph.D. thesis, Computer Science Division, University of California at Berkeley, 1993.

Title: Tubular Reactor Model

Source: K. Meerbergen and D. Roose, Katholieke Universiteit Leuven, Belgium

Discipline: computational fluid dynamics

Further details: The conservation of reactant and energy in a homogeneous tube of length L in dimensionless form is modeled by

$$
\begin{aligned}
\frac{L}{v}\frac{dy}{dt} &= -\frac{1}{Pe_m}\frac{\partial^2 y}{\partial X^2} + \frac{\partial y}{\partial X} + Dy\exp(\gamma - \gamma T^{-1}),\\
\frac{L}{v}\frac{dT}{dt} &= -\frac{1}{Pe_h}\frac{\partial^2 T}{\partial X^2} + \frac{\partial T}{\partial X} + \beta(T - T_0) - BDy\exp(\gamma - \gamma T^{-1}),
\end{aligned}
$$

where y and T represent concentration and temperature and $0 \leq X \leq 1$ denote the spatial coordinate. The boundary conditions are $y'(0) = Pe_m y(0)$, $T'(0) = Pe_h T(0)$, $y'(1) = 0$ and $T'(1) = 0$. Central differences are used to discretize in space. For $x^T = [y_1, T_1, y_2, T_2, \ldots, y_{N/2}, T_{N/2}]$, the equations can be written as $\dot{x} = f(x)$. The parameters in the differential equation are set to $Pe_m = Pe_h = 5, B = 0.5, \gamma = 25, \beta = 3.5$ and $D = 0.2662$. One seeks the rightmost eigenvalues of the Jacobi matrix $A = \partial f/\partial x$. A is a banded matrix with bandwidth 5.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
TUB100	100	396	real
TUB1000	1000	3996	real

References:

R. F. Heinemann and A. B. Poore, Multiplicity, stability, and oscillatory dynamics of a tubular reactor, Chem. Eng. Sci. 36:1411-1419, 1981

T. J. Garratt, The numerical detection of Hopf bifurcations in large systems arising in fluid mechanics, PhD thesis, University of Bath, UK, 1991

K. Meerbergen and D. Roose, Matrix transformation for computing rightmost eigenvalues of large sparse nonsymmetric matrices, Report TW 206, Department of Computer Science, Katheolieke Universiteit Leuven, Belgium, 1994 (revised April 1995).

Title: The Olmstead model

Source: K. Meerbergen, Katholieke Universiteit Leuven, Belgium

Discipline: Hydrodynamics

Further details: The Olmstead model represents the flow of a layer of viscoelastic fluid heated from below. The equations are

$$\begin{aligned}\frac{\partial u}{\partial t} &= (1-C)\frac{\partial^2 v}{\partial X^2} + C\frac{\partial^2 u}{\partial X^2} + Ru - u^3 \\ B\frac{\partial v}{\partial t} &= u - v\end{aligned}$$

with boundary conditions $u(0) = u(1) = 0$ and $v(0) = v(1) = 0$. u represents the speed of the fluid and v is related to viscoelastic forces. The equation was discretised with central differences with grid size $h = 1/(N/2)$. After discretization the equation can be written as $\dot{x} = f(x)$ with $x^T = [u_1, v_1, u_2, v_2, \ldots, u_{N/2}, v_{N/2}]$. One seeks the rightmost eigenvalues of the Jacobi matrix $A = \partial f/\partial x$ with parameters $B = 2$, $C = 0.1$ and $R = 4.7$.

Subroutine: FORTRAN calling sequences for forming matrix-vector Jx and $J^T x$

Data files:

Filename/Key	Order	Number of nonzeros	Data type
OLM100	100	396	real
OLM500	500	1996	real
OLM1000	1000	3996	real
OLM2000	2000	7996	real
OLM5000	5000	19996	real

References:

W. E. Olmstead, W. E. Davis, S. H. Rosenblat and W. L. Kath, Bifurcation with memory, SIAM J. Appl. Math. 46:171–188, 1986

K. Meerbergen and A. Spence, A spectral transformation for finding complex eigenvalues of large sparse nonsymmetric matrices, Report TW 219, Department of Computer Science, Katheolieke Universiteit Leuven, Belgium, 1994

K. Meerbergen and D. Roose, Matrix transformation for computing rightmost eigenvalues of large sparse nonsymmetric matrices, Report TW 206, Department of Computer Science, Katheolieke Universiteit Leuven, Belgium, 1994 (revised April 1995).

Title: Reaction-diffusion Brusselator Model

Source: K. Meerbergen, Katholieke Universiteit Leuven, Belgium and A. Spence, University of Bath, UK.

Discipline: Chemical engineering

Further details: The equations

$$\begin{aligned}\frac{\partial u}{\partial t} &= \frac{D_u}{L^2}\left(\frac{\partial^2 u}{\partial X^2}+\frac{\partial^2 u}{\partial Y^2}\right) - (B+1)u + u^2 v + C\\ \frac{\partial v}{\partial t} &= \frac{D_v}{L^2}\left(\frac{\partial^2 v}{\partial X^2}+\frac{\partial^2 v}{\partial Y^2}\right) - u^2 v + Bu\end{aligned}$$

for u and $v \in (0,1)\times(0,1)$ with homogeneous Dirichlet boundary conditions form a 2D reaction-diffusion model where u and v represent the concentrations of two reactions. The equations are discretized with central differences with grid size $h_u = h_v = 1/(n+1)$ with $n = (N/2)^{1/2}$. For $x^T = [u_{1,1}, v_{1,1}, u_{1,2}, v_{1,2}, \ldots, u_{n,n}, v_{n,n}]$, the disretized equations can be written as $\dot{x} = f(x)$. One wants to compute the rightmost eigenvalues of the Jacobi matrix $A = \partial f/\partial x$. Where the parameters $B = 5.45, C = 2, D_u = 0.004, D_v = 0.008$. The parameter L is chosen different.

Data files:

Filename/Key	Order	Number of nonzeros	Data type	L
RDB200	200	1120	real	0.5
RDB450	450	2580	real	0.5
RDB1250	1250	7300	real	0.5
RDB2048	2048	12032	real	0.5
RDB200L	200	1120	real	1.0
RDB450L	450	2580	real	1.0
RDB800L	800	4640	real	1.0
RDB1250L	1250	7300	real	1.0
RDB2048L	2048	12032	real	1.0
RDB3200L	3200	18880	real	1.0

References:

B. D. Hassard, N. Kazarinoff and Y. H. Wan, Theory and Applications of Hopf Bifurcation, Cambridge University Press, Cambridge, 1981

K. Meerbergen and A. Spence, A spectral transformation for finding complex eigenvalues of large sparse nonsymmetric matrices, Report TW 219, Department of Computer Science, Katheolieke Universiteit Leuven, Belgium, 1994

Appendix B

Matrices in Matrix-Vector Multiplication Format

Title	Subroutine Names
Brusselator wave model in chemical reaction	MVMBWM
Model 2-D convection-diffusion differential operator	MVMMCD
Grcar matrix	MVMGRC
Ising model of ferromagnetic materials	MVMISG
Model eigenvalue problem of ODE	MVMODE
Markov chain modeling (random walk)	MVMRWK
Tolosa matrix	MVMTLS

Title: Brusselator wave model in chemical reaction
Subroutine name: MVMBWM

Source: Y. Saad, University of Minnesota

Discipline: Chemical engineering

Further details: This problem models the concentration waves for reaction and transport interaction of chemical solutions in a tubular reactor. The concentrations $x(t,z)$ and $y(t,z)$ of two reacting and diffusing components are modeled by the system

$$\frac{\partial x}{\partial t} = \frac{\delta_1}{L^2}\frac{\partial^2 x}{\partial^2 z} + f(x,y), \tag{1}$$

$$\frac{\partial y}{\partial t} = \frac{\delta_2}{L^2}\frac{\partial^2 y}{\partial^2 z} + g(x,y), \tag{2}$$

with the initial conditions $x(0,z) = x_0(z)$, $y(0,z) = y_0(z)$ and the Dirichlet boundary conditions $x(t,0) = x(t,1) = x^*$, $y(t,0) = y(t,1) = y^*$, where $0 \le z \le 1$ is the space coordinate along the tube, and t is time. Raschman *et al* considered in particular the so-called Brusselator wave model in which

$$f(x,y) = \alpha - (\beta+1)x + x^2 y, \quad g(x,y) = \beta x - x^2 y.$$

Then, the above system admits the trivial stationary solution $x^* = \alpha$, $y^* = \beta/\alpha$. In this problem one is primarily interested in the existence of stable periodic solutions to the system as the bifurcation parameter L varies. This occurs when the eigenvalues of largest real parts of the Jacobian of the right hand side of (1) and (2), evaluated at the steady station solution, is purely imaginary. For the purpose of verifying this fact numerically, one first needs to discretize the equations with respect to the variable z and compute the eigenvalues with largest real parts of the resulting discrete Jacobian.

If we discretize the interval $[0,1]$ using n interior points with the mesh size $h = 1/(m+1)$. Then the discretized Jacobian of the system is a 2×2 block matrix of the form

$$A = \begin{pmatrix} \tau_1 T + (\beta-1)I & \alpha^2 I \\ -\beta I & \tau_2 T - \alpha^2 I \end{pmatrix}$$

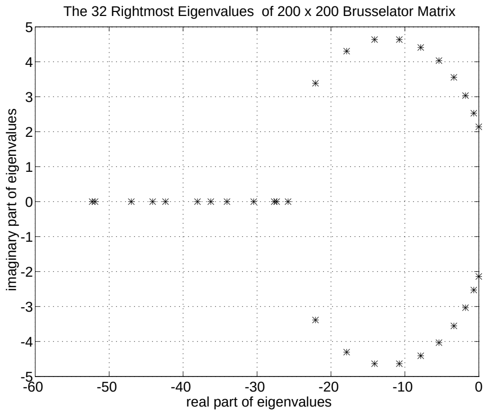
where $T = \text{tridiag}\{1,-2,1\}$, $\tau_1 = \frac{1}{h^2}\frac{\delta_1}{L^2}$ and $\tau_2 = \frac{1}{h^2}\frac{\delta_2}{L^2}$

The exact eigenvalues of J are known since there exists a quadratic relation between the eigenvalues of the matrix A and those of the classical difference matrix $T = \text{tridiag}\{1,-2,1\}$. The following segment is the Matlab M-file for computing the $2m$ eigenvalues of A:

```
h = 1/(m+1); tau1  = delta1/(h*L)^2; tau2  = delta2/(h*L)^2;
for j=1:m,
   eigofT(j) = -2*(1- cos(pi*j*h) );  % eigenvalues of T
end;
for j=1:m,
   coeff(1) = 1;
   coeff(2) = alpha^2 - (beta - 1) - (tau1+tau2)*eigofT(j);
```

```
    coeff(3) = beta*alpha^2 + tau1*tau2*eigofT(j)^2 + ...
               tau2*(beta-1)*eigofT(j) - ...
               alpha^2*tau1*eigofT(j) - alpha^2*(beta-1);
    d = roots(coeff);
    Aeig(j) = d(1);  Aeig(m+j) = d(2); % eigenvalues of A
end;
```

The following figure shows the 32 rightmost eigenvalue distribution of 200 by 200 of the matrix A ($m = 100$) corresponding to the set of parameters $\delta_1 = 0.008$, $\delta_2 = \frac{1}{2}\delta_1 = 0.004$, $\alpha = 2$, $\beta = 5.45, L = 0.51302$ as used in Saad's book.



Subroutine: FORTRAN calling sequence for forming matrix-vector AX or A^TX is

```
SUBROUTINE MVMBWM( TRANS, N, M, X, LDX, Y, LDY )
```

with

TRANS	(input) INTEGER if TRANS $= 0$, computes the product AX, if TRANS $= 1$, computes the product A^TX,
N	(input) INTEGER The order of matrix A. N has to be an even number.
M	(input) INTEGER The number of columns of X.
X	(input) DOUBLE PRECISION array, dimension (LDX, M) contains the vector X.
LDX	(input) INTEGER The leading dimension of the array X, LDX $\geq$ max(1, N).
Y	(output) DOUBLE PRECISION array, dimension (LDY, M) contains the product AX or A^TX.
LDY	(input) INTEGER The leading dimension of the array Y, LDY $\geq$ max(1, N).

In addition, the parameters $\delta_1, \delta_2, L, \alpha$ and β are set as internal parameters.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
BW200	200	796	real
BW2000	2000	7996	real

References:

P. Raschman, M. Kubicek and M. Maros, Waves in distributed chemical systems: experiments and computations, P. J. Holmes ed., New Approaches to Nonlinear Problems in Dynamics - Proceedings of the Asilomar Conference Ground, Pacific Grove, California 1979. The Engineering Foundation, SIAM, pp.271–288, 1980.

Y. Saad, Numerical Methods for Large Eigenvalue Problems, Halsted Press, Div. of John Wiley & Sons, Inc., New York, 1992

Title: Model 2-D Convection Diffusion Operator
Subroutine name: MVMMCD

Source: unclear

Discipline: computational fluid dynamics

Further details: This test matrix is from the following constant-coefficient convection diffusion equation which is widely used for testing and analyzing numerical methods for the solution of linear system of equations,

$$\begin{aligned} -\Delta u + 2p_1 u_x + 2p_2 u_y - p_3 u &= f \quad \text{in} \quad [0,1]^2 \\ u &= g \quad \text{on} \quad \partial[0,1]^2 \end{aligned}$$

where p_1, p_2 and p_3 are positive constants. Discretization by the finite difference scheme with a 5-point stencil on a uniform $m \times m$ grid gives rise to a sparse linear system of equations

$$Au = b$$

where A is of order m^2 and u and b are now vectors of size m^2. Centered differences are used for the first derivatives. If the grid points are numbered using the rowwise natural ordering, then A is a block tridiagonal matrix of the form

$$A = \begin{pmatrix} T & (\beta-1)I & & & \\ -(\beta+1)I & T & (\beta-1)I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & (\beta-1)I \\ & & & -(\beta+1)I & T \end{pmatrix}$$

with

$$T = \begin{pmatrix} 4-\sigma & \gamma-1 & & & \\ -\gamma-1 & 4-\sigma & \gamma-1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma-1 \\ & & & -\gamma-1 & 4-\sigma \end{pmatrix},$$

where $\beta = p_1 h, \gamma = p_2 h, \sigma = p_3 h^2$ and $h = 1/(m+1)$.

The spectral decomposition of the convection diffusion matrix is known. For $1 \leq i, j \leq m$, if Δ is a diagonal matrix with $((i-1)m+j)$th diagonal entry

$$\left(\frac{1+\beta}{1-\beta}\right)^{\frac{i-1}{2}} \left(\frac{1+\gamma}{1-\gamma}\right)^{\frac{j-1}{2}},$$

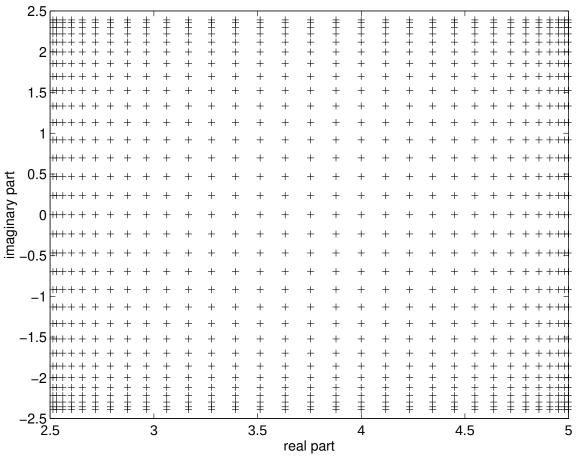
then $\Delta^{-1}A\Delta$ is symmetric. For $1 \leq k, l \leq m$, let (k,l) denote $(k-1)m+l$. Then the (k,l)th unnormalized eigenvector of $\Delta^{-1}A\Delta$ has (i,j)th entry

$$\sin(ikh\pi)\sin(jlh\pi).$$

The reader may now verify that the (k, l)th eigenvalue of A is

$$\lambda_{(k,l)} = 4 - \sigma + 2(1-\beta^2)^{1/2}\cos(kh\pi) + 2(1-\gamma^2)^{1/2}\cos(lh\pi)$$

The following figure shows the eigenvalue distribution of 961 by 961 convection diffusion matrix with $p_1 = 25, p_2 = 50$ and $p_3 = 250$.



Since the normalized eigenvectors of a symmetric matrix are orthogonal, the eigenvectors of A are graded like the diagonal of Δ and the condition number of the eigenvalue problem for A is

$$\mathrm{cond}(\Delta) = \left(\frac{(1+\beta)(1+\gamma)}{(1-\beta)(1-\gamma)}\right)^{\frac{m-1}{2}} .$$

We note that, in practice, the choice of the mesh size h and the coefficients p_1, p_2 and p_3 have to satisfy certain conditions for the discretization to be stable. We refer the reader to the references for the discussion of this issue.

Subroutine: FORTRAN calling sequence for forming matrix-vector AX or A^TX is

```
SUBROUTINE MVMMCD( TRANS, N, M, X, LDX, Y, LDY )
```

with

`TRANS` (input) INTEGER
if `TRANS` $= 0$, computes the product AX,
if `TRANS` $= 1$, computes the product A^TX,

`N` (input) INTEGER
The order of the matrix A. N has to be the square of an integer number.

`M` (input) INTEGER
The number of columns of `X`.

`X` (input) DOUBLE PRECISION array, dimension (`LDX, M`)
contains the vector X.

`LDX` (input) INTEGER
The leading dimension of the array `X`, `LDX` $\geq$ max(1, `N`).

`Y`	(output) DOUBLE PRECISION array, dimension (`LDY, M`) contains the product AX or A^TX.
`LDY`	(input) INTEGER The leading dimension of the array `Y`, `LDY` $\geq$ max(1, `N`).

In addition, p_1, p_2 and p_3 are set as internal parameters.

Data files:

Elman and Streit tested preconditioners for linear systems on six convection-diffusion matrices arising on a 31 by 31 grid. Note that when p_1 and p_2 are large compared to the grid size, the local error in the discretization is significant. Also note that when p_1 and p_2 are large the solution, u, forms boundary layers which are not practical to resolve using regular grids. The matrices correspond to the following choices of p_1,p_2 and p_3.

Filename/Key	Order	Number of nonzeros	Data type	(p_1, p_2, p_3)
CDDE1	961	4681	real	(1,2,30)
CDDE2	961	4681	real	(25,50,30)
CDDE3	961	4681	real	(1,2,80)
CDDE4	961	4681	real	(25,50,80)
CDDE5	961	4681	real	(1,2,250)
CDDE6	961	4681	real	(25,50,250)

References:

H. C. Elman and R. L Streit, Polynomial iteration for nonsymmetric indefinite linear systems, Lec. Notes in Math. Vol. 1230, J. P. Hennart, ed. Numerical Analysis Proceedings, Gauuajsato, Mexico, Springe Verlag, 1984.

Y. Saad, Variations on Arnoldi's method for computing eigenelements of large unsymmetric matrices, Lin. Alg. Appl. 34:269–295, 1980.

Z. Bai and G. W. Stewart, SRRIT – A FORTRAN subroutine to calculator the dominant invariant subspaces of a nonsymmetric matrix, Comp. Sci. Dept. Tech. Rep. TR-2908, Univ. of Maryland, MD, April 1992, (submitted to ACM TOMS).

Z. Jia, Some numerical methods for large unsymmetric eigenproblems, Ph.D. thesis, The faculty of Mathematics, University of Bielefeld, Germany, Feb. 1994.

R. B. Lehoucq, Analysis and implementation of an implicitly Restarted Arnoldi Iteration, Ph.D thesis, Department of Computational and Applied Methematics, Rice University, TR95-13, May 1995.

Title: Grcar Matrix
Subroutine name: MVMGRC

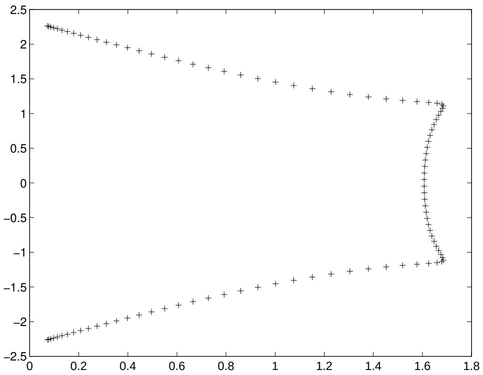
Source: J. Grcar, Sandia National Lab.

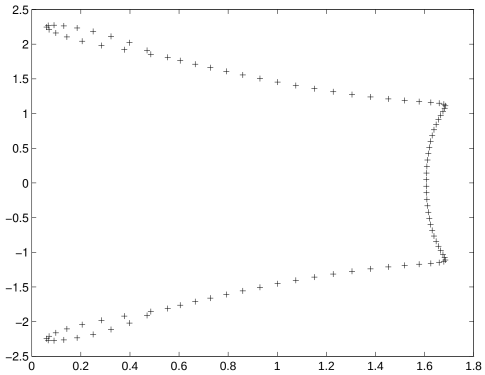
Discipline: numerical linear algebra

Further details: An $n \times n$ Grcar matrix is a nonsymmetric Toeplitz matrix:

$$A = \begin{pmatrix} 1 & 1 & 1 & 1 & & & & \\ -1 & 1 & 1 & 1 & 1 & & & \\ & -1 & 1 & 1 & 1 & 1 & & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & & -1 & 1 & 1 & 1 & 1 \\ & & & & -1 & 1 & 1 & 1 \\ & & & & & -1 & 1 & 1 \\ & & & & & & -1 & 1 \end{pmatrix}$$

The matrix has sensitive eigenvalues. The following figures are the eigenvalue distribution of 100 by 100 Grcar matrix A and A^T, computed by QR algorithm in Matlab.





Subroutine: FORTRAN calling sequence for forming matrix-vector AX or A^TX is

```
SUBROUTINE MVMGRC( TRANS, N, M, X, LDX, Y, LDY )
```

with

`TRANS` (input) INTEGER
if `TRANS` $= 0$, computes the product AX,
if `TRANS` $= 1$, computes the product A^TX,

`N` (input) INTEGER
The order of the matrix A.

`M` (input) INTEGER
The number of columns of `X`.

`X` (input) DOUBLE PRECISION array, dimension (`LDX, M`)
contains the vector X.

`LDX` (input) INTEGER
The leading dimension of the array `X`, `LDX` $\geq$ max(1, `N`).

`Y` (output) DOUBLE PRECISION array, dimension (`LDY, M`)
contains the product AX or $A^T X$.

`LDY` (input) INTEGER
The leading dimension of the array `Y`, `LDY` $\geq$ max(1, `N`).

References:

J. Grcar, Operator coefficient methods for linear equations, Sandia National Lab. Rep. SAND89-8691, Nov. 1989.

N.M. Nachtigal, L. Reichel and L.N. Trefethen, A hybrid GMRES algorithm for non-symmetric linear systems, SIAM J. Matrix Anal. Appl., 13 (1992), pp. 796-825.

N. J. Higham, A collection of test matrices in MATLAB, ACM Trans. Math. Softw. 17:289–305, 1991.

Title: Ising model for ferromagnetic materials
Subroutine name: MVMISG

Source: B. Friedman

Discipline: Material science

Further details: This test matrix is from the analysis of the Ising model for ferromagnetic materials. The matrix A is the product of the two $2m$ by $2m$ matrices K and L,

$$A = KL$$

where

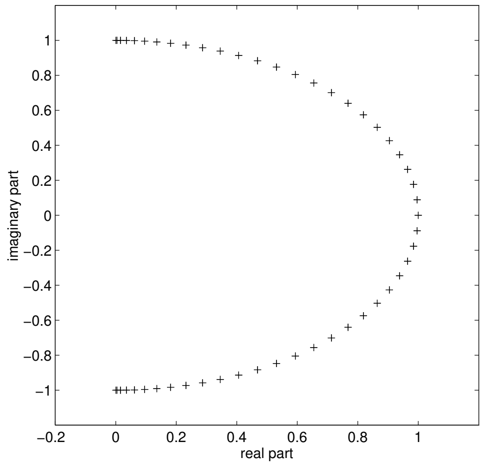
$$K = \begin{pmatrix} E & & & & \\ & E & & & \\ & & \ddots & & \\ & & & E & \\ & & & & E \end{pmatrix}, \qquad L = \begin{pmatrix} \cos\beta & & & & -\sin\beta \\ & F & & & \\ & & \ddots & & \\ & & & F & \\ \sin\beta & & & & \cos\beta \end{pmatrix}$$

$$E = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}, \qquad F = \begin{pmatrix} \cos\beta & \sin\beta \\ -\sin\beta & \cos\beta \end{pmatrix}.$$

It can be shown that the eigenvalues of A are the $2m$ numbers that are obtained by computing the eigenvalues of the m 2 by 2 matrices

$$\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \cos\beta & -\theta^k \sin\beta \\ \theta^{m-k}\sin\beta & \cos\beta \end{pmatrix}$$

for $k = 1, 2, \ldots, m$, where $\theta = e^{i2\pi/m}$. The following figure shows the eigenvalue distribution of 100 by 100 Ising matrix with $\alpha = \pi/4$ and $\beta = \pi/4$



Subroutine: FORTRAN calling sequence for forming matrix-vector AX or $A^T X$ is

```
SUBROUTINE MVMISG( TRANS, N, M, X, LDX, Y, LDY )
```

with

`TRANS`	(input) INTEGER if `TRANS` $= 0$, computes the product AX, if `TRANS` $= 1$, computes the product $A^T X$,
`N`	(input) INTEGER The order of the matrix A. N has to be an even number.
`M`	(input) INTEGER The number of columns of `X`.
`X`	(input) DOUBLE PRECISION array, dimension (`LDX, M`) contains the vector X.
`LDX`	(input) INTEGER The leading dimension of the array `X`, `LDX` $\geq$ max(1, `N`).
`Y`	(output) DOUBLE PRECISION array, dimension (`LDY, M`) contains the product AX or $A^T X$.
`LDY`	(input) INTEGER The leading dimension of the array `Y`, `LDY` $\geq$ max(1, `N`).

In addition, α and β are set as internal parameters.

References:

B. Kaufman, Crystal statistics II, Phys. Rev. 76, pp.1232, 1949.

B. Friedman, Eigenvalues of Composite matrices, Proc. Cambridge Philos. Soc. 57, pp.37-49, 1961

M. Marcus and H. Minc, A survey of Matrix Theory and matrix inequalities, Dover edition, New York, 1992.

Afternotes:

This Ising model was proposed to explain properties of ferromagnets but since then it has found application to topics in chemistry and biology as well as physics. For any reader unfamiliar with the model an excellent introduction is [B. A. Cipra, An Introduction to the Ising Model, American Mathematical Monthly, 94:937–959, 1987].

A numerical method for approximating the leading eigenvalues of 2D Ising models using a transfer matrix of order 2^n with $n = 30$ is reported in [B. Parlett and W. Heng, The Method of Minimal Representations in 2D Ising Model Calculations, J. Comp. Phy. 114, pp.257–264, 1994].

We plan to include the transfer matrix in the future version of this collection.

Title: Model Eigenvalue Problem of ODE
Subroutine name: MVMODE

Source: G. W. Stewart, University of Maryland

Discipline: Model eigenvalue problem of ordinary differential equation.

Further details: Consider the following eigenvalue problem of an ordinary differential equation

$$y'' + \mu^2 y = 0 \tag{3}$$

with the boundary conditions

$$y(0) = 0 \quad \text{and} \quad y'(0) + \gamma y'(1) = 0, \quad 0 < \gamma < 1.$$

It can be shown that the eigenvalues μ are given by

$$\mu = i \cosh^{-1}(-\gamma^{-1}),$$

which are complex. The solutions of this equation are of the form

$$\mu^2 = ((2k+1)^2\pi^2 - \ln^2 \sigma) - i(2(2k+1)\pi \ln \sigma),$$

for $k = 0, \pm 1, \pm 2, \ldots$, where $\sigma = 1/\gamma \pm \sqrt{1/\gamma^2 - 1}$.

The eigenproblem of (3) can be approximated by finite differences as follows. Let y_i denote the approximate solution at the point $x_i = i/(n+1)$ $(i = 0, 1, \ldots, n)$. Replacing the second derivatives in (3) with a centered difference operators to obtain the generalized matrix eigenvalue problem

$$Ay = -\mu^2 By, \tag{4}$$

for $y = (y_1, y_2, \ldots, y_{n+1})^{\mathrm{T}}$, where

$$A = \begin{pmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ 4 & -1 & \cdots & \gamma & -4\gamma & 3\gamma \end{pmatrix}$$

and $B = h^2 \mathrm{diag}(1, 1, \ldots, 1, 0)$. Problem (4) can be recast as the standard eigenvalue problem

$$Cy = -\frac{1}{\mu^2} y,$$

where $C = A^{-1}B$.

Subroutine: The matrix-vector products $Y = CX$ can be formed by solving the linear system $AY = BX$ for Y using the banded Gaussian elimination.

FORTRAN calling sequence for forming matrix-vector product $Y = CX$ is

```
SUBROUTINE MVMODE( N, M, X, LDX, Y, LDY )
```

with

`N`	(input) INTEGER The order of the matrix C.
`M`	(input) INTEGER The number of columns of `X`.
`X`	(input) DOUBLE PRECISION array, dimension (`LDX, M`) contains the vector X.
`LDX`	(input) INTEGER The leading dimension of the array `X`, `LDX` $\geq$ max(1, `N`).
`Y`	(output) DOUBLE PRECISION array, dimension (`LDY, M`) contains the product CX.
`LDY`	(input) INTEGER The leading dimension of the array `Y`, `LDY` $\geq$ max(1, `N`).

In addition, γ is set as an internal parameters.

2`N` workspace is required for the banded Gaussian elimination. As a default value, 3*2001 workspace is set internally. As a result, `N` should be less and equal to 2001. Otherwise, user should set a larger workspace.

Data files: In the data files, $\gamma = 1/100$.

Filename/Key	Order	Number of nonzeros	Data type
ODEP400A	400	1201	real
ODEP400B	400	399	real

References:

G. W. Stewart, SRRIT – A FORTRAN subroutine to calculator the dominant invariant subspaces of a real matrix, Comp. Sci. Dept. Tech. Rep. TR-514, Univ. of Maryland, College Park, Nov. 1978.

Z. Bai and G. W. Stewart, SRRIT – A FORTRAN subroutine to calculator the dominant invariant subspaces of a nonsymmetric matrix, Comp. Sci. Dept. Tech. Rep. TR-2908, Univ. of Maryland, MD, April 1992, (submitted to ACM TOMS).

Title: Markov Chain Transition Matrix
Subroutine name: MVMRWK

Source: G. W. Stewart, University of Maryland

Discipline: Probability theory and its applications

Further details: Consider a random walk on an $(m+1)\times(m+1)$ triangular grid, illustrated below for $m = 6$.

$$\begin{array}{cccccccc}
6 & \bullet & & & & & & \\
5 & \bullet & \bullet & & & & & \\
4 & \bullet & \bullet & \bullet & & & & \\
3 & \bullet & \bullet & \bullet & \bullet & & & \\
2 & \bullet & \bullet & \bullet & \bullet & \bullet & & \\
1 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \\
0 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\
j/i & 0 & 1 & 2 & 3 & 4 & 5 & 6
\end{array}$$

The points of the grid are labeled (j, i), $(i = 0, \ldots, m, j = 0, \ldots, m-i)$. From the point (j, i), a transition may take place to one of the four adjacent points $(j + 1, i), (j, i + 1), (j - 1, i), (j, i - 1)$. The probability of jumping to either of the nodes $(j - 1, i)$ or $(j, i - 1)$ is

$$pd(j, i) = \frac{j + i}{m} \tag{5}$$

with the probability being split equally between the two nodes when both nodes are on the grid. The probability of jumping to either of the nodes $(j + 1, i)$ or $(j, i + 1)$ is

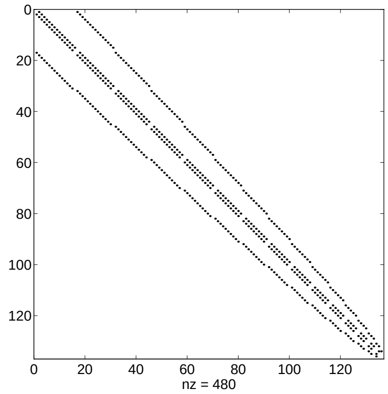
$$pu(j, i) = 1 - pd(j, i). \tag{6}$$

with the probability again being split when both nodes are on the grid.

If the $(m + 1)(m + 2)/2$ nodes (j, i) are numbered $1, 2, \ldots, (m + 1)(m + 2)/2$ in some fashion, then the random walk can be expressed as a finite Markov chain with transition matrix A of order $n = (m + 1)(m + 2)/2$ consisting of the probabilities a_{kl} of jumping from node l to node k (A is actually the transpose of the usual transition matrix; see [Feller]).

We are primarily interested in the steady state probabilities of the chain, which is ordinarily the appropriately scaled eigenvector corresponding to the eigenvalue unity.

The following plot shows the sparsity pattern of the resulted random walk matrix of order 136 (i.e. $m = 15$).



Subroutine: To calculate the ith element of the vector Ax one need only regard the components of q as the average number of individuals at the nodes of the grid and use the probabilities (5) and (6) to calculate how many individuals will be at node i after the next transition.

FORTRAN calling sequence for forming matrix-vector product $Y = AX$ is

```
SUBROUTINE MVMRWK( N, M, X, LDX, Y, LDY )
```

with

- `N` (input) INTEGER
  The order of the matrix A. `N` has to be equal to $(m+1)(m+2)/2$ for some integer $m \geq 0$.
- `M` (input) INTEGER
  The number of columns of `X`.
- `X` (input) DOUBLE PRECISION array, dimension (`LDX, M`)
  contains the vector X.
- `LDX` (input) INTEGER
  The leading dimension of the array `X`, `LDX` $\geq$ max(1, `N`).
- `Y` (output) DOUBLE PRECISION array, dimension (`LDY, M`)
  contains the product AX.
- `LDY` (input) INTEGER
  The leading dimension of the array `Y`, `LDY` $\geq$ max(1, `N`).

Data files:

Filename/Key	Order	Number of nonzeros	Data type
RW136	136	479	real
RW496	496	1859	real
RW5151	5151	20199	real

References:

W. Feller, An introduction to probability theory and its applications, John Wiley, New York, 1961

G. W. Stewart, SRRIT – A FORTRAN subroutine to calculator the dominant invariant subspaces of a real matrix, Comp. Sci. Dept. Tech. Rep. TR-514, Univ. of Maryland, College Park, Nov. 1978.

Y. Saad, Numerical methods for large eigenvalue problems. Halsted Press, Div. of John Wiley & Sons, Inc., New York, 1992.

I. S. Duff and J. A. Scott, Computing selected eigenvalues of sparse unsymmetric matrices using subspace iteration, ACM TOMS 19:137-159, 1993

Z. Bai and G. W. Stewart, SRRIT – A FORTRAN subroutine to calculator the dominant invariant subspaces of a nonsymmetric matrix, Comp. Sci. Dept. Tech. Rep. TR-2908, Univ. of Maryland, MD, April 1992 (submitted to ACM TOMS).

Title: Tolosa Matrix
Subroutine name: MVMTLS

Source: S. Godet-Thobie, CERFACS and C. Bès, Aerospatiale, France

Discipline: Aeroelasticity

Future details: The Tolosa matrix arises in the stability analysis of a model of an airplane in flight. The interesting modes of this system are described by complex eigenvalues whose imaginary parts lie in a prescribed frequency range. The task is to compute the eigenvalues with largest imaginary parts. The problem has been analyzed at CERFACS (Centre Europeen de Recherche et de Formation Avancee en Calcul Scientifique) in cooperation with the Aerospatiale Aircraft Division[3].

The matrix is a sparse 5×5 block matrix of order $n = 90 + 5k$ for an integer $k >= 0$. When $n = 90$, each block is of dimension 18×18 and

$$A = \begin{pmatrix} 0 & I & 0 & 0 & 0 \\ X_1 & X_2 & X_3 & X_4 & X_5 \\ 0 & I & L_1 & 0 & 0 \\ 0 & I & 0 & L_2 & 0 \\ 0 & I & 0 & 0 & L_3 \end{pmatrix}$$

where $L_i = \beta_i I$, $i = 1, 2, 3$, and X_i and β_i are given data. When $n > 90$,

$$A = \begin{pmatrix} 0 & I & 0 & 0 & 0 \\ Y_1 & Y_2 & Y_3 & Y_4 & Y_5 \\ 0 & I & L_1 & 0 & 0 \\ 0 & I & 0 & L_2 & 0 \\ 0 & I & 0 & 0 & L_3 \end{pmatrix}$$

where

$$\begin{aligned} Y_1 &= \begin{pmatrix} X_1 & 0 \\ 0 & \mathrm{diag}(x_i) \end{pmatrix}, \quad x_i = -\omega_i^2, i = 1, \ldots, m-18, \\ Y_2 &= \begin{pmatrix} X_2 & 0 \\ 0 & \mathrm{diag}(y_i) \end{pmatrix}, \quad y_i = -2\alpha_i\omega_i, \quad i = 1, \ldots, m-18, \\ Y_i &= \begin{pmatrix} X_i & 0 \\ 0 & 0 \end{pmatrix}, \quad i = 3, 4, 5, \end{aligned}$$

and

$$\omega_i = 150 + 6i, \qquad \alpha_i = c_1 i + c_2, \qquad c_1 = \frac{.299}{n/5 - 18}, \qquad c_2 = 0.001 - c_1.$$

The following fugures show the eigenvalue distribution of Tolosa matrices of orders 90 and 340.

Subroutine: FORTRAN calling sequence for forming matrix-vector AX or $A^T X$ is

[3] Tolosa is the latin name of Toulouse, France, the location of CERFACS.

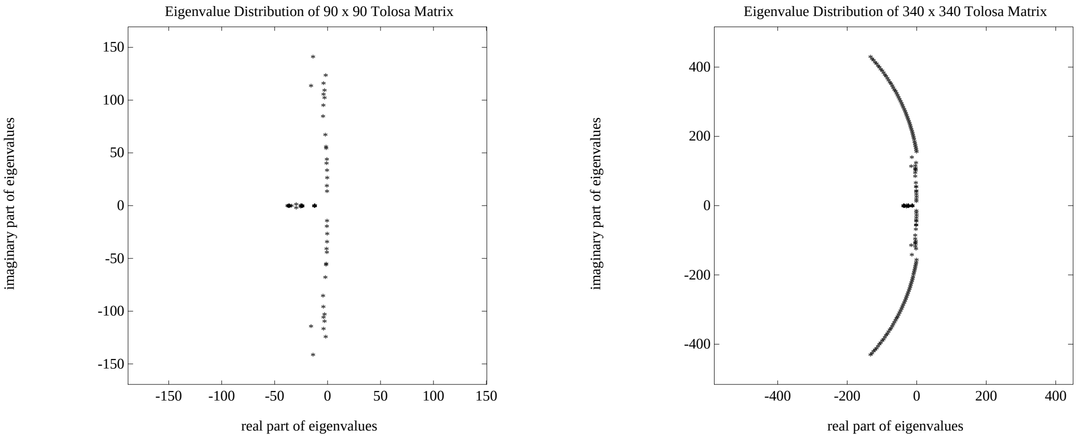


Figure 1: Eigenvalue distribution of 90 by 90 and 340 by 340 Tolosa matrices

```
SUBROUTINE MVMTLS( TRANS, N, M, X, LDX, Y, LDY )
```

with

TRANS	(input) INTEGER if TRANS $= 0$, computes the product AX, if TRANS $= 1$, computes the product $A^T X$,
N	(input) INTEGER The order of the matrix A. N has to be 90+5*K for a negative integer K.
M	(input) INTEGER The number of columns of X.
X	(input) DOUBLE PRECISION array, dimension (LDX, M) contains the vector X.
LDX	(input) INTEGER The leading dimension of the array X, LDX $\geq$ max(1, N).
Y	(output) DOUBLE PRECISION array, dimension (LDY, M) contains the product AX or $A^T X$.
LDY	(input) INTEGER The leading dimension of the array Y, LDY $\geq$ max(1, N).

It is required to read a data file in the main program to initialize the data structure and pass it as a common block to the subroutine MVMTLS. The data file is `block`. `readb.f` is the FORTRAN subroutine for reading the data file. The following is a short deomonstration program in FORTRAN.

```
.
      PROGRAM  TEST
      INTEGER            N, I, LDX, LDY
      PARAMETER          ( LDX = 500, LDY = LDX )
      DOUBLE PRECISION   X( LDX ), Y( LDY )
```

```
*
      DOUBLE PRECISION   ONE
      PARAMETER          ( ONE = 1.0D+0 )
*
      DOUBLE PRECISION   BLK( 18,90 )
      COMMON             BLK( 18,90 )
*
*     Read matrix size
*
      READ(*,*)N
*
*     Data check
*
      IF( N.LT.90 .OR. MOD( N-90,5 ).NE.0 )THEN
         WRITE( *,111 )
         GO TO 20
      ELSE IF( N.GT.LDX )THEN
         WRITE( *,112 )
         GO TO 20
      END IF
*
*     Read in data
*
      CALL READTL( BLK )
*
*     Set an input vector X
*
      DO 10 I = 1, N
         X( I ) = ONE
   10 CONTINUE
*
*     Compute Y = A*X
*
      CALL MVMTLS( 0, N, 1, X, LDX, Y, LDY )
*
   20 CONTINUE
*
  111 FORMAT( 'Error: N must be 90 + 5K' )
  112 FORMAT( 'Error: N must not be larger than LDA' )
*
      STOP
      END
```

Data files:

Filename/Key	Order	Number of nonzeros	Data type
TOLS90	90	1746	real
TOLS340	340	2196	real
TOLS1090	1090	3546	real
TOLS2000	2000	5184	real
TOLS4000	4000	8784	real

References S. Godet-Thobie, Eigenvalues of large highly nonnormal matrices, Ph.D. thesis, Paris IX Dauphine University, Dec. 1992. CERFACS thesis report TH/PA/93/06.

F. Chatelin and S. Godet-Thobie, Stability analysis in aeronautical industries, in Proceedings of the 2nd Symposium on High-Performance Computing, Montpellier, France, M. Durand and F. El Dabaghi eds, Elsevier/North-Holland, pp.415-422, 1991

A. Ruhe, Rational Krylov, a practical algorithm for large sparse nonsymmetric matrix pencils. Computer Science Division UCB/CSD-95-871, University of California, Berkeley, CA, April 1995.

Z. Bai, D. Day and Q. Ye, ABLE: an adaptive block Lanczos method for non-Hermitian eigenvalue problems, Research Report 95-04, Department of Mathematics, University of Kentucky, May 1995

Appendix C

Matrices in Subroutine Format

Title	Subroutine Names
Random Sparse Matrix Model elliptic Partial Differential Equation	MATRAN MATPDE

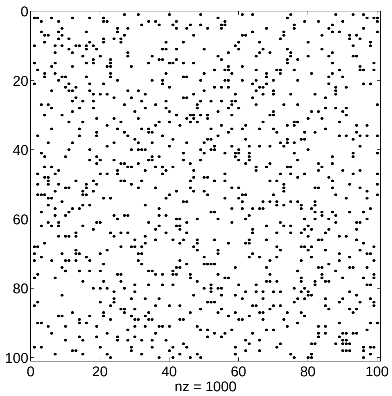
Title: Random Sparse Matrix
Subroutine name: MVMRAN

Source: authors

Discipline: numerical linear algebra

Further details: Random matrices are always the favorite test matrices in an algorithm test suit. We provide a subroutine which generates a random sparse matrix. Users can specify the matrix size, the number of nonzero entries in each column. The random numbers are from the uniform distribution on (-1,1). The generated matrix is stored in compressed column format. Utility routine `dspmvc.f` can be used for computing the matrix-vector products Ax and $A^T x$.

The following figure shows an example of the sparsity pattern of a random 100 by 100 matrix with 10 nonzero entries in each column.



Subroutine: FORTRAN calling sequences for generating a random sparse matrices with NZR nonzero elements per column is

```
SUBROUTINE MATRAN( N, NZR, ISEED, A, COLPRT, ROWIND )
```

with

`N` (input) INTEGER
The order of the matrix A.

`NZR` (input) INTEGER
The number of nonzero entries per column.

`ISEED` (input/output) INTEGER array, dimensio(4) on entry, the seed of the random number generator; the array elements must be between 0 and 4095, and ISEED(4) must be odd. On exit, the seed is updated.

`A` (output) DOUBLE PRECISION array, dimension (`N*NZR`)
the numerical values of the generated matrix.

`COLPTR` (output) INTEGER array, dimension (`N+1`)
the column start pointers.

ROWIND (output) INTEGER array, dimension (N*NZR)
The row indices.

References:

LAPACK random number generator DLARAN is used to generate random numbers.

Title: Partial differential equation
Subroutine name: MVMPDE

Source: H. Elman, University of Maryland

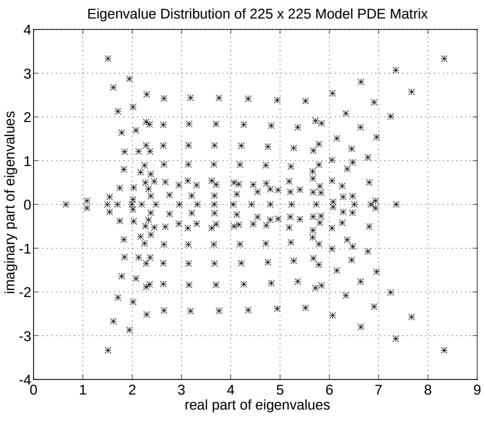
Discipline: partial differential equation

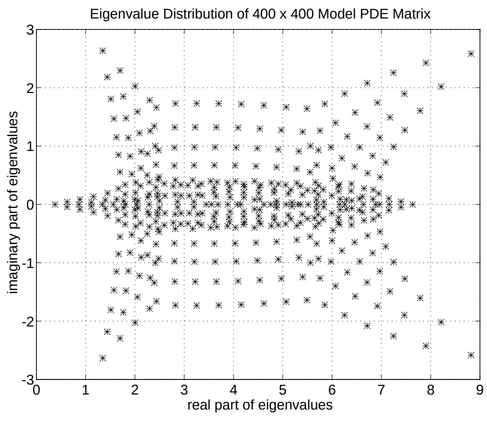
Further details: This test matrix is obtained from the finite difference discretization of the following two-dimensional partial differential operator

$$\begin{aligned}\mathcal{L}u &= -\frac{\partial}{\partial x}\left(e^{-xy}\frac{\partial u}{\partial x}\right) - \frac{\partial}{\partial y}\left(e^{xy}\frac{\partial u}{\partial y}\right) + \beta(x+y)\frac{\partial u}{\partial x} + \beta\frac{\partial}{\partial x}((x+y)u) + \\ &\quad \gamma(x+y)\frac{\partial u}{\partial y} + \gamma\frac{\partial}{\partial y}((x+y)u) + \frac{1}{1+x+y}u\end{aligned}$$

on the unit square $(0,1)\times(0,1)$ with Dirichlet boundary conditions, where $\beta, \gamma \in \mathbb{R}$ are parameters used to control the degree of nonormality of the matrices generated. We discretize the operator using central differences on an $m \times m$ grid with mesh size $h = 1/(m+1)$. This leads to a nonsymmetric matrix A of order $n = m^2$. It is suggested to use values of β and γ between 0 and 250. The object is to estimate those eigenvalues with the largest real parts and to determine whether or not there are significant gaps in the spectrum.

The following figure shows the eigenvalue distribution for orders 225 ($m = 15$) and 400 ($m = 20$) of the matrix with $\beta = 20$ and $\gamma = 0$.





Subroutine: FORTRAN calling sequences for generating a matrix A (which is stored in compressed row format) is

```
SUBROUTINE MATRAN( N, NZR, ISEED, A, ROWPRT, COLIND )
```

with

`N` (output) INTEGER
The order of the matrix A. `N` = `NX*NY`.

NX	(input) INTEGER The number of mesh points in the X-axis
NY	(input) INTEGER The number of mesh points in the Y-axis
A	(output) DOUBLE PRECISION array, dimension (NZ) the numerical values of the generated matrix, where the number of nonzero elements NZ = NX*NY + (NX-1)*NY*2 + NX*(NY-1)*2.
ROWPTR	(output) INTEGER array, dimension (N+1) the row start pointers.
COLIND	(output) INTEGER array, dimension (N*NZR) The column indices.
RHS	(output) DOUBLE PRECISION array, dimension (N) The right hand side of the linear system of equation $Ax = f$.

In addition, β and γ are set as internal parameters, which may be altered.

The utility routine `dspmvr.f` can be used for computing the matrix-vector products Ax and $A^T x$.

Data files:

Filename/Key	Order	Number of nonzeros	Data type
PDE225	225	1065	real
PDE900	900	4380	real
PDE2961	2961	14585	real

References:

H. Elman, Iterative Methods for Large Sparse Nonsymmetric Systems of Linear Equations. PhD thesis, Yale University, New Haven, CT, 1982.

J. Cullum and R. A. Willoughby, A Practical Procedure for Computing Eigenvalues of Large Sparse Nonsymmetric Matrices, In Large Scale Eigenvalue Problem, J. Cullum and R. A. Willoughby eds. Elsevier Science Pub. North-Holland, 1986.

R. W. Freund, M. H. Gutknecht, and N. M. Nachtigal. An implementation of the look-ahead Lanczos algorithm for non-Hermitian matrices. *SIAM J. Sci. Comput.*, 14:137–158, 1993.

Appendix C: List of Utility Routines

`dprtmt.f` FORTRAN subroutine for writing a real sparse matrix in the standard HB sparse format. It is assumed that the matrix is stored in the compressed column format.

`zprtmt.f` complex version of `dprtmt.f` .

`dreadm.f` FORTRAN subroutine for reading a real sparse matrix which is in standard HB sparse format.

`zreadm.f` complex version of `dreadm.f` .

`dreadhb.c` C subroutine for reading a real sparse matrix which is in standard HB sparse format.

`dm2hb.m` Matlab M-file for writing a real sparse matrix in the standard HB sparse format.

`zm2hb.m` complex version of `dm2hb.m` .

`dspmvc.f` FORTRAN subroutine for computing the matrix-vector product Ax or $A^T x$, it is assumed that A is stored in compressed column format.

`zspmvc.f` complex version of `dspmvc.f`.

`dspmvr.f` FORTRAN subroutine for computing the matrix-vector product Ax or $A^T x$, it is assumed that A is stored in compressed row format.

`zspmvr.f` complex version of `dspmvr.f`.

`mvm2hb.f` FORTRAN program to illustrate that if one has a matrix-vector product subroutine, how to write it in the standard HB sparse matrix format.

In addition, file `hb2matlabinfo` provides information how to get software from MathWork to read a HB sparse matrix format into Matlab.