

# Tutorial 4

## Numerical Linear Algebra

### Math 475/CS 475

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This tutorial is devoted to discussion of the computational methods used in numerical linear algebra. Topics discussed include, matrix multiplication, matrix transformations, numerical methods for solving systems of linear equations, the linear least squares, orthogonality, singular value decomposition, the matrix eigenvalue problem, and computations with sparse matrices.

#### 4.1 MATLAB functions used in Tutorial 4

The following MATLAB functions will be used in this tutorial.

| Function      | Description                                 |
|---------------|---|
| <b>abs</b>    | Absolute value                              |
| <b>chol</b>   | Cholesky factorization                      |
| <b>cond</b>   | Condition number                            |
| <b>det</b>    | Determinant                                 |
| <b>diag</b>   | Diagonal matrices and diagonals of a matrix |
| <b>diff</b>   | Difference and approximate derivative       |
| <b>eps</b>    | Floating point relative accuracy            |
| <b>eye</b>    | Identity matrix                             |
| <b>fliplr</b> | Flip matrix in left/right direction         |
| <b>flipud</b> | Flip matrix in up/down direction            |
| <b>flops</b>  | Floating point operation count              |
| <b>full</b>   | Convert sparse matrix to full matrix        |
| <b>funm</b>   | Evaluate general matrix function            |
| <b>hess</b>   | Hessenberg form                             |
| <b>hilb</b>   | Hilbert matrix                              |
| <b>imag</b>   | Complex imaginary part                      |
| <b>inv</b>    | Matrix inverse                              |
| <b>length</b> | Length of vector                            |
| <b>lu</b>     | LU factorization                            |
| <b>max</b>    | Largest component                           |

|               |                                      |
|---------------|--------------------------------------|
| <b>min</b>    | Smallest component                   |
| <b>norm</b>   | Matrix or vector norm                |
| <b>ones</b>   | Ones array                           |
| <b>pascal</b> | Pascal matrix                        |
| <b>pinv</b>   | Pseudoinverse                        |
| <b>qr</b>     | Orthogonal-triangular decomposition  |
| <b>rand</b>   | Uniformly distributed random numbers |
| <b>randn</b>  | Normally distributed random numbers  |
| <b>rank</b>   | Matrix rank                          |
| <b>real</b>   | Complex real part                    |
| <b>repmat</b> | Replicate and tile an array          |
| <b>schur</b>  | Schur decomposition                  |
| <b>sign</b>   | Signum function                      |
| <b>size</b>   | Size of matrix                       |
| <b>sqrt</b>   | Square root                          |
| <b>sum</b>    | Sum of elements                      |
| <b>svd</b>    | Singular value decomposition         |
| <b>tic</b>    | Start a stopwatch timer              |
| <b>toc</b>    | Read the stopwach timer              |
| <b>trace</b>  | Sum of diagonal entries              |
| <b>tril</b>   | Extract lower triangular part        |
| <b>triu</b>   | Extract upper triangular part        |
| <b>zeros</b>  | Zeros array                          |

## 4.2 The matrix-matrix product

Computation of the product of two or more matrices is one of the basic operations in the numerical linear algebra. Number of flops needed for computing a product of two matrices **A** and **B** can be decreased drastically if a special structure of matrices **A** and **B** is utilized properly. For instance, if both **A** and **B** are upper (lower) triangular, then the product of **A** and **B** is an upper (lower) triangular matrix.

```
function C = prod2t(A, B)

% Product C = A*B of two upper triangular matrices A and B.

[m,n] = size(A);
[u,v] = size(B);
if (m ~= n) | (u ~= v)
    error('Matrices must be square')
end
if n ~= u
    error('Inner dimensions must agree')
end
C = zeros(n);
for i=1:n
    for j=i:n
        C(i,j) = A(i,i:j)*B(i:j,j);
    end
end
end
```

In the following example a product of two random triangular matrices is computed using function `prod2t`. Number of flops is also determined.

```
A = triu(randn(4)); B = triu(rand(4));
flops(0)
C = prod2t(A, B)
nflps = flops

C =
   -0.4110   -1.2593   -0.6637   -1.4261
         0    0.9076    0.6371    1.7957
         0         0   -0.1149   -0.0882
         0         0         0     0.0462
nflps =
     36
```

For comparison, using MATLAB's "general purpose" matrix multiplication operator `*`, the number of flops needed for computing the product of matrices **A** and **B** is

```
flops(0)
A*B;
flops

ans =
    128
```

Product of two Hessenberg matrices **A** and **B**, where **A** is a lower Hessenberg and **B** is an upper Hessenberg can be computed using function `Hessprod`.

```
function C = Hessprod(A, B)

% Product C = A*B, where A and B are the lower and
% upper Hessenberg matrices, respectively.

[m, n] = size(A);
C = zeros(n);
for i=1:n
    for j=1:n
        if( j<n )
            l = min(i,j)+1;
        else
            l = n;
        end
        C(i,j) = A(i,1:l)*B(1:l,j);
    end
end
```

We will run this function on Hessenberg matrices obtained from the Hilbert matrix **H**

```
H = hilb(10);
```

```

A = tril(H,1);    B = triu(H,-1);

flops(0)

C = Hessprod(A,B);

nflps = flops

nflps =
    1039

```

Using the multiplication operator `*` the number of flops used for the same problem is

```

flops(0)

C = A*B;

nflps = flops

nflps =
    2000

```

For more algorithms for computing the matrix-matrix products see the subsequent sections of this tutorial.

## 4.3 Matrix transformations

The goal of this section is to discuss important matrix transformations that are used in numerical linear algebra.

On several occasions we will use function `ek(k, n)` – the  $k$ th coordinate vector in the  $n$ -dimensional Euclidean space

```

function v = ek(k, n)

% The k-th coordinate vector in the n-dimensional Euclidean space.

v = zeros(n,1);
v(k) = 1;

```

### 4.3.1 Gauss transformation

In many problems that arise in applied mathematics one wants to transform a matrix to an upper triangular one. This goal can be accomplished using the *Gauss transformation* (synonym: *elementary matrix*).

Let  $\mathbf{m}, \mathbf{e}_k \in \mathbb{R}^n$ . The Gauss transformation  $\mathbf{M}_k \equiv \mathbf{M}$  is defined as  $\mathbf{M} = \mathbf{I} - \mathbf{m}\mathbf{e}_k^T$ . Vector  $\mathbf{m}$  used here is called the *Gauss vector* and  $\mathbf{I}$  is the  $n$ -by- $n$  identity matrix. In this section we present two functions for computations with this transformation. For more information about this transformation the reader is referred to [3].

```

function m = Gaussv(x, k)

% Gauss vector m from the vector x and the position
% k (k > 0) of the pivot entry.

if x(k) == 0
    error('Wrong vector')
end;
n = length(x);
x = x(:);
if ( k > 0 & k < n )
    m = [zeros(k,1);x(k+1:n)/x(k)];
else
    error('Index k is out of range')
end

```

Let  $\mathbf{M}$  be the Gauss transformation. The matrix-vector product  $\mathbf{M}*\mathbf{b}$  can be computed without forming the matrix  $\mathbf{M}$  explicitly. Function **Gaussprod** implements a well-known formula for the product in question.

```

function c = Gaussprod(m, k, b)

% Product c = M*b, where M is the Gauss transformation
% determined by the Gauss vector m and its column
% index k.

n = length(b);
if ( k < 0 | k > n-1 )
    error('Index k is out of range')
end
b = b(:);
c = [b(1:k);-b(k)*m(k+1:n)+b(k+1:n)];

```

Let

```

x = 1:4; k = 2;
m = Gaussv(x,k)

```

```

m =
     0
     0
  1.5000
  2.0000

```

Then

```

c = Gaussprod(m, k, x)

c =
     1
     2
     0
     0

```

### 4.3.2 Householder transformation

The *Householder transformation*  $\mathbf{H}$ , where  $\mathbf{H} = \mathbf{I} - 2\mathbf{u}\mathbf{u}^T$ , also called the *Householder reflector*, is a frequently used tool in many problems of numerical linear algebra. Here  $\mathbf{u}$  stands for the real unit vector. In this section we give several functions for computations with this matrix.

```
function u = Housv(x)

% Householder reflection unit vector u from the vector x.

m = max(abs(x));
u = x/m;
if u(1) == 0
    su = 1;
else
    su = sign(u(1));
end
u(1) = u(1)+su*norm(u);
u = u/norm(u);
u = u(:);
```

Let

```
x = [1 2 3 4]';
```

Then

```
u = Housv(x)
```

```
u =
    0.7690
    0.2374
    0.3561
    0.4749
```

The Householder reflector  $\mathbf{H}$  is computed as follows

```
H = eye(length(x))-2*u*u'
```

```
H =
   -0.1826   -0.3651   -0.5477   -0.7303
   -0.3651    0.8873   -0.1691   -0.2255
   -0.5477   -0.1691    0.7463   -0.3382
   -0.7303   -0.2255   -0.3382    0.5490
```

An efficient method of computing the matrix-vector or matrix-matrix products with Householder matrices utilizes a special form of this matrix.

```

function P = Houspre(u, A)

% Product P = H*A, where H is the Householder reflector
% determined by the vector u and A is a matrix.

[n, p] = size(A);
m = length(u);
if m ~= n
    error('Dimensions of u and A must agree')
end
v = u/norm(u);
v = v(:);
P = [];
for j=1:p
    aj = A(:,j);
    P = [P aj-2*v*(v'*aj)];
end

```

Let

```
A = pascal(4);
```

and let

```
u = Housv(A(:,1))
```

```

u =
    0.8660
    0.2887
    0.2887
    0.2887

```

Then

```
P = Houspre(u, A)
```

```

P =
   -2.0000   -5.0000  -10.0000  -17.5000
   -0.0000   -0.0000   -0.6667   -2.1667
   -0.0000    1.0000    2.3333    3.8333
   -0.0000    2.0000    6.3333   13.8333

```

In some problems that arise in numerical linear algebra one has to compute a product of several Householder transformations. Let the Householder transformations are represented by their normalized reflection vectors stored in columns of the matrix  $\mathbf{V}$ . The product in question, denoted by  $\mathbf{Q}$ , is defined as

$$\mathbf{Q} = \mathbf{V}(:, 1) * \mathbf{V}(:, 2) * \dots * \mathbf{V}(:, n)$$

where  $n$  stands for the number of columns of the matrix  $\mathbf{V}$ .

```

function Q = Housprod(V)

% Product Q of several Householder transformations
% represented by their reflection vectors that are
% saved in columns of the matrix V.

[m, n] = size(V);
Q = eye(m)-2*V(:,n)*V(:,n)';
for i=n-1:-1:1
    Q = Houspre(V(:,i),Q);
end

```

Among numerous applications of the Householder transformation the following one: reduction of a square matrix to the upper Hessenberg form and reduction of an arbitrary matrix to the upper bidiagonal matrix, are of great importance in numerical linear algebra. It is well known that any square matrix  $A$  can always be transformed to an upper Hessenberg matrix  $H$  by orthogonal similarity (see [7] for more details). Householder reflectors are used in the course of computations. Function **Hessred** implements this method

```

function [A, V] = Hessred(A)

% Reduction of the square matrix A to the upper
% Hessenberg form using Householder reflectors.
% The reflection vectors are stored in columns of
% the matrix V. Matrix A is overwritten with its
% upper Hessenberg form.

[m,n] =size(A);
if A == triu(A,-1)
    V = eye(m);
    return
end
V = [];
for k=1:m-2
    x = A(k+1:m,k);
    v = Housv(x);
    A(k+1:m,k:m) = A(k+1:m,k:m) - 2*v*(v'*A(k+1:m,k:m));
    A(1:m,k+1:m) = A(1:m,k+1:m) - 2*(A(1:m,k+1:m)*v)*v';
    v = [zeros(k,1);v];
    V = [V v];
end

```

Householder reflectors used in these computations can easily be reconstructed from the columns of the matrix  $V$ . Let

```
A = [0 2 3;2 1 2;1 1 1];
```

To compute the upper Hessenberg form  $H$  of the matrix  $A$  we run function **Hessred** to obtain

```
[H, V] = Hessred(A)
```

```
H =
      0   -3.1305   1.7889
    -2.2361   2.2000  -1.4000
      0   -0.4000  -0.2000
V =
      0
     0.9732
     0.2298
```

The only Householder reflector  $\mathbf{P}$  used in the course of computations is shown below

```
P = eye(3)-2*V*V'
P =
     1.0000         0         0
         0    -0.8944   -0.4472
         0    -0.4472    0.8944
```

To verify correctness of these results it suffices to show that  $\mathbf{P}^*\mathbf{H}*\mathbf{P} = \mathbf{A}$ . We have

```
P*H*P
ans =
      0   2.0000   3.0000
     2.0000   1.0000   2.0000
     1.0000   1.0000   1.0000
```

Another application of the Householder transformation is to transform a matrix to an upper bidiagonal form. This reduction is required in some algorithms for computing the *singular value decomposition* (SVD) of a matrix. Function `upbid` works with square matrices only

```
function [A, V, U] = upbid(A)

% Bidiagonalization of the square matrix A using the
% Golub- Kahan method. The reflection vectors of the
% left Householder matrices are saved in columns of
% the matrix V, while the reflection vectors of the
% right Householder reflections are saved in columns
% of the matrix U. Matrix A is overwritten with its
% upper bidiagonal form.

[m, n] = size(A);
if m ~= n
    error('Matrix must be square')
end
if tril(triu(A),1) == A
    V = eye(n-1);
    U = eye(n-2);
end
V = [];
U = [];
```

```

for k=1:n-1
    x = A(k:n,k);
    v = Housv(x);
    l = k:n;
    A(l,l) = A(l,l) - 2*v*(v'*A(l,l));
    v = [zeros(k-1,1);v];
    V = [V v];
    if k < n-1
        x = A(k,k+1:n)';
        u = Housv(x);
        p = 1:n;
        q = k+1:n;
        A(p,q) = A(p,q) - 2*(A(p,q)*u)*u';
        u = [zeros(k,1);u];
        U = [U u];
    end
end
end

```

Let (see [1], Example 10.9.2, p.579)

```
A = [1 2 3;3 4 5;6 7 8];
```

Then

```
[B, V, U] = upbid(A)
```

```

B =
   -6.7823    12.7620    -0.0000
    0.0000     1.9741    -0.4830
    0.0000     0.0000    -0.0000
V =
    0.7574         0
    0.2920    -0.7248
    0.5840     0.6889
U =
         0
   -0.9075
   -0.4201

```

Let the matrices **V** and **U** be the same as in the last example and let

```
Q = Housprod(V); P = Housprod(U);
```

Then

```
Q'*A*P
```

```

ans =
   -6.7823    12.7620    -0.0000
    0.0000     1.9741    -0.4830
    0.0000    -0.0000     0.0000

```

which is the same as the bidiagonal form obtained earlier.

### 4.3.3 Givens transformation

*Givens transformation* (synonym: Givens rotation) is an orthogonal matrix used for zeroing a selected entry of the matrix. See [1] for details. Functions included here deal with this transformation.

```
function J = GivJ(x1, x2)

% Givens plane rotation J = [c s;-s c]. Entries c and s
% are computed using numbers x1 and x2.

if x1 == 0 & x2 == 0
    J = eye(2);
    return
end
if abs(x2) >= abs(x1)
    t = x1/x2;
    s = 1/sqrt(1+t^2);
    c = s*t;
else
    t = x2/x1;
    c = 1/sqrt(1+t^2);
    s = c*t;
end
J = [c s;-s c];
```

Premultiplication and postmultiplication by a Givens matrix can be performed without computing a Givens matrix explicitly.

```
function A = preGiv(A, J, i, j)

% Premultiplication of A by the Givens rotation
% which is represented by the 2-by-2 planar rotation
% J. Integers i and j describe position of the
% Givens parameters.

A([i j],:) = J*A([i j],:);
```

Let

```
A = [1 2 3;-1 3 4;2 5 6];
```

Our goal is to zero the (2,1) entry of the matrix **A**. First the Givens matrix **J** is created using function **GivJ**

```
J = GivJ(A(1,1), A(2,1))
```

```
J =
-0.7071    0.7071
-0.7071   -0.7071
```

Next, using function `preGiv` we obtain

```
A = preGiv(A,J,1,2)

A =
   -1.4142    0.7071    0.7071
         0   -3.5355   -4.9497
         2.0000    5.0000    6.0000
```

Postmultiplication by the Givens rotation can be accomplished using function `postGiv`

```
function A = postGiv(A, J, i, j)

% Postmultiplication of A by the Givens rotation
% which is represented by the 2-by-2 planar rotation
% J. Integers i and j describe position of the
% Givens parameters.

A(:,[i j]) = A(:,[i j])*J;
```

An important application of the Givens transformation is to compute the QR factorization of a matrix.

```
function [Q, A] = Givred(A)

% The QR factorization A = Q*R of the rectangular
% matrix A using Givens rotations. Here Q is the
% orthogonal matrix. On the output matrix A is
% overwritten with the matrix R.

[m, n] = size(A);
if m == n
    k = n-1;
elseif m > n
    k = n;
else
    k = m-1;
end
Q = eye(m);
for j=1:k
    for i=j+1:m
        J = GivJ(A(j,j),A(i,j));
        A = preGiv(A,J,j,i);
        Q = preGiv(Q,J,j,i);
    end
end
Q = Q';
```

Let

```
A = pascal(4)
```

```
A =
    1     1     1     1
    1     2     3     4
    1     3     6    10
    1     4    10    20
```

Then

```
[Q, R] = Givred(A)
```

```
Q =
    0.5000    -0.6708     0.5000    -0.2236
    0.5000    -0.2236    -0.5000     0.6708
    0.5000     0.2236    -0.5000    -0.6708
    0.5000     0.6708     0.5000     0.2236

R =
    2.0000     5.0000    10.0000    17.5000
    0.0000     2.2361     6.7082    14.0872
    0.0000         0     1.0000     3.5000
   -0.0000         0    -0.0000     0.2236
```

A relative error in the computed QR factorization of the matrix  $\mathbf{A}$  is

```
norm(A-Q*R)/norm(A)
```

```
ans =
    1.4738e-016
```

## 4.4 Solving systems of linear equations

A good numerical algorithm for solving a system of linear equations should, among other things, minimize computational complexity. If the matrix of the system has a special structure, then this fact should be utilized in the design of the algorithm. In this section, we give an overview of MATLAB's functions for computing a solution vector  $\mathbf{x}$  to the linear system  $\mathbf{Ax} = \mathbf{b}$ . To this end, we will assume that the matrix  $\mathbf{A}$  is a square matrix.

### 4.4.1 Triangular systems

If the matrix of the system is either a lower triangular or upper triangular, then one can easily design a computer code for computing the vector  $\mathbf{x}$ . We leave this task to the reader (see Problems 2 and 3).

### 4.4.2 The LU factorization

MATLAB's function `lu` computes the LU factorization  $\mathbf{PA} = \mathbf{LU}$  of the matrix  $\mathbf{A}$  using a partial pivoting strategy. Matrix  $\mathbf{L}$  is unit lower triangular,  $\mathbf{U}$  is upper triangular, and  $\mathbf{P}$  is the permutation matrix. Since  $\mathbf{P}$  is orthogonal, the linear system  $\mathbf{Ax} = \mathbf{b}$  is equivalent to  $\mathbf{LUx} = \mathbf{P}^T \mathbf{b}$ . This method is recommended for solving linear systems with multiple right hand sides.

Let

```
A = hilb(5);    b = [1 2 3 4 5]';
```

The following commands are used to compute the LU decomposition of  $\mathbf{A}$ , the solution vector  $\mathbf{x}$ , and the upper bound on the relative error in the computed solution

```
[L, U, P] = lu(A);
```

```
x = U \ (L \ (P' * b))
```

```
x =
 1.0e+004 *
    0.0125
   -0.2880
    1.4490
   -2.4640
    1.3230
```

```
r1_err = cond(A)*norm(b-A*x)/norm(b)
```

```
r1_err =
 4.3837e-008
```

Number of *decimal digits of accuracy* in the computed solution  $\mathbf{x}$  is defined as the negative decimal logarithm of the relative error (see e.g., [6]). Vector  $\mathbf{x}$  of the last example has

```
dda = -log10(r1_err)
```

```
dda =
 7.3582
```

about seven decimal digits of accuracy.

### 4.4.3 Cholesky factorization

For linear systems with symmetric positive definite matrices the recommended method is based on the Cholesky factorization  $\mathbf{A} = \mathbf{H}^T \mathbf{H}$  of the matrix  $\mathbf{A}$ . Here  $\mathbf{H}$  is the upper triangular matrix with positive diagonal entries. MATLAB's function `chol` calculates the matrix  $\mathbf{H}$  from  $\mathbf{A}$  or generates an error message if  $\mathbf{A}$  is not positive definite. Once the matrix  $\mathbf{H}$  is computed, the solution  $\mathbf{x}$  to  $\mathbf{Ax} = \mathbf{b}$  can be found using the trick used in 4.4.2.

## 4.5 The least squares solution and orthogonalization

In some problems of applied mathematics one seeks a solution to the *overdetermined linear system*  $\mathbf{Ax} = \mathbf{b}$ . In general, such a system is inconsistent. The least squares solution to this system is a vector  $\mathbf{x}$  that minimizes the Euclidean norm of the residual  $\mathbf{r} = \mathbf{b} - \mathbf{Ax}$ . Vector  $\mathbf{x}$  always exists, however it is not necessarily unique. For more details, see e.g., [7], p. 81. In this section we discuss methods for computing the least squares solution.

### 4.5.1 Using MATLAB built-in functions

MATLAB's backslash operator `\` can be used to find the least squares solution  $\mathbf{x} = \mathbf{A} \backslash \mathbf{b}$ . For the rank deficient systems a warning message is generated during the course of computations. A second MATLAB's function that can be used for computing the least squares solution is the `pinv` command. The solution is computed using the following command  $\mathbf{x} = \text{pinv}(\mathbf{A}) * \mathbf{b}$ . Here `pinv` stands for the *pseudoinverse* matrix. This method however, requires more flops than the backslash method does. For more information about the pseudoinverses, see Section 4.7 of this tutorial.

### 4.5.2 Normal equations

This classical method, which is due to C.F. Gauss, finds a vector  $\mathbf{x}$  that satisfies the *normal equations*  $\mathbf{A}^T \mathbf{A} \mathbf{x} = \mathbf{A}^T \mathbf{b}$ . The method under discussion is adequate when the condition number of  $\mathbf{A}$  is small.

```
function [x, dist] = lsqne(A, b)

% The least-squares solution x to the overdetermined
% linear system Ax = b. Matrix A must be of full column
% rank.

% Input:
%     A- matrix of the system
%     b- the right-hand sides
% Output:
%     x- the least-squares solution
%     dist- Euclidean norm of the residual b - Ax

[m, n] = size(A);
if (m <= n)
    error('System is not overdetermined')
end
if (rank(A) < n)
    error('Matrix must be of full rank')
end
H = chol(A'*A);
x = H \ (H' \ (A'*b));
r = b - A*x;
dist = norm(r);
```

Throughout the sequel the following matrix  $\mathbf{A}$  and the vector  $\mathbf{b}$  will be used to test various methods for solving the least squares problem

```
format long
```

```
A = [.5 .501;.5 .5011;0 0;0 0]; b = [1;-1;1;-1];
```

Using the method of normal equations we obtain

```
[x,dist] = lsqne(A,b)
```

```
x =
    1.0e+004 *
     2.00420001218025
    -2.00000001215472
dist =
    1.41421356237310
```

One can judge a quality of the computed solution by verifying orthogonality of the residual to the column space of the matrix  $\mathbf{A}$ . We have

```
err = A'*(b - A*x)
```

```
err =
    1.0e-011 *
     0.18189894035459
     0.24305336410179
```

### 4.5.3 Methods based on the QR factorization of a matrix

Most numerical methods for finding the least squares solution to the overdetermined linear systems are based on the orthogonal factorization of the matrix  $\mathbf{A} = \mathbf{QR}$ . There are two variants of the QR factorization method: the *full* and the *reduced* factorization. In the full version of the QR factorization the matrix  $\mathbf{Q}$  is an  $m$ -by- $m$  orthogonal matrix and  $\mathbf{R}$  is an  $m$ -by- $n$  matrix with an  $n$ -by- $n$  upper triangular matrix stored in rows 1 through  $n$  and having zeros everywhere else. The reduced factorization computes an  $m$ -by- $n$  matrix  $\mathbf{Q}$  with orthonormal columns and an  $n$ -by- $n$  upper triangular matrix  $\mathbf{R}$ . The QR factorization of  $\mathbf{A}$  can be obtained using one of the following methods:

- (i) Householder reflectors
- (ii) Givens rotations
- (iii) Modified Gram-Schmidt orthogonalization

#### Householder QR factorization

MATLAB function `qr` computes matrices  $\mathbf{Q}$  and  $\mathbf{R}$  using Householder reflectors. The command `[Q, R] = qr(A)` generates a full form of the QR factorization of  $\mathbf{A}$  while `[Q, R] = qr(A, 0)` computes the reduced form. The least squares solution  $\mathbf{x}$  to  $\mathbf{Ax} = \mathbf{b}$  satisfies the system of equations  $\mathbf{R}^T \mathbf{Rx} = \mathbf{A}^T \mathbf{b}$ . This follows easily from the fact that the associated residual  $\mathbf{r} = \mathbf{b} - \mathbf{Ax}$  is orthogonal to the column space of  $\mathbf{A}$ . Thus no explicit knowledge of the matrix  $\mathbf{Q}$  is required. Function `mylsq` will be used on several occasions to compute a solution to the overdetermined linear system  $\mathbf{Ax} = \mathbf{b}$  with known QR factorization of  $\mathbf{A}$

```
function x = mylsq(A, b, R)

% The least squares solution x to the overdetermined
% linear system Ax = b. Matrix R is such that R = Q'A,
% where Q is a matrix whose columns are orthonormal.

m = length(b);
[n,n] = size(R);
```

```

if m < n
    error('System is not overdetermined')
end
x = R \ (R' \ (A' * b));

```

Assume that the matrix **A** and the vector **b** are the same as above. Then

```

[Q,R] = qr(A,0);           % Reduced QR factorization of A

x = mylsq(A,b,R)

x =
    1.0e+004 *
    2.004200000000159
   -2.000000000000159

```

### Givens QR factorization

Another method of computing the QR factorization of a matrix uses Givens rotations rather than the Householder reflectors. Details of this method are discussed earlier in this tutorial. This method, however, requires more flops than the previous one. We will run function **Givred** on the overdetermined system introduced earlier in this chapter

```

[Q,R]= Givred(A);

x = mylsq(A,b,R)

x =
    1.0e+004 *
    2.004200000000026
   -2.000000000000026

```

### Modified Gram-Schmidt orthogonalization

The third method is a variant of the classical Gram-Schmidt orthogonalization. A version used in the function **mgs** is described in detail in [4]. Mathematically the Gram-Schmidt and the modified Gram-Schmidt method are equivalent, however the latter is more stable. This method requires that matrix **A** is of a full column rank

```

function [Q, R] = mgs(A)

% Modified Gram-Schmidt orthogonalization of the
% matrix A = Q*R, where Q is orthogonal and R upper
% is an upper triangular matrix. Matrix A must be
% of a full column rank.

[m, n] = size(A);
for i=1:n
    R(i,i) = norm(A(:,i));
    Q(:,i) = A(:,i)/R(i,i);
    for j=i+1:n

```

```

    R(i,j) = Q(:,i)'*A(:,j);
    A(:,j) = A(:,j) - R(i,j)*Q(:,i);
end
end

```

Running function `mgs` on our test system we obtain

```

[Q,R] = mgs(A);

x = mylsq(A,b,R)

```

```

x =
 1.0e+004 *
 2.004200000000022
-2.000000000000022

```

This small size overdetermined linear system was tested using three different functions for computing the QR factorization of the matrix **A**. In all cases the least squares solution was found using function `mylsq`. The flop count and the check of orthogonality of **Q** are contained in the following table. As a measure of closeness of the computed **Q** to its exact value is determined by  $\text{errorQ} = \text{norm}(\mathbf{Q}'\mathbf{Q} - \text{eye}(\mathbf{k}))$ , where  $\mathbf{k} = 2$  for the reduced form and  $\mathbf{k} = 4$  for the full form of the QR factorization

| Function             | Flop count | errorQ      |
|----------------------|------------|-------------|
| <code>qr(, 0)</code> | 138        | 2.6803e-016 |
| <code>Givred</code>  | 488        | 2.2204e-016 |
| <code>mgs</code>     | 98         | 2.2206e-012 |

For comparison the number of flops used by the backslash operator was equal to 122 while the `pinv` command found a solution using 236 flops.

Another method for computing the least squares solution finds first the QR factorization of the augmented matrix  $[\mathbf{A} \ \mathbf{b}]$  i.e.,  $\mathbf{QR} = [\mathbf{A} \ \mathbf{b}]$  using one of the methods discussed above. The least squares solution **x** is then found solving a linear system  $\mathbf{Ux} = \mathbf{Qb}$ , where **U** is an n-by- n principal submatrix of **R** and **Qb** is the n+1<sup>st</sup> column of the matrix **R**. See e.g., [7] for more details. Function `mylsqf` implements this method

```

function x = mylsqf(A, b, f, p)

% The least squares solution x to the overdetermined
% linear system Ax = b using the QR factorization.
% The input parameter f is the string holding the
% name of a function used to obtain the QR factorization.
% Fourth input parameter p is optional and should be
% set up to 0 if the reduced form of the qr function
% is used to obtain the QR factorization.

[m, n] = size(A);
if m <= n

```

```

    error('System is not overdetermined')
end
if nargin == 4
    [Q, R] = qr([A b],0);
else
    [Q, R] = feval(f,[A b]);
end
Qb = R(1:n,n+1);
R = R(1:n,1:n);
x = R\Qb;

```

A choice of a numerical algorithm for solving a particular problem is often a complex task. Factors that should be considered include numerical stability of a method used and accuracy of the computed solution, to mention the most important ones. It is not our intention to discuss these issues in this tutorial. The interested reader is referred to [5] and [3].

## 4.6 Singular value decomposition of a matrix

Many properties of a matrix can be derived from its *singular value decomposition* (SVD). The SVD is motivated by the following fact: the image of the unit sphere under the  $m$ -by- $n$  matrix is a hyperellipse. Function **SVDdemo** takes a 2-by-2 matrix and generates two graphs: the original circle together with two perpendicular vectors and their images under the transformation used. In the example that follows the function under discussion a unit circle **C** with center at the origin is transformed using a 2-by-2 matrix **A**.

```

function SVDdemo(A)

% This illustrates a geometric effect of the application
% of the 2-by-2 matrix A to the unit circle C.

t = linspace(0,2*pi,200);
x = sin(t);
y = cos(t);
[U,S,V] = svd(A);
vx = [0 V(1,1) 0 V(1,2)];
vy = [0 V(2,1) 0 V(2,2)];
axis equal
h1_line = plot(x,y,vx,vy);
set(h1_line(1), 'LineWidth',1.25)
set(h1_line(2), 'LineWidth',1.25, 'Color',[0 0 0])
grid
title('Unit circle C and right singular vectors v_i')
pause(5)
w = [x;y];
z = A*w;
U = U*S;
udx = [0 U(1,1) 0 U(1,2)];
udy = [0 U(2,1) 0 U(2,2)];
figure
h1_line = plot(udx,udy,z(1,:),z(2,:));
set(h1_line(2), 'LineWidth',1.25, 'Color',[0 0 1])
set(h1_line(1), 'LineWidth',1.25, 'Color',[0 0 0])
grid

```

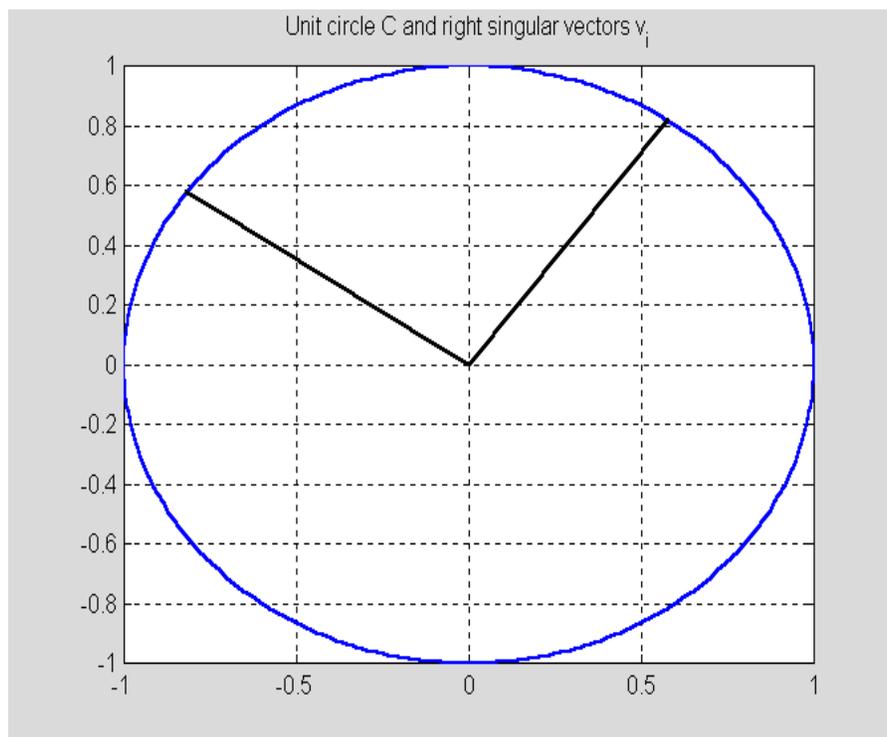
```
title('Image A*C of C and vectors \sigma_iu_i')
```

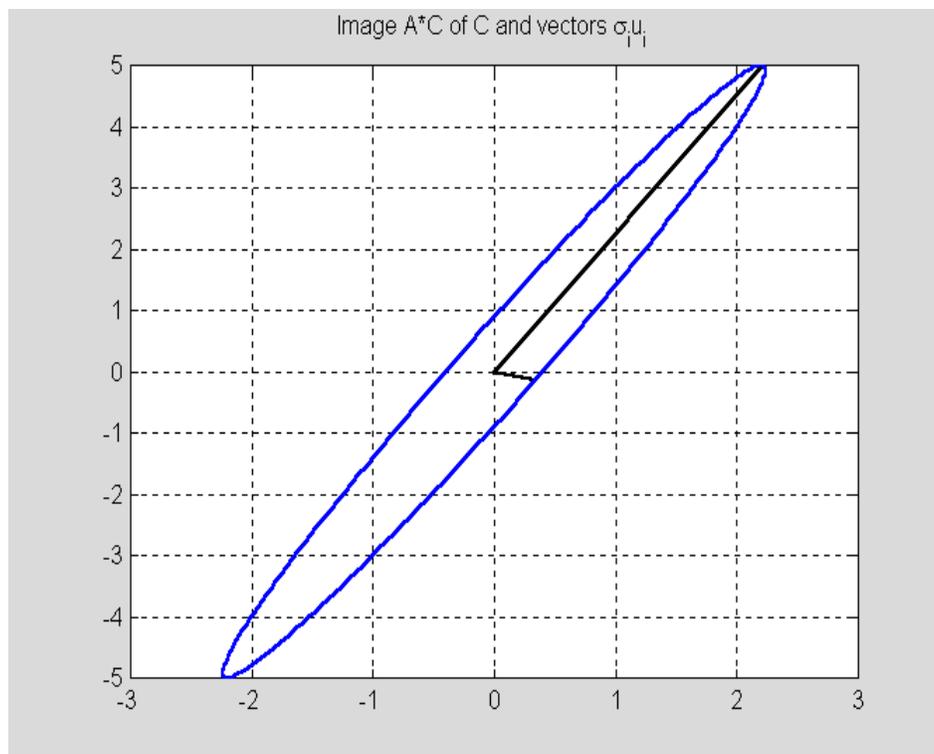
Define a matrix

```
A = [1 2;3 4];
```

Then

```
SVDdemo(A)
```





The *full form* of the singular value decomposition of the  $m$ -by- $n$  matrix  $\mathbf{A}$  (real or complex) is the factorization of the form  $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^*$ , where  $\mathbf{U}$  and  $\mathbf{V}$  are unitary matrices of dimensions  $m$  and  $n$ , respectively and  $\mathbf{S}$  is an  $m$ -by- $n$  diagonal matrix with nonnegative diagonal entries stored in the nonincreasing order. Columns of matrices  $\mathbf{U}$  and  $\mathbf{V}$  are called the *left singular vectors* and the *right singular vectors*, respectively. The diagonal entries of  $\mathbf{S}$  are the *singular values* of the matrix  $\mathbf{A}$ . MATLAB's function `svd` computes matrices of the SVD of  $\mathbf{A}$  by invoking the command `[U, S, V] = svd(A)`. The *reduced form* of the SVD of the matrix  $\mathbf{A}$  is computed using function `svd` with a second input parameter being set to zero `[U, S, V] = svd(A, 0)`. If  $m > n$ , then only the first  $n$  columns of  $\mathbf{U}$  are computed and  $\mathbf{S}$  is an  $n$ -by- $n$  matrix.

Computation of the SVD of a matrix is a nontrivial task. A common method used nowadays is the *two-phase method*. Phase one reduces a given matrix  $\mathbf{A}$  to an upper bidiagonal form using the Golub-Kahan method. Phase two computes the SVD of  $\mathbf{A}$  using a variant of the QR factorization. Function `mysvd` implements a method proposed in Problem 4.15 in [4]. This code works for the 2-by-2 real matrices only.

```
function [U, S, V] = mysvd(A)
```

```
% Singular value decomposition A = U*S*V' of a
% 2-by-2 real matrix A. Matrices U and V are orthogonal.
% The left and the right singular vectors of A are stored
% in columns of matrices U and V, respectively. Singular
% values of A are stored, in the nonincreasing order, on
% the main diagonal of the diagonal matrix S.
```

```

if A == zeros(2)
    S = zeros(2);
    U = eye(2);
    V = eye(2);
    return
end
[S, G] = symmat(A);
[S, J] = diagmat(S);
U = G'*J;
V = J;
d = diag(S);
s = sign(d);
for j=1:2
    if s(j) < 0
        U(:,j) = -U(:,j);
    end
end
d = abs(d);
S = diag(d);
if d(1) < d(2)
    d = flipud(d);
    S = diag(d);
    U = fliplr(U);
    V = fliplr(V);
end
end

```

In order to run this function two other functions **symmat** and **diagmat** must be in MATLAB's search path

```

function [S, G] = symmat(A)

% Symmetric 2-by-2 matrix S from the matrix A. Matrices
% A, S, and G satisfy the equation G*A = S, where G
% is the Givens plane rotation.

if A(1,2) == A(2,1)
    S = A;
    G = eye(2);
    return
end
t = (A(1,1) + A(2,2))/(A(1,2) - A(2,1));
s = 1/sqrt(1 + t^2);
c = -t*s;
G(1,1) = c;
G(2,2) = c;
G(1,2) = s;
G(2,1) = -s;
S = G*A;

function [D, G] = diagmat(A);

% Diagonal matrix D obtained by an application of the
% two-sided Givens rotation to the matrix A. Second output
% parameter G is the Givens rotation used to diagonalize
% matrix A, i.e., G.'*A*G = D.

```

```

if A ~= A'
    error('Matrix must be symmetric')
end
if abs(A(1,2)) < eps & abs(A(2,1)) < eps
    D = A;
    G = eye(2);
    return
end
r = roots([-1 (A(1,1)-A(2,2))/A(1,2) 1]);
[t, k] = min(abs(r));
t = r(k);
c = 1/sqrt(1+t^2);
s = c*t;
G = zeros(size(A));
G(1,1) = c;
G(2,2) = c;
G(1,2) = s;
G(2,1) = -s;
D = G.'*A*G;

```

Let

```
A = [1 2;3 4];
```

Then

```
[U,S,V] = mysvd(A)
```

```

U =
    0.4046   -0.9145
    0.9145    0.4046
S =
    5.4650    0
         0    0.3660
V =
    0.5760    0.8174
    0.8174   -0.5760

```

To verify this result we compute

```
AC = U*S*V'
```

```

AC =
    1.0000    2.0000
    3.0000    4.0000

```

and the relative error in the computed SVD decomposition

```
norm(AC-A)/norm(A)
```

```

ans =
    1.8594e-016

```

Another algorithm for computing the least squares solution  $\mathbf{x}$  of the overdetermined linear system  $\mathbf{Ax} = \mathbf{b}$  utilizes the singular value decomposition of  $\mathbf{A}$ . Function `lsqsvd` should be used for ill-conditioned or rank deficient matrices.

```
function x = lsqsvd(A, b)

% The least squares solution x to the overdetermined
% linear system Ax = b using the reduced singular
% value decomposition of A.

[m, n] = size(A);
if m <= n
    error('System must be overdetermined')
end
[U,S,V] = svd(A,0);
d = diag(S);
r = sum(d > 0);
b1 = U(:,1:r)'\*b;
w = d(1:r).\*b1;
x = V(:,1:r)*w;
re = b - A*x;           % One step of the iterative
b1 = U(:,1:r)'\*re;    % refinement
w = d(1:r).\*b1;
e = V(:,1:r)*w;
x = x + e;
```

The linear system with

```
A = ones(6,3); b = ones(6,1);
```

is ill-conditioned and rank deficient. Therefore the least squares solution to this system is not unique

```
x = lsqsvd(A,b)
```

```
x =
    0.3333
    0.3333
    0.3333
```

## 4.7 The pseudoinverse of a matrix

Another application of the SVD is for computing the *pseudoinverse* of a matrix. Singular or rectangular matrices always possess the pseudoinverse matrix. Let the matrix  $\mathbf{A}$  be defined as follows

```
A = [1 2 3;4 5 6]
```

```
A =
     1     2     3
     4     5     6
```

Its pseudoinverse is

```
B = pinv(A)
```

```
B =
  -0.9444    0.4444
  -0.1111    0.1111
   0.7222   -0.2222
```

The pseudoinverse **B** of the matrix **A** satisfy the *Penrose conditions*

$$\mathbf{ABA} = \mathbf{A}, \mathbf{BAB} = \mathbf{B}, (\mathbf{AB})^T = \mathbf{AB}, (\mathbf{BA})^T = \mathbf{BA}$$

We will verify the first condition only

```
norm(A*B*A-A)
```

```
ans =
  3.6621e-015
```

and leave it to the reader to verify the remaining ones.

## 4.8 The matrix eigenvalue problem

The matrix eigenvalue problem, briefly discussed in Tutorial 3, is one of the central problems in the numerical linear algebra. It is formulated as follows.

Given a square matrix  $\mathbf{A} = [a_{ij}]$ ,  $1 \leq i, j \leq n$ , find a nonzero vector  $\mathbf{x} \in \mathbb{R}^n$  and a number  $\lambda$  that satisfy the equation  $\mathbf{Ax} = \lambda\mathbf{x}$ . Number  $\lambda$  is called the *eigenvalue* of the matrix **A** and **x** is the associated *right eigenvector* of **A**.

In this section we will show how to localize the eigenvalues of a matrix using celebrated Gershgorin's Theorem. Also, we will present MATLAB's code for computing the dominant eigenvalue and the associated eigenvector of a matrix. The *QR iteration* for computing all eigenvalues of the symmetric matrices is also discussed.

Gershgorin Theorem states that each eigenvalue  $\lambda$  of the matrix **A** satisfies at least one of the following inequalities  $|\lambda - a_{kk}| \leq r_k$ , where  $r_k$  is the sum of all off-diagonal entries in row **k** of the matrix  $|\mathbf{A}|$  (see, e.g., [1], pp.400-403 for more details). Function **Gershg** computes the centers and the radii of the Gershgorin circles of the matrix **A** and plots all Gershgorin circles. The eigenvalues of the matrix **A** are also displayed.

```
function [C] = Gershg(A)
```

```
% Gershgorin's circles C of the matrix A.
```

```
d = diag(A);
cx = real(d);
cy = imag(d);
B = A - diag(d);
```

```

[m, n] = size(A);
r = sum(abs(B'));
C = [cx cy r(:)];
t = 0:pi/100:2*pi;
c = cos(t);
s = sin(t);
[v,d] = eig(A);
d = diag(d);
u1 = real(d);
v1 = imag(d);
hold on
grid on
axis equal
xlabel('Re')
ylabel('Im')
h1_line = plot(u1,v1,'or');
set(h1_line,'LineWidth',1.5)
for i=1:n
x = zeros(1,length(t));
y = zeros(1,length(t));
    x = cx(i) + r(i)*c;
    y = cy(i) + r(i)*s;
    h2_line = plot(x,y);
    set(h2_line,'LineWidth',1.2)
end
hold off
title('Gershgorin circles and the eigenvalues of a')

```

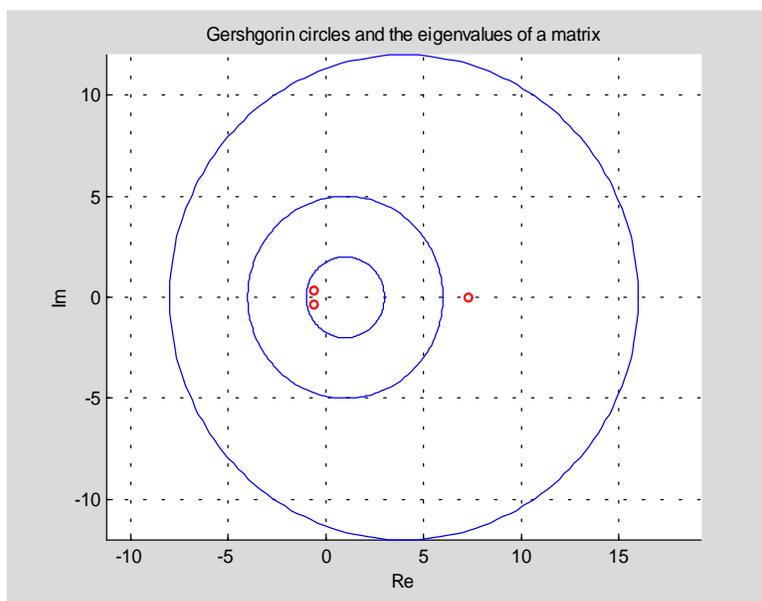
To illustrate functionality of this function we define a matrix **A**, where

```
A = [1 2 3;3 4 9;1 1 1];
```

Then

```
C = Gershg(A)
```

```
C =
    1     0     5
    4     0    12
    1     0     2
```



Information about each circle (coordinates of the origin and its radius) is contained in successive rows of the matrix  $\mathbf{C}$ .

It is well known that the eigenvalues are sensitive to small changes in the entries of the matrix (see, e.g., [3]). The *condition number of the simple eigenvalue*  $\lambda$  of the matrix  $\mathbf{A}$  is defined as follows

$$\mathbf{Cond}(\lambda) = 1/|\mathbf{y}^T \mathbf{x}|$$

where  $\mathbf{y}$  and  $\mathbf{x}$  are the left and right eigenvectors of  $\mathbf{A}$ , respectively with  $\|\mathbf{x}\|_2 = \|\mathbf{y}\|_2 = 1$ . Recall that a nonzero vector  $\mathbf{y}$  is said to be a *left eigenvector* of  $\mathbf{A}$  if  $\mathbf{y}^T \mathbf{A} = \lambda \mathbf{y}^T$ . Clearly  $\mathbf{Cond}(\lambda) \geq 1$ . Function `eigsen` computes the condition number of all eigenvalues of a matrix.

```
function s = eigsen(A)

% Condition numbers s of all eigenvalues of the diagonalizable
% matrix A.

[n,n] = size(A);
[v1,la1] = eig(A);
[v2,la2] = eig(A');
[d1, j] = sort(diag(la1));
v1 = v1(:,j);
[d2, j] = sort(diag(la2));
v2 = v2(:,j);
s = [];
for i=1:n
    v1(:,i) = v1(:,i)/norm(v1(:,i));
    v2(:,i) = v2(:,i)/norm(v2(:,i));
    s = [s;1/abs(v1(:,i)'\*v2(:,i))];
end
```

In this example we will illustrate sensitivity of the eigenvalues of the celebrated Wilkinson's matrix  $\mathbf{W}$ . Its is an upper bidiagonal 20-by-20 matrix with diagonal entries 20, 19, ..., 1. The superdiagonal entries are all equal to 20. We create this matrix using some MATLAB functions that are discussed in Section 4.9.

```
W = spdiags([(20:-1:1)', 20*ones(20,1)],[0 1], 20,20);
format long
s = eigsen(full(W))
```

```
s =
 1.0e+012 *
 0.00008448192546
 0.00145503286853
 0.01206523295175
 0.06389158525507
 0.24182386727359
 0.69411856608888
 1.56521713930244
 2.83519277292867
 4.18391920177580
 5.07256664475500
 5.07256664475500
 4.18391920177580
 2.83519277292867
 1.56521713930244
 0.69411856608888
 0.24182386727359
 0.06389158525507
 0.01206523295175
 0.00145503286853
 0.00008448192546
```

Clearly all eigenvalues of the Wilkinson's matrix are sensitive.

Let us perturb the  $w_{20,1}$  entry of  $\mathbf{W}$

```
W(20,1)=1e-5;
```

and next compute the eigenvalues of the perturbed matrix

```
eig(full(W))

ans =
-1.00978219090288
-0.39041284468158 + 2.37019976472684i
-0.39041284468158 - 2.37019976472684i
 1.32106082150033 + 4.60070993953446i
 1.32106082150033 - 4.60070993953446i
 3.88187526711025 + 6.43013503466255i
 3.88187526711025 - 6.43013503466255i
 7.03697639135041 + 7.62654906220393i
```

```

7.03697639135041 - 7.62654906220393i
10.499999999999714 + 8.04218886506797i
10.499999999999714 - 8.04218886506797i
13.96302360864989 + 7.62654906220876i
13.96302360864989 - 7.62654906220876i
17.11812473289285 + 6.43013503466238i
17.11812473289285 - 6.43013503466238i
19.67893917849915 + 4.60070993953305i
19.67893917849915 - 4.60070993953305i
21.39041284468168 + 2.37019976472726i
21.39041284468168 - 2.37019976472726i
22.00978219090265

```

Note a dramatic change in the eigenvalues.

In some problems only selected eigenvalues and associated eigenvectors are needed. Let the eigenvalues  $\{\lambda_k\}$  be rearranged so that  $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ . The *dominant eigenvalue*  $\lambda_1$  and/or the associated eigenvector can be found using one of the following methods: power iteration, inverse iteration, and Rayleigh quotient iteration. Functions **powerit** and **Rqi** implement the first and the third method, respectively.

```
function [la, v] = powerit(A, v)
```

```

% Power iteration with the Rayleigh quotient.
% Vector v is the initial estimate of the eigenvector of
% the matrix A. Computed eigenvalue la and the associated
% eigenvector v satisfy the inequality% norm(A*v - la*v,1) < tol,
% where tol = length(v)*norm(A,1)*eps.

```

```

if norm(v) ~= 1
    v = v/norm(v);
end
la = v'*A*v;
tol = length(v)*norm(A,1)*eps;
while norm(A*v - la*v,1) >= tol
    w = A*v;
    v = w/norm(w);
    la = v'*A*v;
end

```

```
function [la, v] = Rqi(A, v, iter)
```

```

% The Rayleigh quotient iteration.
% Vector v is an approximation of the eigenvector associated with the
% dominant eigenvalue la of the matrix A. Iterative process is
% terminated either if norm(A*v - la*v,1) < norm(A,1)*length(v)*eps
% or if the number of performed iterations reaches the allowed number
% of iterations iter.

```

```

if norm(v) > 1
    v = v/norm(v);
end
la = v'*A*v;
tol = norm(A,1)*length(v)*eps;
for k=1:iter

```

```

    if norm(A*v - la*v,1) < tol
        return
    else
        w = (A - la*eye(size(A)))\v;
        v = w/norm(w);
        la = v'*A*v;
    end
end

```

Let ([7], p.208, Example 27.1)

```
A = [2 1 1;1 3 1;1 1 4]; v = ones(3,1);
```

Then

```
format long
```

```
flops(0)
```

```
[la, v] = powerit(A, v)
```

```
la =
```

```
5.21431974337753
```

```
v =
```

```
0.39711254978701
```

```
0.52065736843959
```

```
0.75578934068378
```

```
flops
```

```
ans =
```

```
3731
```

Using function **Rqi**, for computing the dominant eigenpair of the matrix **A**, we obtain

```
flops(0)
```

```
[la, v] = Rqi(A,ones(3,1),5)
```

```
la =
```

```
5.21431974337754
```

```
v =
```

```
0.39711254978701
```

```
0.52065736843959
```

```
0.75578934068378
```

```
flops
```

```
ans =
```

```
512
```

Once the dominant eigenvalue (eigenpair) is computed one can find another eigenvalue or eigenpair by applying a process called *deflation*. For details the reader is referred to [4], pp. 127-128.

```
function [l2, v2, B] = defl(A, v1)

% Deflated matrix B from the matrix A with a known eigenvector v1 of A.
% The eigenpair (l2, v2) of the matrix A is computed.
% Functions Housv, Houspre, Housmvp and Rqi are used
% in the body of the function defl.

n = length(v1);
v1 = Housv(v1);
C = Houspre(v1,A);
B = [];
for i=1:n
    B = [B Housmvp(v1,C(i,:))];
end
l1 = B(1,1);
b = B(1,2:n);
B = B(2:n,2:n);
[l2, y] = Rqi(B, ones(n-1,1),10);
if l1 ~= l2
    a = b*y/(l2-l1);
    v2 = Housmvp(v1,[a;y]);
else
    v2 = v1;
end
```

Let **A** be an 5-by-5 *Pei matrix*, i.e.,

```
A = ones(5)+diag(ones(5,1))
```

```
A =
     2     1     1     1     1
     1     2     1     1     1
     1     1     2     1     1
     1     1     1     2     1
     1     1     1     1     2
```

Its dominant eigenvalue is  $\lambda_1 = 6$  and all the remaining eigenvalues are equal to one. To compute the dominant eigenpair of **A** we use function **Rqi**

```
[l1,v1] = Rqi(A,rand(5,1),10)
```

```
l1 =
 6.000000000000000
v1 =
 0.44721359549996
 0.44721359549996
 0.44721359549996
 0.44721359549996
 0.44721359549996
```

and next apply function **defl** to compute another eigenpair of **A**

```
[l2,v2] = defl(A,v1)
```

```
l2 =
    1.000000000000000
v2 =
   -0.894427190999992
    0.22360679774998
    0.22360679774998
    0.22360679774998
    0.22360679774998
```

To check these results we compute the norms of the "residuals"

```
[norm(A*v1-l1*v1);norm(A*v2-l2*v2)]
```

```
ans =
    1.0e-014 *
    0.07691850745534
    0.14571016336181
```

To this end we will deal with the *symmetric eigenvalue problem*. It is well known that the eigenvalues of a symmetric matrix are all real. One of the most efficient algorithms is the QR iteration with or without shifts. The algorithm included here is the two-phase algorithm. Phase one reduces a symmetric matrix  $\mathbf{A}$  to the symmetric tridiagonal matrix  $\mathbf{T}$  using MATLAB's function `hess`. Since  $\mathbf{T}$  is orthogonally similar to  $\mathbf{A}$ ,  $\text{sp}(\mathbf{A}) = \text{sp}(\mathbf{T})$ . Here  $\text{sp}$  stands for the *spectrum* of a matrix. During the phase two the off diagonal entries of  $\mathbf{T}$  are annihilated. This is an iterative process, which theoretically is an infinite one. In practice, however, the off diagonal entries approach zero fast. For details the reader is referred to [2] and [7].

Function `qrsft` computes all eigenvalues of the symmetric matrix  $\mathbf{A}$ . Phase two uses *Wilkinson's shift*. The latter is computed using function `wsft`.

```
function [la, v] = qrsft(A)

% All eigenvalues la of the symmetric matrix A.
% Method used: the QR algorithm with Wilkinson's shift.
% Function wsft is used in the body of the function qrsft.

[n, n] = size(A);
A = hess(A);
la = [];
i = 0;
while i < n
    [j, j] = size(A);
    if j == 1
        la = [la;A(1,1)];
        return
    end
    mu = wsft(A);
    [Q, R] = qr(A - mu*eye(j));
    A = R*Q + mu*eye(j);
```

```

    if abs(A(j,j-1)) < 10*(abs(A(j-1,j-1))+abs(A(j,j)))*eps
        la = [la;A(j,j)];
        A = A(1:j-1,1:j-1);
        i = i + 1;
    end
end
end

```

```
function mu = wsft(A)
```

```
% Wilkinson's shift mu of the symmetric matrix A.
```

```

[n, n] = size(A);
if A == diag(diag(A))
    mu = A(n,n);
    return
end
mu = A(n,n);
if n > 1
    d = (A(n-1,n-1)-mu)/2;
    if d ~= 0
        sn = sign(d);
    else
        sn = 1;
    end
    bn = A(n,n-1);
    mu = mu - sn*bn^2/(abs(d) + sqrt(d^2+bn^2));
end
end

```

We will test function `qrsft` on the matrix `A` used earlier in this section

```
A = [2 1 1;1 3 1;1 1 4];
```

```
la = qrsft(A)
```

```

la =
    5.21431974337753
    2.46081112718911
    1.32486912943335

```

Function `eigv` computes both the eigenvalues and the eigenvectors of a symmetric matrix provided the eigenvalues are distinct. A method for computing the eigenvectors is discussed in [1], Algorithm 8.10.2, pp. 452-454

```
function [la, V] = eigv(A)
```

```
% Eigenvalues la and eigenvectors V of the symmetric
% matrix A with distinct eigenvalues.
```

```

V = [];
[n, n] = size(A);
[Q,T] = schur(A);
la = diag(T);

```

```

if nargin == 2
    d = diff(sort(la));
    for k=1:n-1
        if d(k) < 10*eps
            d(k) = 0;
        end
    end
    if ~all(d)
        disp('Eigenvalues must be distinct')
    else
        for k=1:n
            U = T - la(k)*eye(n);
            t = U(1:k,1:k);
            y1 = [];
            if k>1
                t11 = t(1:k-1,1:k-1);
                s = t(1:k-1,k);
                y1 = -t11\s;
            end
            y = [y1;1];
            z = zeros(n-k,1);
            y = [y;z];
            v = Q*y;
            V = [V v/norm(v)];
        end
    end
end

```

We will use this function to compute the eigenvalues and the eigenvectors of the matrix **A** of the last example

```
[la, V] = eigv(A)
```

```

la =
    1.32486912943335
    2.46081112718911
    5.21431974337753
V =
    0.88765033882045   -0.23319197840751    0.39711254978701
   -0.42713228706575   -0.73923873953922    0.52065736843959
   -0.17214785894088    0.63178128111780    0.75578934068378

```

To check these results let us compute the residuals  $\mathbf{A}\mathbf{v} - \lambda\mathbf{v}$

```
A*V-V*diag(la)
```

```

ans =
    1.0e-014 *
         0   -0.09992007221626    0.13322676295502
   -0.02220446049250   -0.42188474935756    0.44408920985006
         0    0.11102230246252   -0.13322676295502

```

## 4.9 Sparse matrices in MATLAB

MATLAB has several built-in functions for computations with sparse matrices. A partial list of these functions is included here.

| Function         | Description                          |
|------------------|--------------------------------------|
| <b>condest</b>   | Condition estimate for sparse matrix |
| <b>eigs</b>      | Few eigenvalues                      |
| <b>find</b>      | Find indices of nonzero entries      |
| <b>full</b>      | Convert sparse matrix to full matrix |
| <b>issparse</b>  | True for sparse matrix               |
| <b>nnz</b>       | Number of nonzero entries            |
| <b>nonzeros</b>  | Nonzero matrix entries               |
| <b>sparse</b>    | Create sparse matrix                 |
| <b>spdiags</b>   | Sparse matrix formed from diagonals  |
| <b>speye</b>     | Sparse identity matrix               |
| <b>spfun</b>     | Apply function to nonzero entries    |
| <b>sprand</b>    | Sparse random matrix                 |
| <b>sprandsym</b> | Sparse random symmetric matrix       |
| <b>spy</b>       | Visualize sparsity pattern           |
| <b>svds</b>      | Few singular values                  |

Function **spy** works for matrices in full form as well.

### Computations with sparse matrices

The following MATLAB functions work with sparse matrices: **chol**, **det**, **inv**, **jordan**, **lu**, **qr**, **size**, **\**.

Command **sparse** is used to create a *sparse* form of a matrix.

Let

```
A = [0 0 1 1; 0 1 0 0; 0 0 0 1];
```

Then

```
B = sparse(A)
```

```
B =
      (2,2)      1
      (1,3)      1
      (1,4)      1
      (3,4)      1
```

Command **full** converts a sparse form of a matrix to the full form

```
C = full(B)
```

```
C =
    0     0     1     1
    0     1     0     0
    0     0     0     1
```

Command **sparse** has the following syntax

```
sparse(k,l,s,m,n)
```

where **k** and **l** are arrays of row and column indices, respectively, **s** is an array of nonzero numbers whose indices are specified in **k** and **l**, and **m** and **n** are the row and column dimensions, respectively.

Let

```
S = sparse([1 3 5 2], [2 1 3 4], [1 2 3 4], 5, 5)
```

```
S =
    (3,1)      2
    (1,2)      1
    (5,3)      3
    (2,4)      4
```

```
F = full(S)
```

```
F =
    0     1     0     0     0
    0     0     0     4     0
    2     0     0     0     0
    0     0     0     0     0
    0     0     3     0     0
```

To create a sparse matrix with several diagonals parallel to the main diagonal one can use the command **spdiags**. Its syntax is shown below

```
spdiags(B, d, m, n)
```

The resulting matrix is an m-by-n sparse matrix. Its diagonals are the columns of the matrix **B**. Location of the diagonals are described in the vector **d**.

Function **mytrid** creates a sparse form of the tridiagonal matrix with constant entries along the diagonals.

```
function T = mytrid(a,b,c,n)
```

```
% The n-by-n tridiagonal matrix T with constant entries  
% along diagonals. All entries on the subdiagonal, main  
% diagonal, and the superdiagonal are equal a, b, and c,  
% respectively.
```

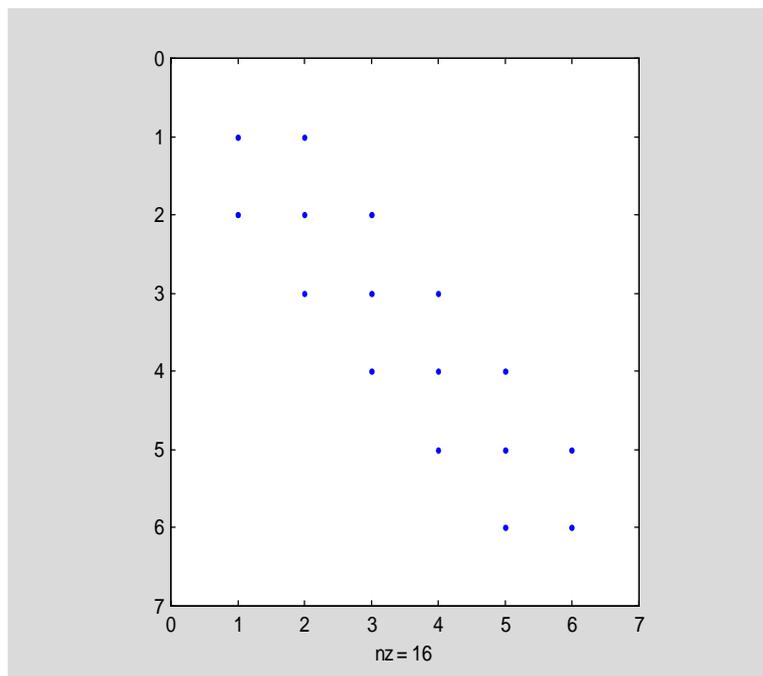
```
e = ones(n,1);
T = spdiags([a*e b*e c*e],[-1:1,n,n]);
```

To create a symmetric 6-by-6-tridiagonal matrix with all diagonal entries are equal 4 and all subdiagonal and superdiagonal entries are equal to one execute the following command

```
T = mytrid(1,4,1,6);
```

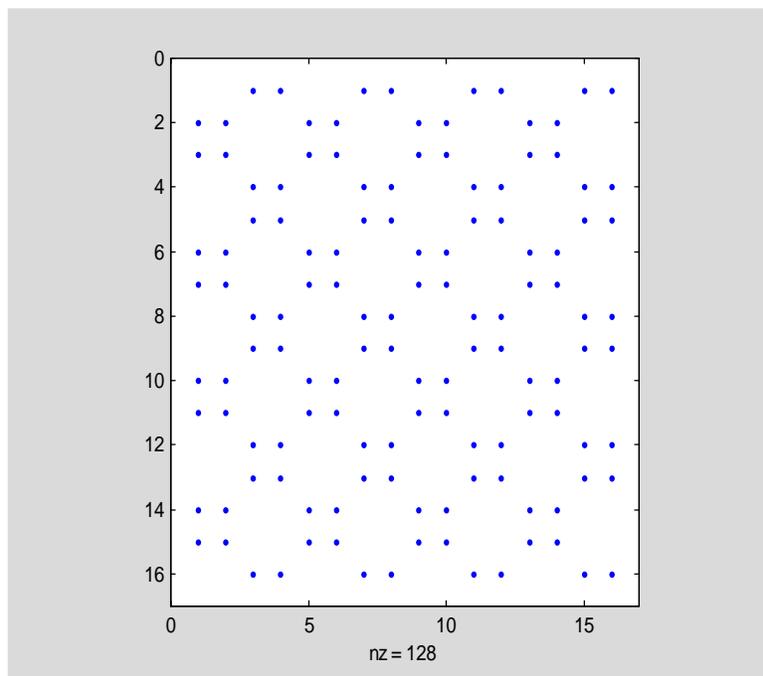
Function `spy` creates a graph of the matrix. The nonzero entries are displayed as the dots.

```
spy( T )
```



The following is the example of a sparse matrix created with the aid of the nonsparse matrix `magic`

```
spy(rem(magic(16),2))
```



Using a sparse form rather than the full form of a matrix one can reduce a number of flops used.  
Let

```
A = sprand(50,50,.25);
```

The above command generates a 50-by-50 random sparse matrix **A** with a density of about 25%.  
We will use this matrix to solve a linear system **Ax = b** with

```
b = ones(50,1);
```

Number of flops used is determined in usual way

```
flops(0)
```

```
A\b;
```

```
flops
```

```
ans =  
54757
```

Using the full form of **A** the number of flops needed to solve the same linear system is

```
flops(0)
```

```
full(A)\b;
```

```
flops
```

```
ans =  
    72014
```

## References

- [1] B.N. Datta, Numerical Linear Algebra and Applications, Brooks/Cole Publishing Company, Pacific Grove, CA, 1995.
- [2] J.W. Demmel, Applied Numerical Linear Algebra, SIAM, Philadelphia, PA, 1997.
- [3] G.H. Golub and Ch.F. Van Loan, Matrix Computations, Second edition, Johns Hopkins University Press, Baltimore, MD, 1989.
- [4] M.T. Heath, Scientific Computing: An Introductory Survey, McGraw-Hill, Boston, MA, 1997.
- [5] N.J. Higham, Accuracy and Stability of Numerical Algorithms, SIAM, Philadelphia, PA, 1996.
- [6] R.D. Skeel and J.B. Keiper, Elementary Numerical Computing with *Mathematica*, McGraw-Hill, New York, NY, 1993.
- [7] L.N. Trefethen and D. Bau III, Numerical Linear Algebra, SIAM, Philadelphia, PA, 1997.

## Problems

- Let  $\mathbf{A}$  be an  $n$ -by- $n$  matrix and let  $\mathbf{v}$  be an  $n$ -dimensional vector. Which of the following methods is faster?
  - $(\mathbf{v}*\mathbf{v}')*\mathbf{A}$
  - $\mathbf{v}*(\mathbf{v}'*\mathbf{A})$
- Suppose that  $\mathbf{L} \in \mathbb{R}^{n \times n}$  is lower triangular and  $\mathbf{b} \in \mathbb{R}^n$ . Write MATLAB function  $\mathbf{x} = \mathbf{ltri}(\mathbf{L}, \mathbf{b})$  that computes a solution  $\mathbf{x}$  to the linear system  $\mathbf{L}\mathbf{x} = \mathbf{b}$ .
- Repeat Problem 2 with  $\mathbf{L}$  being replaced by the upper triangular matrix  $\mathbf{U}$ . Name your function  $\mathbf{utri}(\mathbf{U}, \mathbf{b})$ .
- Let  $\mathbf{A} \in \mathbb{R}^{n \times n}$  be a triangular matrix. Write a function  $\mathbf{dettri}(\mathbf{A})$  that computes the determinant of the matrix  $\mathbf{A}$ .
- Write MATLAB function  $\mathbf{MA} = \mathbf{Gausspre}(\mathbf{A}, \mathbf{m}, \mathbf{k})$  that overwrites matrix  $\mathbf{A} \in \mathbb{R}^{n \times p}$  with the product  $\mathbf{MA}$ , where  $\mathbf{M} \in \mathbb{R}^{n \times n}$  is the Gauss transformation which is determined by the Gauss vector  $\mathbf{m}$  and its column index  $\mathbf{k}$ .  
**Hint:** You may wish to use the following formula  $\mathbf{MA} = \mathbf{A} - \mathbf{m}(\mathbf{e}_k^T \mathbf{A})$ .
- A system of linear equations  $\mathbf{Ax} = \mathbf{b}$ , where  $\mathbf{A}$  is a square matrix, can be solved applying successively Gauss transformations to the augmented matrix  $[\mathbf{A}, \mathbf{b}]$ . A solution  $\mathbf{x}$  then can be found using back substitution, i.e., solving a linear system with an upper triangular matrix. Using functions  $\mathbf{Gausspre}$  of Problem 5,  $\mathbf{Gaussv}$  described in Section 4.3, and  $\mathbf{utri}$  of Problem 3, write a function  $\mathbf{x} = \mathbf{sol}(\mathbf{A}, \mathbf{b})$  which computes a solution  $\mathbf{x}$  to the linear system  $\mathbf{Ax} = \mathbf{b}$ .
- Add a few lines of code to the function  $\mathbf{sol}$  of Problem 6 to compute the determinant of the matrix  $\mathbf{A}$ . The header of your function might look like this function  $[\mathbf{x}, \mathbf{d}] = \mathbf{sol}(\mathbf{A}, \mathbf{b})$ . The second output parameter  $\mathbf{d}$  stands for the determinant of  $\mathbf{A}$ .
- The purpose of this problem is to test function  $\mathbf{sol}$  of Problem 6.
  - Construct at least one matrix  $\mathbf{A}$  for which function  $\mathbf{sol}$  fails to compute a solution. Explain why it happened.
  - Construct at least one matrix  $\mathbf{A}$  for which the computed solution  $\mathbf{x}$  is poor. For comparison of a solution you found using function  $\mathbf{sol}$  with an acceptable solution you may wish to use MATLAB's backslash operator  $\backslash$ . Compute the relative error in  $\mathbf{x}$ . Compare numbers of flops used by function  $\mathbf{sol}$  and MATLAB's command  $\backslash$ . Which of these methods is faster in general?
- Given a square matrix  $\mathbf{A}$ . Write MATLAB function  $[\mathbf{L}, \mathbf{U}] = \mathbf{mylu}(\mathbf{A})$  that computes the LU decomposition of  $\mathbf{A}$  using partial pivoting.

10. Change your working format to **format long e** and run function **mylu** of Problem 11 on the following matrices

- (i)  $A = [\text{eps } 1; 1 \ 1]$
- (ii)  $A = [1 \ 1; \text{eps } 1]$
- (iii)  $A = \text{hilb}(10)$
- (iv)  $A = \text{rand}(10)$

In each case compute the error  $\|A - LU\|_F$ .

11. Let  $A$  be a tridiagonal matrix that is either diagonally dominant or positive definite. Write MATLAB's function  $[L, U] = \text{trilu}(a, b, c)$  that computes the LU factorization of  $A$ . Here  $a$ ,  $b$ , and  $c$  stand for the subdiagonal, main diagonal, and superdiagonal of  $A$ , respectively.

12. The following function computes the Cholesky factor  $L$  of the symmetric positive definite matrix  $A$ . Matrix  $L$  is lower triangular and satisfies the equation  $A = LL^T$ .

```
function L = mychol(A)

% Cholesky factor L of the matrix A; A = L*L'.

[n, n] = size(A);
for j=1:n
    for k=1:j-1
        A(j:n,j) = A(j:n,j) - A(j:n,k)*A(j,k);
    end
    A(j,j) = sqrt(A(j,j));
    A(j+1:n,j) = A(j+1:n,j)/A(j,j);
end
L = tril(A);
```

Add a few lines of code that generates the error messages when  $A$  is neither

- symmetric nor
- positive definite

Test the modified function **mychol** on the following matrices

- (i)  $A = [1 \ 2 \ 3; 2 \ 1 \ 4; 3 \ 4 \ 1]$
- (ii)  $A = \text{rand}(5)$

13. Prove that any 2-by-2 Householder reflector is of the form

$H = [\cos \theta \ \sin \theta; \sin \theta \ -\cos \theta]$ . What is the Householder reflection vector  $u$  of  $H$ ?

14. Find the eigenvalues and the associated eigenvectors of the matrix  $H$  of Problem 13.

15. Write MATLAB function  $[Q, R] = \text{myqr}(A)$  that computes a full QR factorization  $A = QR$  of  $A \in \mathbb{R}^{m \times n}$  with  $m \geq n$  using Householder reflectors. The output matrix  $Q$  is an  $m$ -by- $m$  orthogonal matrix and  $R$  is an  $m$ -by- $n$  upper triangular with zero entries in rows  $n+1$  through  $m$ .

- Hint:** You may wish to use function **Housprod** in the body of the function **myqr**.
16. Let  $\mathbf{A}$  be an  $n$ -by-3 random matrix generated by the MATLAB function **rand**. In this exercise you are to plot the error  $\|\mathbf{A} - \mathbf{QR}\|_F$  versus  $n$  for  $n = 3, 5, \dots, 25$ . To compute the QR factorization of  $\mathbf{A}$  use the function **myqr** of Problem 15. Plot the graph of the computed errors using MATLAB's function **semilogy** instead of the function **plot**. Repeat this experiment several times. Does the error increase as  $n$  does?
  17. Write MATLAB function  $\mathbf{V} = \mathbf{Vandm}(\mathbf{t}, \mathbf{n})$  that generates Vandermonde's matrix  $\mathbf{V}$  used in the polynomial least-squares fit. The degree of the approximating polynomial is  $\mathbf{n}$  while the  $x$ -coordinates of the points to be fitted are stored in the vector  $\mathbf{t}$ .
  18. In this exercise you are to compute coefficients of the least squares polynomials using four methods, namely the normal equations, the QR factorization, modified Gram-Schmidt orthogonalization and the singular value decomposition.  
Write MATLAB function  $\mathbf{C} = \mathbf{lspol}(\mathbf{t}, \mathbf{y}, \mathbf{n})$  that computes coefficients of the approximating polynomials. They should be saved in columns of the matrix  $\mathbf{C} \in \mathbb{R}^{(n+1) \times 4}$ . Here  $\mathbf{n}$  stands for the degree of the polynomial,  $\mathbf{t}$  and  $\mathbf{y}$  are the vectors holding the  $x$ - and the  $y$ -coordinates of the points to be approximated, respectively. Test your function using  $\mathbf{t} = \mathbf{linspace}(1.4, 1.8)$ ,  $\mathbf{y} = \mathbf{sin}(\mathbf{tan}(\mathbf{t})) - \mathbf{tan}(\mathbf{sin}(\mathbf{t}))$ ,  $\mathbf{n} = 2, 4, 8$ . Use **format long** to display the output to the screen.  
**Hint:** To create the Vandermonde matrix needed in the body of the function **lspol** you may wish to use function **Vandm** of Problem 17.
  19. Modify function **lspol** of Problem 18 adding a second output parameter **err** so that the header of the modified function should look like this  
function  $[\mathbf{C}, \mathbf{err}] = \mathbf{lspol}(\mathbf{t}, \mathbf{y}, \mathbf{n})$ . Parameter **err** is the least squares error in the computed solution  $\mathbf{c}$  to the overdetermined linear system  $\mathbf{V}\mathbf{c} \approx \mathbf{y}$ . Run the modified function on the data of Problem 18. Which of the methods used seems to produce the least reliable numerical results? Justify your answer.
  20. Write MATLAB function  $[\mathbf{r}, \mathbf{c}] = \mathbf{nrceig}(\mathbf{A})$  that computes the number of real and complex eigenvalues of the real matrix  $\mathbf{A}$ . You cannot use MATLAB function **eig**. Run function **nrceig** on several random matrices generated by the functions **rand** and **randn**.  
**Hint:** You may wish to use the following MATLAB functions **schur**, **diag**, **find**. Note that the **diag** function takes a second optional argument.
  21. Assume that an eigenvalue of a matrix is sensitive if its condition number is greater than  $10^3$ . Construct an  $n$ -by- $n$  matrix ( $5 \leq n \leq 10$ ) whose all eigenvalues are real and sensitive.
  22. Write MATLAB function  $\mathbf{A} = \mathbf{pent}(\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}, \mathbf{e}, \mathbf{n})$  that creates the full form of the  $n$ -by- $n$  pentadiagonal matrix  $\mathbf{A}$  with constant entries  $\mathbf{a}$  along the second subdiagonal, constant entries  $\mathbf{b}$  along the subdiagonal, etc.
  23. Let  $\mathbf{A} = \mathbf{pent}(1, 26, 66, 26, 1, \mathbf{n})$  be an  $n$ -by- $n$  symmetric pentadiagonal matrix generated by function **pent** of Problem 22. Find the eigenvalue decomposition  $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$  of  $\mathbf{A}$  for various values of  $\mathbf{n}$ . Repeat this experiment using random numbers in the band of the matrix  $\mathbf{A}$ . Based on your observations, what conjecture can be formulated about the eigenvectors of  $\mathbf{A}$ ?
  24. Write MATLAB function  $[\mathbf{la}, \mathbf{x}] = \mathbf{smeig}(\mathbf{A}, \mathbf{v})$  that computes the smallest

(in magnitude) eigenvalue of the nonsingular matrix  $\mathbf{A}$  and the associated eigenvector  $\mathbf{x}$ . The input parameter  $\mathbf{v}$  is an estimate of the eigenvector of  $\mathbf{A}$  that is associated with the largest (in magnitude) eigenvalue of  $\mathbf{A}$ .

25. In this exercise you are to experiment with the eigenvalues and eigenvectors of the partitioned matrices. Begin with a square matrix  $\mathbf{A}$  with known eigenvalues and eigenvectors. Next construct a matrix  $\mathbf{B}$  using MATLAB's built-in function `repmat` to define the matrix  $\mathbf{B}$  as  $\mathbf{B} = \text{repmat}(\mathbf{A}, 2, 2)$ . Solve the matrix eigenvalue problem for the matrix  $\mathbf{B}$  and compare the eigenvalues and eigenvectors of matrices  $\mathbf{A}$  and  $\mathbf{B}$ . You may wish to continue in this manner using larger values for the second and third parameters in the function `repmat`. Based on the results of your experiment, what conjecture about the eigenvalues and eigenvectors of  $\mathbf{B}$  can be formulated?