Numerieke technieken en optimalisatie

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All computation may be done with Matlab.

Exercise 2.1: QU Decomposition in MATLAB

Consider the following 4×4 matrix A

$$A = \begin{pmatrix} 4 & 1 & -2 & 2 \\ 1 & 2 & 0 & 1 \\ -2 & 0 & 3 & 2 \\ 2 & 1 & -2 & -1 \end{pmatrix}.$$

Use MATLAB to perform $Givens\ rotations$, and bring the matrix A to QU form. Check your results against MATLAB.

Answer.

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\% A = \begin{bmatrix} 4 & 1 & -2 & 2 \\ 1 & 2 & 0 & 1 \\ 0 & 1 & -2 & 0 & 3 & 2 \\ 0 & 2 & 1 & -2 & -1 \end{bmatrix}
\% A = [1 \ 2 \ 0; \ 1 \ 1 \ 1; \ 2 \ 1 \ 0];
A = [1 2 ; 0 3; 0 4];
n = size(A, 1);
U = A;
Q = eye(n);
for i=1:n-1 %Columns
for j = i+1:n \% rows (to be zero)
if U(j,i) \sim 0 \% Only for non-zero
r = sqrt(U(i,i)^2+U(j,i)^2);
c = U(i, i)/r;
s = U(j, i)/r;
% Rotation matrix
G = eye(n);
G([i,j],[i,j]) = [c s; -s c];
% Matrices QU (see definition)
U = G*U;
Q = Q*G';
end
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end end

% Checking it

$$[Q1, U1] = qr(A);$$

Exercise 2.2: (Householder reflection matrix)

For any vector $v \in \mathbb{R}^n$, one defines a matrix

$$Q_v := I_n - \frac{2}{\|v\|_2^2} v v^T.$$

- a) Show that
 - 1) Q_v is a symmetric, orthogonal matrix and $Q_v^2 = I_n$.

Answer.

- Symmetry:

$$Q_v^T = \left(I_n - \frac{2}{\|v\|_2} v v^T\right)^T$$

$$= (I_n)^T - \left(\frac{2}{\|v\|_2} v v^T\right)^T$$

$$= I_n - \frac{2}{\|v\|_2} (v^T)^T v^T$$

$$= I_n - \frac{2}{\|v\|_2} v v^T = Q_v$$

- Orthogonality:

$$Q_{v} Q_{v}^{T} = \left(I_{n} - \frac{2}{\|v\|_{2}} vv^{T}\right) \left(I_{n} - \frac{2}{\|v\|_{2}} vv^{T}\right)$$

$$= I_{n} - \frac{2}{\|v\|_{2}} vv^{T} - \frac{2}{\|v\|_{2}} vv^{T} + \left(\frac{2}{\|v\|_{2}} vv^{T}\right) \left(\frac{2}{\|v\|_{2}} vv^{T}\right)$$

$$= I_{n} - \frac{4}{\|v\|_{2}^{2}} vv^{T} + \frac{4}{\|v\|_{2}^{2}} \left(vv^{T}\right) \left(vv^{T}\right) = I_{n}$$

-
$$Q_v^2 = I_n$$
:

$$Q_v^2 = Q_v Q_v$$

$$= (Q_v)^T Q_v$$

$$= (Q_v)^{-1} Q_v = I_n$$

2) For any $u \in \mathbb{R}^n$ that is orthogonal to v (i.e. in the hyperplane orthogonal to v),

$$Q_v u = u, \qquad Q_v v = -v.$$

Answer.

$$Q_v u = \left(I_n - \frac{2}{\|v\|_2} v v^T\right) u$$
$$= I_n u - \frac{2}{\|v\|_2} v(v^T u) = u$$

$$Q_{v}v = \left(I_{n} - \frac{2}{\|v\|_{2}}vv^{T}\right)v$$
$$= I_{n}v - \frac{2}{\|v\|_{2}}v(v^{T}v) = -v$$

3) Q_v has only eigenvalues ± 1 and $\det(Q_v) = -1$.

Answer. Let λ and x be the eigenvalues and eigenvectors of Q_v , i.e

$$Q_v x = \lambda x$$

Moreover,

$$||Q_v x||^2 = ||\lambda x||^2 = \lambda^2 ||x||^2$$

and

$$||Q_v x||^2 = (Q_v x)^T (Q_v x) = x^T Q_v^T Q_v x = x^T x = ||x||^2$$

then

$$\lambda = \pm 1$$

If u is orthogonal to v then $Q_v u = u$, it means that u is an eigenvector with eigenvalue 1. Since there are n-1 vectors (L.I) orthogonal to v then 1 is an eigenvalue of multiplicity n-1.

$$\det(Q_v) = (1)^{n-1} \cdot (-1) = -1$$

b) Let
$$x = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$
, find the reflect vector $v \in \mathbb{R}^3$ such that $Q_v x = -\|x\|_2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$.

Answer. The right reflection is through a hyperplane that bisects the angle between x and $Q_v x$

$$v = \alpha(x - Q_v x) = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} - \|x\|_2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 - \|x\|_2 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} -2.74 \\ 2 \\ 3 \end{pmatrix}$$

Exercise 2.3: (Sparse matrices and the CRS format) Self-study

A matrix $A \in \mathbb{R}^{n \times n}$ is called *sparse* if most of its entries are zero. (More precisely, we say that it has at most O(n) nonzero entries.) We consider the *compressed row storage* (CRS) format. Let A have N nonzero entries, with $N \ll n^2$. Instead of saving the matrix A as a one-dimensional array of size n^2 , one uses three arrays: entries and colmns are arrays of size N, row_pointer is an array of size n+1. entries saves the nonzero entries of the matrix A in the order of their occurrence (left to right, then top to bottom) and colmns saves the corresponding column indices. row_pointer[i] saves the index of entries where the first entry in row i-1 is located, i.e., entries[row_pointer[i]] gives the first element of row i (note that array indices start at 0), row_pointer[n] gives the size of entries.

a) Let

$$A := \begin{pmatrix} 12 & 22 & 0 \\ 0 & 23 & 33 \\ 0 & 0 & 44 \end{pmatrix}.$$

Give the CRS format of A.

Answer. Entries: [12 22 23 33 44]
Columns: [0 1 1 2 2]
Row pointer: [0 2 4 5]

b) Recover the matrix from the CRS format given below

entries = [5 8 3 6]
columns = [0 1 2 1]
row_pointer = [0 0 2 3 4]

Answer.

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 5 & 8 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 6 & 0 & 0 \end{pmatrix}$$

c) A matrix resulting from a discretization of a one-dimensional Laplace operator is given as

$$A := \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & -1 & 2 & -1 \\ & & & & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{n \times n}$$

for $h := \frac{1}{n+1}$. We assume real numbers are saved as double, i.e., required memory is 8 byte; and indices are saved as int, i.e., required memory is 4 byte. Take n = 50,000 and compute the memory required to save A completely, i.e., including the zero entries or in CRS format.

Answer. - Complete matrix: $(n \times n) \cdot 8 = 2^1 \cdot 10^{10}$ bytes = 20 GB. - CRS: $24n - 16 + 16n - 4 = 40n - 20 = 1.999.980 \approx 2.000.000$ bytes = 0.002 GB + Non-zeros: $n + 2(n - 1) = 3n - 2 \rightarrow (3n - 2) \cdot 8 = 24n - 16 = 1.199.984$ + Indices: $n + 2(n - 1) + (n + 1) = 4n - 1 \rightarrow (4n - 1) \cdot 4 = 16n - 4 = 799.996$

Exercise 2.4: (Convergence of iterative solvers)

Let $\|\cdot\|$ be a norm on $\mathbb{R}^{n\times n}$ that is induced by a vector norm, i.e.,

$$||A|| := \sup_{0 \neq x \in \mathbb{R}^n} \frac{||Ax||}{||x||}.$$

By $\rho(A)$, we denote the spectral radius of a matrix A, i.e.,

$$\rho(A) := \max\{|\lambda| | \lambda \text{ is an eigenvalue of } A\}.$$

a) Show that for all matrices $A \in \mathbb{R}^{n \times n}$,

$$\rho(A) \leq ||A||$$
.

Answer. Let λ be an eigenvalue of A and $v \neq 0$ be a corresponding eigenvector

$$\lambda v = Av \to ||\lambda v|| = ||Av||$$

 $|\lambda|||v|| = ||Av|| \le ||A||||v|| \to |\lambda| \le ||A||$

In conclusion, for all λ we have $|\lambda| \leq ||A||$ and this implies $\max_{\lambda} (|\lambda|) \leq ||A||$

b) Compute the spectral radius of the matrix

$$A = \begin{pmatrix} a & 4 \\ 0 & a \end{pmatrix}.$$

When is $\rho(A) < 1$? Check that $||A^k||^{\frac{1}{k}}$ can be greater than one in this case.

Answer.

$$\det(A - \lambda I) = (a - \lambda)^2 - 0 = 0 \iff \lambda = a$$

Then $\rho(A) \leq 1 \iff |\lambda| \leq 1 \iff |a| \leq 1$ and with this we can show that:

$$||A||_{\infty} = |a| + 4 \rightarrow 4 < ||A||_{\infty} < 5$$

 $||A||_{1} = |a| + 4 \rightarrow 4 < ||A||_{1} < 5$