

Numerical Algorithms (MU4IN910)

Lecture 2: Matrix computation

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Summary of the previous lecture

- Introduction to floating-point arithmetic
- Introduction to MATLAB
- Matrix storage
- Efficient tools for matrix manipulations: the BLAS

We consider computations involving **dense matrices** (matrices that do not have a large number of zero elements)

We need to

- 1 **efficiently** manipulate those matrices on computers
- 2 choose the right **decomposition** to solve the problem we consider

Classic problems in linear algebra

Solving linear systems: given a matrix A of size $n \times n$ and a vector b of size n , find x such that

$$Ax = b$$

Solving least-square problems: given a matrix A of size $m \times n$ (with $m > n$) and a vector b of size m , solve

$$\min_x \|b - Ax\|$$

Solving eigenvalue/eigenvector problems: given a matrix A of size $n \times n$, find a vector $x \neq 0$ and a scalar λ such that

$$Ax = \lambda x$$

Outline of the lecture

- ➊ Matrix manipulation
 - ➊ How matrices are stored on computers?
 - ➋ Basic tools for matrix manipulation: the BLAS
- ➋ Matrix decompositions and their uses
 - ➊ LU
 - ➋ QR
 - ➌ Eigendecomposition (diagonalization, etc.)
 - ➍ SVD (singular value decomposition)
- ➌ Software

- **Scientific Computing with Case Studies**, D. O’Leary, SIAM, 2009
- Applied Numerical Linear Algebra, J. Demmel, SIAM, 1997
- Numerical Linear Algebra, L. N. Trefethen and D. Bau, SIAM, 1997
- Matrix Computations, G. Golub and C. Van Loan, Johns Hopkins University Press, 4th edition, 2013
- Matrix Algorithms. Volume I: Basic Decompositions, G. W. Stewart, SIAM, 2001
- Matrix Algorithms. Volume II: Eigensystems, G. W. Stewart, SIAM, 2001

Notation

- All vectors are column vectors
- Matrices are upper case letters; vectors and scalars are lower case
- The element of a matrix A at the (i, j) th entry will be denoted a_{ij} or $A(i, j)$
- I is the **identity matrix** and e_i is the i th column of I
- $B = A^T$ means that B is the **transpose** of A : $b_{ij} = a_{ji}$
- $B = A^*$ means that B is the **complex conjugate transpose** of A : $b_{ij} = \overline{a_{ji}}$
- We will often use MATLAB notation. For example $A(i : j, k : l)$ denotes the submatrix of A with row entries between i and j and column entries between k and l
- An **orthogonal matrix** U satisfies $U^T U = I$
- A **unitary matrix** U satisfies $U^* U = I$
- Two matrices A and B are **similar** if there exists an invertible matrix X such that $B = XAX^{-1}$

Vector and matrix norms

Definition 1

A **vector norm** is a function $\| \cdot \| : \mathbb{C}^n \rightarrow \mathbb{R}^+$ satisfying the following conditions:

- ❶ $\|x\| = 0$ iff $x = 0$
- ❷ $\|\alpha x\| = |\alpha| \|x\|$ for all $\alpha \in \mathbb{C}$ and $x \in \mathbb{C}^n$
- ❸ $\|x + y\| \leq \|x\| + \|y\|$ for all $x, y \in \mathbb{C}^n$

Example 1

- $\|x\|_1 = |x_1| + \dots + |x_n| = \sum_{i=1}^n |x_i|$
- $\|x\|_2 = (|x_1|^2 + \dots + |x_n|^2)^{1/2} = \left(\sum_{i=1}^n |x_i|^2\right)^{1/2}$
- $\|x\|_\infty = \max_{1 \leq i \leq n} |x_i|$

Vector and matrix norms (cont'd)

Definition 2

A **matrix norm** is a function $\|\cdot\| : \mathbb{C}^{m \times n} \rightarrow \mathbb{R}^+$ satisfying the same properties as vector norms.

Example 2

Subordinate matrix norms to vector norms: $\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|=1} \|Ax\|$

- $\|A\|_1 = \sup_{x \neq 0} \frac{\|Ax\|_1}{\|x\|_1} = \max_{1 \leq j \leq n} \sum_{i=1}^m |a_{ij}|$
- $\|A\|_\infty = \sup_{x \neq 0} \frac{\|Ax\|_\infty}{\|x\|_\infty} = \max_{1 \leq i \leq m} \sum_{j=1}^n |a_{ij}|$
- $\|A\|_2 = \sup_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}$

Matrix decompositions and their uses

We are going to study the four following decompositions:

- 1 LU
- 2 QR
- 3 Eigendecomposition (diagonalization, etc.)
- 4 SVD (singular value decomposition)

Permutation matrix

A permutation matrix is a square matrix that satisfies the following conditions:

- All the coefficients are either 0 or 1
- There is exactly one entry of 1 in each row
- There is exactly one entry of 1 in each column

Multiply on the left by a permutation matrix results in permuting the rows of the matrix A . For example:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \end{pmatrix} = \begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} \\ a_{3,1} & a_{3,2} & a_{3,3} \\ a_{2,1} & a_{2,2} & a_{2,3} \end{pmatrix}$$

LU decomposition

Definition 3

The LU decomposition of an invertible matrix A of size $n \times n$ is defined by $PA = LU$ where

- P is a **permutation matrix**
- L is a **unit lower triangular matrix** (Low) (zero above the main diagonal and ones on the main diagonal)
- U is an **upper triangular matrix** (Up)

$$P \begin{pmatrix} a_{1,1} & \dots & a_{1,n} \\ \vdots & & \vdots \\ a_{n,1} & \dots & a_{n,n} \end{pmatrix} = \begin{pmatrix} 1 & & \\ \vdots & \ddots & \\ \ell_{n,1} & \dots & 1 \end{pmatrix} \begin{pmatrix} u_{1,1} & \dots & u_{1,n} \\ & \ddots & \vdots \\ & & u_{n,n} \end{pmatrix}$$

This corresponds to the **Gaussian elimination algorithm**

How to compute a LU decomposition

Principle of the algorithm

- The matrix A is reduced to an upper triangular matrix by putting zeros below the main diagonal, column by column, by subtracting a multiple of the current pivot from all rows below it
- Multipliers form the entries of L
- For numerical stability it is necessary to pivot or interchange rows. Changes are stored in P

In MATLAB: $[L,U,P]=lu(A)$ or $[PtL,U]=lu(A)$ to compute $P^T L$ and U

Cost: $n^3/3$ multiplications

Example of LU decomposition

$$L_2^{-1}A = \begin{pmatrix} 1 & 0 & 0 \\ -1/2 & 1 & 0 \\ -1/4 & 0 & 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 8 \\ 2 & 8 & 7 \\ 1 & 3 & 6 \end{pmatrix} = \begin{pmatrix} 4 & 4 & 8 \\ 0 & 6 & 3 \\ 0 & 2 & 4 \end{pmatrix}$$

$$L_1^{-1}L_2^{-1}A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/3 & 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 8 \\ 0 & 6 & 3 \\ 0 & 2 & 4 \end{pmatrix} = \begin{pmatrix} 4 & 4 & 8 \\ 0 & 6 & 3 \\ 0 & 0 & 3 \end{pmatrix} = U$$

Finally,

$$A = L_2L_1U = \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 1/4 & 1/3 & 1 \end{pmatrix} \begin{pmatrix} 4 & 4 & 8 \\ 0 & 6 & 3 \\ 0 & 0 & 3 \end{pmatrix} = LU$$

Why a permutation matrix is needed (1)

What about

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}?$$

The pivot is zero, so we factorize the matrix:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

Why a permutation matrix is needed (2)

What about

$$A = \begin{pmatrix} 10^{-20} & 1 \\ 1 & \mathbf{1} \end{pmatrix}?$$

$$\text{We have } A = LU = \begin{pmatrix} 1 & 0 \\ 10^{20} & 1 \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \\ 0 & 1 - 10^{20} \end{pmatrix}$$

If the arithmetic uses only 16 decimal digits, then $1 - 10^{20}$ is rounded to the number -10^{20} .

The decomposition is then

$$\tilde{L}\tilde{U} = \begin{pmatrix} 1 & 0 \\ 10^{20} & 1 \end{pmatrix} \begin{pmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{pmatrix} = \begin{pmatrix} 10^{-20} & 1 \\ 1 & \mathbf{0} \end{pmatrix}$$

Use the permutation matrix to use the **largest element in absolute value** as the pivot.

Uses of the LU decomposition

One can use the LU decomposition to solve **linear system**

$$Ax = b,$$

given A and b .

If we factorize A as $PA = LU$ then we have

$$PAx = LUx = Pb$$

Let $y = Ux$, then $Ly = Pb$

To solve $Ax = b$:

- ① one solves $Ly = Pb$ by forward substitution
- ② one solves $Ux = y$ by backward substitution

In MATLAB, the backslash command $x=A \backslash b$ generally uses the LU decomposition to solve a linear system

Uses of the LU decomposition (cont'd)

- To solve $Ax = b$, one first solves $Ly = Pb$ by forward substitution
For $i = 1 : n$

$$y_i = (Pb)_i - \sum_{j=1}^{i-1} l_{ij}y_j$$

- and then solve $Ux = y$ by backward substitution
For $i = n : -1 : 1$,

$$x_i = \left(y_i - \sum_{j=i+1}^n u_{ij}x_j \right) / u_{ii}$$

What about symmetric positive-definite matrices?

A $n \times n$ matrix A is **symmetric positive-definite** if $A^T = A$ and $x^T A x > 0$ for all $x \neq 0$.

If ω is a vector of size $n - 1$ and K a matrix of size $(n - 1) \times (n - 1)$, one step of Gaussian elimination on $\frac{1}{\alpha}A$ with $a_{1,1} = \alpha^2$ gives:

$$A = \begin{pmatrix} \alpha^2 & \omega^T \\ \omega & K \end{pmatrix} = \begin{pmatrix} \alpha & 0 \\ \omega/\alpha & I \end{pmatrix} \begin{pmatrix} \alpha & \omega^T/\alpha \\ 0 & K - \omega\omega^T/\alpha^2 \end{pmatrix}$$

By factorizing the matrix U as follows:

$$\begin{pmatrix} \alpha & \omega^T/\alpha \\ 0 & K - \omega\omega^T/a_{1,1} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & K - \omega\omega^T/a_{1,1} \end{pmatrix} \begin{pmatrix} \alpha & \omega^T/\alpha \\ 0 & I \end{pmatrix}$$

and combining the two operation, we get:

$$A = \begin{pmatrix} \alpha & 0 \\ \omega/\alpha & I \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & K - \omega\omega^T/a_{1,1} \end{pmatrix} \begin{pmatrix} \alpha & \omega^T/\alpha \\ 0 & I \end{pmatrix} = LDL^T$$

Cholesky decomposition

If A is symmetric positive-definite : $A^T = A$ et $x^T A x > 0$ for all $x \neq 0$, then it is more convenient to use the **Choleski** decomposition,

$$A = LL^T$$

with L is a lower triangular matrix, or

$$A = LDL^T$$

where L is a unit lower triangular matrix, and D is a diagonal matrix

This gives a decomposition at half the cost of the LU decomposition

In MATLAB, use the command `chol`

Existence, uniqueness of solutions of linear systems

- If A is **nonsingular** (invertible) then the linear system $Ax = b$ has a **unique solution**
- If A is **singular** then x is a solution of $Ax = b$ if b can be written as a linear combination of some columns of A . In this case, every vector $x + y$ is a solution if $Ay = 0$.

Sensitivity of the solution of a linear system

Assuming that we **perturb** the system such that we now need to solve

$$(A + \Delta A)y = b + \Delta b.$$

We want to know to which **distance** the solution y of the **perturbed system** is from the solution x of the **intial system**

Let

$$\varepsilon_A = \frac{\|\Delta A\|}{\|A\|}$$

$$\varepsilon_b = \frac{\|\Delta b\|}{\|b\|}$$

$$\kappa = \|A\| \|A^{-1}\| \quad \text{condition number of the matrix } A$$

If $\kappa \varepsilon_A < 1$ then

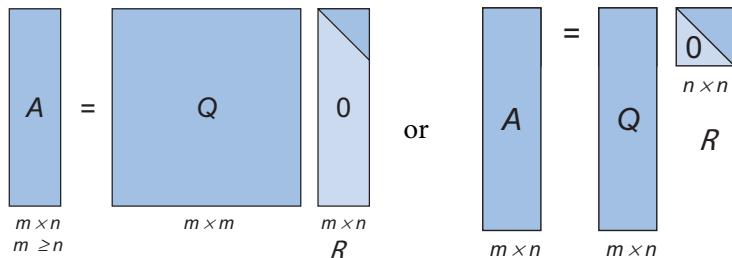
$$\frac{\|x - y\|}{\|x\|} \leq \frac{\kappa}{1 - \kappa \varepsilon_A} (\varepsilon_A + \varepsilon_b)$$

The QR decomposition

Definition 4 (QR decomposition)

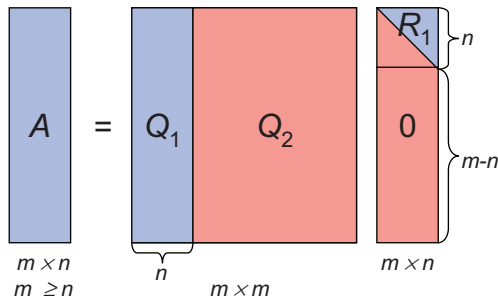
The *QR decomposition* of a matrix A of size $m \times n$ with $m \geq n$ is defined by $A = QR$ where

- Q is an $m \times m$ unitary matrix (orthogonal if A is real) and R is an $m \times n$ matrix with zeros below the main diagonal or
- Q is an $m \times n$ unitary matrix (orthogonal if A is real) and R is an $n \times n$ upper triangular matrix.



The QR decomposition (cont'd)

The compact $m \times n$ decomposition arises because part of the $m \times n$ matrix Q is not needed in the decomposition



$$A = Q_1 R_1 + Q_2 0 = Q_1 R_1$$

Algorithms for computing QR decomposition

There are mainly 3 different algorithms for computing the QR decomposition:

- 1 Givens rotations (good for Q $m \times m$)
- 2 Gram-Schmidt orthogonalization (good for Q $m \times n$)
- 3 Householder reflections

We will study methods 1 and 2 in this lecture. We will see method 3 in the tutorial

Givens rotations

We assume all matrices are real ones (we will see the complex case in the tutorial)

A simple orthogonal matrix, a rotation, can be used to introduce one zero at a time into a real matrix.

A **Givens matrix** is written as

$$G = \begin{pmatrix} c & s \\ -s & c \end{pmatrix}$$

where $c^2 + s^2 = 1$ (c and s have the geometric interpretation of the cosine and sine of an angle θ)

A vector multiplied by G is rotated through an angle θ

How to use Givens rotations?

Problem: Given a vector $z \neq 0$ of size 2, find a matrix G such that $Gz = xe_1$ where $x = \|z\|$

Solution:

$$Gz = \begin{pmatrix} cz_1 + sz_2 \\ -sz_1 + cz_2 \end{pmatrix} = xe_1$$

Multiplying the first equation by c , the second by s , and subtracting yields $(c^2 + s^2)z_1 = cx$ and so $c = z_1/x$.

In the same way, we find that $s = z_2/x$

As $c^2 + s^2 = 1$, we can conclude that $z_1^2 + z_2^2 = x^2$, and so

$$\begin{aligned} c &= \frac{z_1}{\sqrt{z_1^2 + z_2^2}} \\ s &= \frac{z_2}{\sqrt{z_1^2 + z_2^2}} \end{aligned}$$

Givens QR decomposition

So we know how to use Givens matrices to zero out single components of a matrix. We will use the notation G_{ij} to denote an $n \times n$ identity matrix with its i th and j th rows modified to include the Givens rotation.

Example if $n = 6$:

$$G_{25} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c & 0 & 0 & s & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -s & 0 & 0 & c & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

The multiplication of a vector by this matrix leaves all but rows 2 and 5 of the vector unchanged.

Givens QR decomposition (cont'd)

Algorithm 1 (Givens algorithm)

Initialize Q to be the $m \times m$ identity matrix
Initialize R to be the $m \times n$ matrix A
for $i=1:n$
 for $j=i+1:m$
 – Choose the matrix G_{ij} to put a zero in
 position (j,i) of the matrix R , using the
 current value in position (i,i)
 – $R = G_{ij}R$
 – $Q = QG_{ij}^T$
 end
end

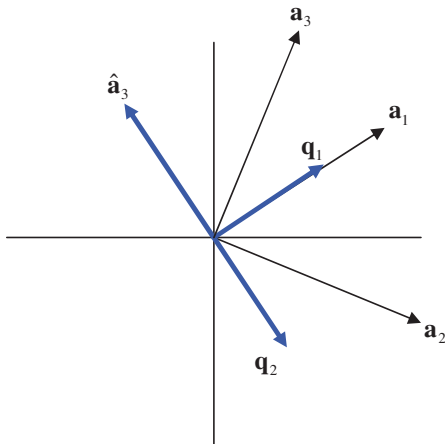
QR by Gram-Schmidt

From the columns $[a_1, \dots, a_n]$ of the matrix A , we create an orthonormal basis $\{q_1, \dots, q_n\}$ and save the coefficients that accomplish this goal in an upper triangular matrix R .

Algorithm 2 (Gram-Schmidt orthogonalization)

```
 $r_{1,1} = \|a_1\|$   
 $q_1 = a_1 / r_{1,1}$   
for  $k = 1 : n - 1$   
     $q_{k+1} = a_{k+1}$   
    for  $i = 1 : k$   
         $r_{i,k+1} = q_i^* q_{k+1}$   
         $q_{k+1} = q_{k+1} - r_{i,k+1} q_i$   
    end  
     $r_{k+1,k+1} = \|q_{k+1}\|$   
     $q_{k+1} = q_{k+1} / r_{k+1,k+1}$   
end
```

QR by Gram-Schmidt (cont'd)



Cost of QR decomposition

- Givens rotations: $2mn^2 - 2/3n^3$ multiplications
- Gram-Schmidt: mn^2 multiplications
- Householder reflections: $mn^2 - 1/3n^3$ multiplications

Uses of QR decomposition

In MATLAB : $[Q, R] = \text{qr}(A)$ for A of size $m \times n$ with $m \geq n$

- $\text{qr}(A, 0)$ returns the compact matrix Q (although the full is computed with Householder reflections)
- QR can get the basis for the range of a full-rank matrix A (the first n columns of Q) and the null-space of A^* (the last $m - n$ columns of Q).
- QR can be used to solve linear least squares problems

Solution of a linear system: $Ax = b$

→ if $A = QR$ then $Rx = Q^*b$

Solving linear least squares problems

Given A of size $m \times n$ (with $m > n$), we want to find

$$\min_x \|Ax - b\|$$

where $\|\cdot\|$ is the Euclidean norm (2-norm).

- Minimizing $\|Ax - b\|$ gives the same solution as minimizing $\|Ax - b\|^2$
- The norm of a vector is invariant under multiplication by Q^* , so $\|y\| = \|Q^*y\|$ for all y
- Suppose we partition the vector y into two pieces:

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

$$\text{Then } \|y\|^2 = \|y_1\|^2 + \|y_2\|^2$$

Solving linear least squares problems (cont'd)

If $A = QR$, we define

$$c = Q^*b = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

with c_1 of size n and c_2 of size $m - n$.

Then

$$\begin{aligned}\|b - Ax\|^2 &= \|Q^*(b - Ax)\|^2 \\ &= \|c - Rx\|^2 \\ &= \|c_1 - R_1x\|^2 + \|c_2 - 0x\|^2 \\ &= \|c_1 - R_1x\|^2 + \|c_2\|^2\end{aligned}$$

The minimum is obtained for x solution of $R_1x = c_1$

In MATLAB, use $x = A \backslash b$

Case study: data fitting

Data (t_i, f_i) represent the amount of a pollutant in a river, measured once a year.

We want to know whether a straight line is a good fit to this data!

We want to solve

$$\min_x \|Ax - b\|$$

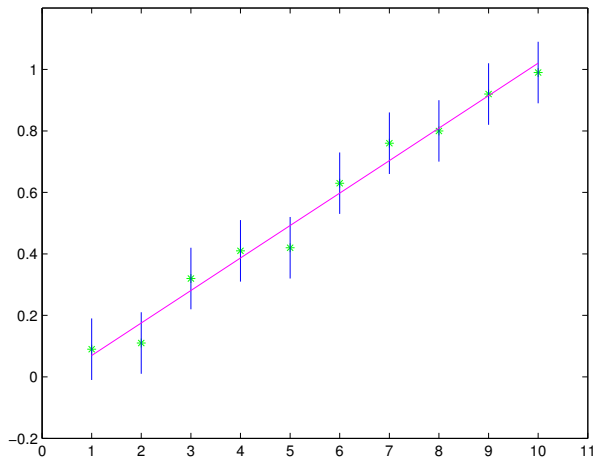
with

$$A = \begin{pmatrix} 1 & t_1 \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ 1 & t_{10} \end{pmatrix}, \quad b = \begin{pmatrix} f_1 \\ \cdot \\ \cdot \\ \cdot \\ f_{10} \end{pmatrix}$$

Case study: data fitting (cont'd)

```
sigma=.05;
t = [1:10];
b = [0.09 0.11 0.32 0.41 0.42 0.63 0.76 0.8 0.92 0.99];
plot(t,b,'g*');
hold on;
for i=1:10
    plot([t(i),t(i)], [b(i)+2*sigma,b(i)-2*sigma]));
end
axis([0 11 -.2 1.2]);
A = [ones(10,1),t'];
x = A \ b';
plot(t,A*x,'m');
```

Case study: data fitting (cont'd)



Eigendecomposition

Definition 5

A matrix A of size $n \times n$ is *diagonalizable* if $A = U\Lambda U^{-1}$ where Λ is a diagonal matrix whose diagonal entries are the *eigenvalues* λ_i . The columns of U are called the *eigenvectors*:

$$Au_i = \lambda_i u_i.$$

The decomposition is guaranteed to exist if

- A is real symmetric or complex Hermitian, or
- A is normal ($AA^* = A^*A$), or
- the eigenvalues of A are distinct.

Otherwise, the decomposition may fail to exist, although it will exist for a nearby matrix.

How to compute the eigendecomposition

Algorithm with 2 steps:

Step 1: reduce the matrix A to compact form, so that it is easy to manipulate.
Find a unitary matrix V so that

$$V^*AV = H$$

where H is

- **tridiagonal** if A is Hermitian (or real symmetric)
- **upper Hessenberg** otherwise

This can be done in $\mathcal{O}(n^3)$ operations.

The matrices A and H being similar, if we find an eigendecomposition of H as

$$H = U\Lambda U^{-1}$$

then we have the eigendecomposition

$$A = (VU)\Lambda(VU)^{-1}$$

for A

How to compute the eigendecomposition (cont'd)

Step 2: Find the eigendecomposition of H by QR iteration:

- Form $H = QR$
- Replace H by RQ

As $Q^*Q = I$ and $H = QR$, we have

$$RQ = (Q^*Q)RQ = Q^*HQ$$

As a consequence, the new H has the same eigenvalues as the old one, and if we have an eigendecomposition of RQ , then we have an eigendecomposition of H

We repeat Step 2 many times (about $5n$, typically), and often some subdiagonal elements of H converge to zero. Once that happens, we can read some eigenvalues off the diagonal.

In MATLAB, `[U,Lambda]=eig(A)`

Cost of eigendecomposition

- The cost of Step 1 is $\mathcal{O}(n^3)$
- The cost of $\mathcal{O}(n)$ iterations of Step 2 is $\mathcal{O}(n^3)$
- The total cost is $\mathcal{O}(n^3)$

Uses of eigendecomposition

- stability analysis in control theory
- convergence of iterative methods
- computation of invariant subspaces
- convergence of A^p when $p \rightarrow +\infty$

The Singular Value Decomposition (SVD)

Definition 6 (SVD)

Every matrix A of dimensions $m \times n$ (with $m \geq n$) can be decomposed as

$$A = U\Sigma V^*$$

where

- U has dimension $m \times m$ and $U^*U = I$
- Σ has dimension $m \times n$, the only nonzeros are on the main diagonal, and they are nonnegative real numbers $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$
- V has dimension $n \times n$ and $V^*V = I$

The σ_i are called the **singular values** of A

The Singular Value Decomposition (SVD)

- Full decomposition:

The diagram illustrates the full SVD decomposition. On the left is a gray rectangle labeled A . To its right is an equals sign. Further right is a gray rectangle labeled U , which is enclosed in a dashed box. To the right of U is a white square labeled Σ , also enclosed in a dashed box. A diagonal line of gray squares runs from the top-left to the bottom-right of Σ . To the right of Σ is a gray rectangle labeled V^* .

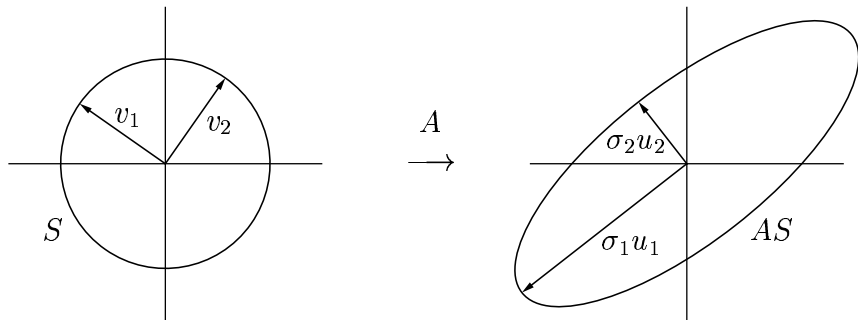
$$A = U \Sigma V^*$$

- Compact decomposition:

The diagram illustrates the compact SVD decomposition. On the left is a gray rectangle labeled A . To its right is an equals sign. Further right is a gray rectangle labeled \hat{U} . To the right of \hat{U} is a white square labeled $\hat{\Sigma}$, which contains a diagonal line of gray squares. To the right of $\hat{\Sigma}$ is a gray rectangle labeled V^* .

$$A = \hat{U} \hat{\Sigma} V^*$$

Geometric interpretation of the SVD



Some useful relations

If $A = U\Sigma V^*$ then

$$A^*A = (U\Sigma V^*)U\Sigma V^* = V\Sigma^*U^*U\Sigma V^* = V\Sigma^*\Sigma V^*$$

Therefore,

- The **singular values** σ_i of A are the square roots of the **eigenvalues** of A^*A
- The columns of V are the right singular vectors of A and the **eigenvectors** of A^*A
- The columns of U are the left singular vectors of A and the **eigenvectors** of AA^*

How to compute the SVD

We can compute the SVD as follows:

- 1 Compute $A^* A$
- 2 Compute the eigendecomposition of $A^* A = V \Lambda V^*$
- 3 Let Σ the $m \times n$ matrix whose diagonal entries are the square root of the diagonal entries of Λ
- 4 Solve $U \Sigma = A V$ with unitary matrix U

This algorithm is unstable! Nevertheless there exists efficient and stable algorithms to compute SVD

In MATLAB, $[U, S, V] = \text{svd}(A)$

Cost: $\mathcal{O}(mn^2)$ with constant usually of order 10

Uses of the SVD: Uses of the SVD include solving ill-conditioned least squares problems, representing the range or null space of a matrix, image compression, image deblurring, etc.

Some tasks to avoid

- **matrix inverse**

We can solve $Ax = b$ by multiplying both sides of the equation by A^{-1} :

$$A^{-1}Ax = x = A^{-1}b$$

Therefore, we can solve linear systems by multiplying the right-hand side b by A^{-1} .

This is a bad idea. It is more expensive than the LU decomposition and it generally computes an answer that has larger error.

Whenever you see a matrix inverse in a formula, think "LU decomposition".

- **Jordan canonical form**

Some matrices do not have an eigendecomposition like

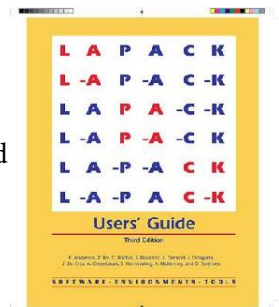
$$A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

but every matrix can be decomposed into Jordan canonical form as,

$$A = WJW^{-1}$$

For computing matrix decompositions and solving matrix problems in Fortran or C, look for LAPACK (<http://www.netlib.org/lapack/>).

- numerically stable algorithms
- uniform interface, making use easy
- row or column oriented implementation, appropriate for the matrix storage scheme used by the language
- built on BLAS and thus efficient (at least efficient when n is large (100 or more). The overhead for small n is quite big)



For Java, we can use JavaNumerics (<http://math.nist.gov/javanumerics/>)

MATLAB is based on LAPACK

A summary of matrix decompositions

Decomposition	Multiplications	Examples of uses
LU	$n^3/3$	<ul style="list-style-type: none">• Solving linear systems• Computing determinants
QR	$mn^2 - 1/3n^3$	<ul style="list-style-type: none">• Solving well-conditioned linear least squares problems• Representing the range or null space of a matrix
Eigendecomposition	$\mathcal{O}(n^3)$	<ul style="list-style-type: none">• Determining eigenvalues or eigenvectors of a matrix• Determining invariant subspaces.• Determining stability of a control system• Determining convergence of A^p when $p \rightarrow +\infty$
SVD	$\mathcal{O}(mn^2)$	<ul style="list-style-type: none">• Solving ill-conditioned linear least squares problems• Representing the range or null space of a matrix• Computing an approximation to a matrix

- We have not discussed **sparse matrices**, those with mostly zero entries. There exists some specific algorithms for those matrices that preserve the sparsity.
- There exists some specific algorithms for structured matrices (for example symmetric, tridiagonal, etc)