Queens College, CUNY, Department of Computer Science

Numerical Methods

CSCI 361 / 761

Fall 2017

Instructor: Dr. Sateesh Mane

October 9, 2017

8 Lecture 8

8.1 Matrices

- We shall study the solution of linear systems of equations by using matrices.
- The topic is also called (applied) **linear algebra.**
- In this lecture we shall examine some basic definitions and properties of matrices, independent of applications to linear algebra.

8.2 Matrices: general remarks

- A **matrix** with n rows and k columns is called an $n \times k$ matrix.
  For example for $n = 2$ and $k = 3$ then

$$M_{2\times 3} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \end{bmatrix} . \tag{8.2.1}$$

- The notation m_{ij} will be employed to denote the elements of a matrix M.

- A **square matrix** ($n \times n$ square matrix) has n rows and n columns.
  For example for $n = 2$ then

$$N_{2\times 2} = \begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix} . \tag{8.2.2}$$

- Both types of rectangular brackets or parentheses will be employed to describe a matrix.

- A **column vector** (with n elements) is an $n \times 1$ matrix. For example for $n = 3$ then

$$\boldsymbol{v} = \begin{bmatrix} a \\ b \\ c \end{bmatrix} . \tag{8.2.3}$$

- A **row vector** (with n elements) is a $1 \times n$ matrix. For example for $n = 4$ then

$$\boldsymbol{r} = \begin{bmatrix} \alpha & \beta & \gamma & \delta \end{bmatrix} . \tag{8.2.4}$$

- If A is an $m \times n$ matrix, then we can add (or subtract) a matrix B to it if and only if B is also an $m \times n$ matrix. The two matrices must have the same size.

- If we multiply a matrix M by a number λ, the matrix elements of λM (also $M\lambda$, because $\lambda M = M\lambda$) are obtained by multiplying all the elements of M by λ.
  An example for $n = 2$ and $k = 3$ is (see eq. (8.2.1)

$$\lambda\, M = M\, \lambda = \begin{bmatrix} \lambda m_{11} & \lambda m_{12} & \lambda m_{13} \\ \lambda m_{21} & \lambda m_{22} & \lambda m_{23} \end{bmatrix} . \tag{8.2.5}$$

- Matrix multiplication: if A is an $m \times n$ matrix and B is an $n \times k$ matrix, then the matrix product AB is an $m \times k$ matrix.

  1. **Note that the matrix product BA does not exist if $k \neq m$.**
  2. The order of matrix multiplication is important: AB might exist but BA might not.
  3. Even if both matrix products AB and BA exist, **they may not be equal**:

$$AB \neq BA \qquad\qquad \text{(in general)}\,. \tag{8.2.6}$$

  4. We say that matrix multiplication is **non-commutative.**

8.3 Matrices: more definitions

- The **zero matrix** has all entries equal to zero. Obvious enough.
- For a square matrix, the **leading diagonal** is the one with elements m_{ij} where $i = j$.
  The leading diagonal is also called the **main diagonal**.
- A **diagonal matrix** has nonzero elements only along its leading diagonal.
  For $n = 3$ an example is

$$D_{3\times 3} = \begin{pmatrix} d_{11} & 0 & 0 \\ 0 & d_{22} & 0 \\ 0 & 0 & d_{33} \end{pmatrix} . \tag{8.3.1}$$

- The **unit (or identity) matrix** is a diagonal matrix will all nonzero elements equal to 1.
  The identity matrix is frequently denoted by the symbol I or $\boldsymbol{I}$.
  The $n \times n$ unit or identity matrix is

$$I_{n\times n} = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ & & \ddots & \\ 0 & 0 & \dots & 1 \end{pmatrix} . \tag{8.3.2}$$

- A **tridiagonal matrix** has nonzero entries only on the leading diagonal and the two diagonals immediately above and below the leading diagonal.
  The matrix must be a square matrix.
  For $n = 5$ an example is

$$M_{\rm tri} = \begin{pmatrix} a_1 & b_1 & 0 & 0 & 0 \\ c_2 & a_2 & b_2 & 0 & 0 \\ 0 & c_3 & a_3 & b_3 & 0 \\ 0 & 0 & c_4 & a_4 & b_4 \\ 0 & 0 & 0 & c_5 & a_5 \end{pmatrix} . \tag{8.3.3}$$

- A **pentadiagonal matrix** is ... *you figure it out.*
- A **banded matrix** has nonzero elements only in diagonals such that $m_{ij} = 0$ if $|i - j| > c$, for some integer constant $c \geq 0$. A diagonal matrix is a banded matrix with $c = 0$. A tridiagonal matrix is a banded matrix with $c = 1$.
- An **upper triangular matrix** U has nonzero entries only on or above the leading diagonal.
  A **lower triangular matrix** L has nonzero entries only on or below the leading diagonal.
  Both the matrices L and U must be square.
  For $n = 4$, examples are

$$L = \begin{pmatrix} \ell_{11} & 0 & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} & 0 \\ \ell_{41} & \ell_{42} & \ell_{43} & \ell_{44} \end{pmatrix} , \qquad U = \begin{pmatrix} u_{11} & u_{12} & u_{13} & u_{14} \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix} . \tag{8.3.4}$$

  For $n \times n$ matrices, the number of independent matrix elements in both cases is $n(n+1)/2$.
  A diagonal matrix is simultaneously both upper and lower triangular.

8.4 Matrix transpose

- The **transpose** of a matrix M is denoted by M^T.
  The transpose M^T is obtained by interchanging the rows and columns of the matrix M.

- If M is an $n \times k$ matrix then M^T is a $k \times n$ matrix.

- The matrix M **need not be square**.

- The transpose matrix always exists and is unique.

- For $n = 2$ and $k = 3$ an example is

$$M = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \end{bmatrix}, \qquad M^T = \begin{bmatrix} m_{11} & m_{21} \\ m_{12} & m_{22} \\ m_{13} & m_{23} \end{bmatrix}. \tag{8.4.1}$$

- The transpose of a column vector is a row vector and vice versa.

- The transpose of a transpose is the original matrix: $(M^T)^T = M$.

- The product of a matrix and its transpose is a square matrix:
  MM^T is an $n \times n$ square matrix and M^TM is a $k \times k$ square matrix.

- The transpose of the matrix product AB is given by

$$(AB)^T = B^T A^T. \tag{8.4.2}$$

  Similarly

$$(ABC)^T = C^T B^T A^T. \tag{8.4.3}$$

  There is an obvious pattern for products of more matrices.

8.5 Matrix inverse

- The **inverse** of a matrix M is denoted by M^{-1}.
- The matrix M must be square.
- **Not every matrix has an inverse: M^{-1} does not always exist.**
- A matrix which does not have an inverse is called **singular**.
- The inverse matrix M^{-1} (if it exists) is defined by the relations

$$MM^{-1} = I\,, \qquad M^{-1}M = I\,. \tag{8.5.1}$$

- **If the inverse matrix M^{-1} exists, then it is unique.**
- The zero matrix (all entries are zero) is obviously singular.
- The inverse of the unit matrix is obviously the unit matrix itself.
- A matrix can equal its own inverse, i.e. $M^2 = I$. Some examples for $n = 2$ are

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,, \qquad M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,. \tag{8.5.2}$$

- Examples of singular matrices are

$$M_{\text{singular}} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\,, \qquad M_{\text{singular}} = \begin{pmatrix} 1 & 2 \\ 2 & 4 \end{pmatrix}\,. \tag{8.5.3}$$

- The inverse of the matrix product AB is given by

$$(AB)^{-1} = B^{-1}A^{-1}\,. \tag{8.5.4}$$

  Similarly

$$(ABC)^{-1} = C^{-1}B^{-1}A^{-1}\,. \tag{8.5.5}$$

  There is an obvious pattern for products of more matrices.

8.5.1 Non-square matrices

- **For your information only. Not for examination.**
- If the matrix M is not square, one can define a "left inverse" L_{inv} and a "right inverse" R_{inv}.
- The theory becomes complicated. Suppose M is $n \times k$, where $n \neq k$.
- If $n > k$, only a left inverse can exist. If it does, there are infinitely many choices. The inverse is not unique.

$$L_{\text{inv}}M = I_{k\times k}\,. \tag{8.5.6}$$

- If $n < k$, only a right inverse can exist. If it does, there are infinitely many choices. The inverse is not unique.

$$MR_{\text{inv}} = I_{n\times n}\,. \tag{8.5.7}$$

8.6 Square matrices: commutation & anticommutation

- Square matrices have some special properties which are important in many applications.
- Consider two square matrices A and B, both of the same size ($n \times n$).
- Then A and B are said to **commute** if $AB = BA$.
- Also A and B are said to **anticommute** if $AB = -BA$.

8.7 Square matrices: symmetric & antisymmetric

- A **symmetric matrix** S is equal to its transpose: $S^T = S$.
- An **antisymmetric matrix** A is equal to the **negative** of its transpose: $A^T = -A$.
- An antisymmetric matrix is also called a **skew-symmetric matrix**.
- Hence the matrix elements satisfy the relations

$$(S^T)_{ij} = S_{ji}\,, \qquad (A^T)_{ij} = -A_{ji}\,. \tag{8.7.1}$$

- The elements on the leading diagonal of an antisymmetric matrix are all zero.
- Every diagonal matrix is symmetric.
- For $n = 3$ an example is

$$S_{3\times3} = \begin{pmatrix} a_{11} & b & c \\ b & a_{22} & d \\ c & d & a_{33} \end{pmatrix}, \qquad A_{3\times3} = \begin{pmatrix} 0 & \beta & \gamma \\ -\beta & 0 & \delta \\ -\gamma & -\delta & 0 \end{pmatrix}. \tag{8.7.2}$$

- An $n \times n$ symmetric matrix has $n(n+1)/2$ independent elements.
- An $n \times n$ antisymmetric matrix has $n(n-1)/2$ independent elements.
- The sum of two symmetric matrices is also symmetric.
- The sum of two antisymmetric matrices is also antisymmetric.
- The product of a symmetric matrix with a number is a symmetric matrix.
- The product of an antiymmetric matrix with a number is an antisymmetric matrix.
- **However, do not jump to conclusions when we multiply symmetric and antisymmetric matrices.**

8.7.1 Products of symmetric and antisymmetric matrices

- **Do not jump to conclusions about the products of symmetric and antisymmetric matrices.**
- The following matrices are symmetric:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{8.7.3}$$

  (Never mind why I call them σ_1 and σ_3. Yes there is also a σ_2.)

- The matrix products $\sigma_3\sigma_3$ and $\sigma_1\sigma_1$ are also symmetric matrices ($\sigma_3^2 = \sigma_1^2 = I$):

$$\sigma_3\sigma_3 = \sigma_1\sigma_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{8.7.4}$$

- **The matrix products $\sigma_1\sigma_3$ and $\sigma_3\sigma_1$ are antisymmetric:**

$$\sigma_1\sigma_3 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} , \qquad \sigma_3\sigma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{8.7.5}$$

- The symmetric matrices σ_1 and σ_3 anticommute. Their product is an antisymmetric matrix.
- Yes the product is proportional to σ_2. If you really want to know,

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} . \tag{8.7.6}$$

  The matrix elements of σ_2 are complex numbers (pure imaginary).

8.8 Square matrices: trace

- The **trace** of a square matrix is the sum of the elements on the main diagonal.
- Some authors also refer to the trace as the **spur** of a matrix.

$$\mathrm{spur}(M) = \mathrm{trace}(M) = \mathrm{Tr}(M) = m_{11} + m_{22} + \cdots + m_{nn} = \sum_{i=1}^{n} m_{ii}\,. \tag{8.8.1}$$

- A **traceless** matrix is one whose trace equals zero.
- An antisymmetric matrix is always traceless.
- The trace of a square matrix is equal to the trace of its transpose:

$$\mathrm{Tr}(M) = \mathrm{Tr}(M^T)\,. \tag{8.8.2}$$

- For two square matrices A and B, the trace of $A+B$ is the sum of the traces

$$\mathrm{Tr}(A+B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)\,. \tag{8.8.3}$$

- Furthermore, for matrices A and B,

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA)\,. \tag{8.8.4}$$

- The trace of a matrix product has a cyclic property. For three matrices A, B and C,

$$\mathrm{Tr}(ABC) = \mathrm{Tr}(BCA) + \mathrm{Tr}(CAB)\,. \tag{8.8.5}$$

- The cyclic property extends in an obvious way to products of more matrices.

8.9 Square matrices: determinant

- The **determinant** of a square matrix is a number obtained from all the rows and colums of the matrix. For a 2×2 matrix, the determinant is given by

$$M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad \det(M) = ad - bc\,. \tag{8.9.1}$$

- In general, for an $n \times n$ square matrix, the determinant is given by a sum of products

$$\det(M) = \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_n=1}^{n} \sigma_{i_1,i_2,\dots,i_n} m_{1i_1} m_{2i_2} \dots m_{ni_n}\,. \tag{8.9.2}$$

  Here $\sigma_{i_1,i_2,\dots,i_n}$ is a sign factor equal to ± 1, given by

$$\sigma_{i_1,i_2,\dots,i_n} = \begin{cases} +1 & ((i_1,i_2,\dots,i_n) = \text{even permutation of } (1,2,\dots,n)) \\ -1 & ((i_1,i_2,\dots,i_n) = \text{odd permutation of } (1,2,\dots,n))\,. \end{cases} \tag{8.9.3}$$

- There are computationally more efficient ways to calculate the determiant of a matrix.
- The determinant of a unit matrix equals unity: $\det(I) = 1$.
- The determinant of a matrix is equal to the determinant of its transpose:

$$\det(M) = \det(M^T)\,. \tag{8.9.4}$$

- For matrices $A_1, \dots, A_n$ the determinant of the product equals the product of the determinants

$$\det(A_1 A_2 \dots A_n) = \det(A_1)\,\det(A_2)\,\dots\det(A_n)\,. \tag{8.9.5}$$

- The inverse M^{-1} of a square matrix M exists if and only if $\det(M) \neq 0$.

8.10 Orthogonal matrices

- **The material in this section is not for examination.**
- **You may skip it if it is too advanced.**
- An **orthogonal matrix** O satisfies the relation

$$O^T O = I \,. \tag{8.10.1}$$

- It is also true that $OO^T = I$ and $O^T = O^{-1}$.
- The determinant of an orthogonal matrix equals ± 1.
- The converse is not true: a square matrix with determinant 1 is not necessarily orthogonal

$$M = \begin{pmatrix} 2 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \qquad\qquad (\textbf{not orthogonal})\,. \tag{8.10.2}$$

- An orthogonal matrix with determinant $+1$ is called a **special orthogonal matrix**.
- The identity matrix is a special orthogonal matrix.
- The negative of the identity matrix $-I_{n\times n}$ has determinant $(-1)^n$.
  It equals 1 if n is even and -1 if n is odd.
- Examples of symmetric and antisymmetric special orthogonal matrices are
  (x is a real number)

$$S = \begin{pmatrix} \cosh(x) & \sinh(x) \\ \sinh(x) & \cosh(x) \end{pmatrix} \,, \qquad A = \begin{pmatrix} \cos(x) & -\sin(x) \\ \sin(x) & \cos(x) \end{pmatrix} \,. \tag{8.10.3}$$

- The following matrix is orthogonal and has determinant -1

$$O = \begin{pmatrix} \cos(x) & \sin(x) \\ \sin(x) & -\cos(x) \end{pmatrix} \,. \tag{8.10.4}$$

- Rotation matrices, in any number of dimensions, are special orthogonal matrices.
- Reflection matrices are orthogonal matrices, not always special orthogonal matrices.

8.11 Complex valued matrices

- **The material in this section is not for examination.**
- **You may skip it if it is too advanced.**
- The elements of a matrix need not be real. They can be complex.
- The **Hermitian conjugate** of a complex valued matrix C is the complex conjugate transpose matrix
$$C^\dagger = (C^T)^* = (C^*)^T \,. \tag{8.11.1}$$
- A **Hermitian matrix** H is equal to its Hermitian conjugate
$$H^\dagger = H \,. \tag{8.11.2}$$
- An **anti-Hermitian** or **skew-Hermitian** matrix A is equal to the negative of its Hermitian conjugate
$$A^\dagger = -A \,. \tag{8.11.3}$$
- The eigenvalues of a Hermitian matrix are real numbers.
  The eigenvalues of a skew-Hermitian matrix are pure imaginary numbers.
- A **unitary matrix** U satisfies the relation
$$U^\dagger U = I \,. \tag{8.11.4}$$
- It is also true that $UU^\dagger = I$ and $U^\dagger = U^{-1}$.
- The determinant of a unitary matrix satisfies $|\det U| = 1$.
  Hence the determinant of a unitary matrix lies on the complex unit circle.
- The eigenvalues of a unitary matrix lie on the complex unit circle.
- A unitary matrix with determinant $+1$ is called a **special unitary matrix**.
- The unit matrix is both a Hermitian matrix and a special unitary matrix.
- Examples of symmetric and antisymmetric special unitary matrices are
$$S = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \,, \qquad A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \,. \tag{8.11.5}$$
- The following matrices are unitary and have determinant -1 and $-i$, respectively
$$iI_{2\times 2} = \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \,, \tag{8.11.6}$$
$$iI_{3\times 3} = \begin{pmatrix} i & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & i \end{pmatrix} \,. \tag{8.11.7}$$

8.12 Matrix exponential

- **The material in this section is not for examination.**
- **You may skip it if it is too advanced.**
- The **exponential** of a square matrix is **defined** by the power series infinite sum

$$\exp(M) = e^M = 1 + M + \frac{M^2}{2!} + \frac{M^3}{3!} + \cdots = \sum_{n=0}^{\infty} \frac{M^n}{n!} . \tag{8.12.1}$$

- Note that this is a **definition.**
- As with the exponential series for a number x, the exponential series for a matrix converges absolutely.
- Be careful: if A and B are square matrices, then in general

$$e^A e^B \neq e^{A+B} . \tag{8.12.2}$$

  The above result is true only if A and B commute.
- The exponential of an antisymmetric matrix is a special orthogonal matrix

$$(e^A)^T e^A = e^{A^T} e^A = e^{-A} e^A = I . \tag{8.12.3}$$

- The exponential of an anti-Hermitian matrix is a special unitary matrix

$$(e^A)^\dagger e^A = e^{A^\dagger} e^A = e^{-A} e^A = I . \tag{8.12.4}$$

8.13 Matrix rank

- **The material in this section is not for examination.**
- **You may skip it if it is too advanced.**
- The matrix M need not be square.
- The **rank** of a matrix M is the dimension of the vector space spanned by the columns of M.
- The rank of M is also equal to the dimension of the vector space spanned by the rows of M.
- Hence the column rank equals the row rank of a matrix.
- **We shall see a little bit of this when we solve a set of simultaneous linear equations, and the equations are not all linearly independent. In that case, if there are n equations, the rank will be less than n. It may or may not be possible to solve the equations in this situation. We shall see.**
- **Nevertheless, concepts such as "vector space" are not for examination.**