• CSCI 5304 • Fall 2019 •

COMPUTATIONAL ASPECTS OF MATRIX THEORY

Class time	:	8:15 – 9:30 TTh
Room	:	ME 108
Instructor	:	Yousef Saad
URL	:	www-users.cselabs.umn.edu/classes/Fall-2019/csci5304/

September 4, 2019

About this class. Instructor and Teaching Assistant

- Me: Yousef Saad
- TA: Jack Perisich

What you will learn and why

– Course title:

“Computational Aspects of Matrix Theory”

– Alternative title:

“Theoretical Aspects of Matrix Computations”

... detailed title:

“Everything you need to know about computations involving matrices that you can learn in one semester – from theory to algorithms, matlab implementations, and applications.”

➤ Topic becoming increasingly important in Computer Science.

➤ At the core of *most* disciplines requiring numerical computing.

Objectives of this course

Set 1 Fundamentals of matrix theory :

- Matrices, subspaces, eigenvectors
- Norms, matrix norms, understanding errors, sensitivity [somewhat theoretical]
- Various decompositions, LU, QR, SVD, ..

set 2 Computational linear algebra / Algorithms

- Solving linear systems, LU factorization
- Solving least-squares problems, QR factorization
- Eigenvalue problems - computing eigenvalues, eigenvectors,

Set 3 Linear algebra in applications

- See how numerical linear algebra is used to solve problems in (a few) computer science-related applications.

- Examples: page-rank, applications in optimization, information retrieval, applications in machine learning, control, ...

Logistics:

- We will use Canvas only to post grades
- Main class web-site is :

`www-users.cselabs.umn.edu/classes/Fall-2019/csci5304/`

- There you will find :

- Lecture notes
- Homeworks [and solutions]
- On occasion: Additional exercises [do before indicated class]
- ... and more

Please Note:

➤ Homeworks and solutions are copyrighted

- *Solutions of HWs and exams are provided to you [login required] with the hope of helping you understand the material better. By accessing them you agree not to send them to others, sell them (%#!!$), or otherwise (help) make them available via external websites.*

Note: The login to access these solutions is *not* you U of M login. [it will be given in class later when needed..]

About lecture notes:

➤ Lecture notes (like this first set) will be posted on the class web-site – usually before the lecture.

➤ Note: format used in lectures may be formatted differently – but same contents.

➤ Review them to get some understanding if possible before class.

➤ Read the relevant section (s) in one of the references listed

➤ Lecture note sets are grouped by topics rather than by lecture.

➤ In the notes the symbol ✍1 indicates suggested easy exercises or questions – often [not always] done in class.

Occasional in-class practice exercises

- Posted in advance – see HWs web-page
- Do them before class. No need to turn in anything. But...
- ... prepare for an occasional follow-up Quiz [!relax: not graded]

Matlab

- You will need to use matlab for testing algorithms.
- No lecture notes on matlab +
- Other documents will be posted in the matlab web-site.
- Most important:
- .. I post the matlab diaries used for the demos (if any).

● If you do not know matlab at all and have difficulties with it see me or one of the TAs at office hours. All you may need is some initial help to get you started.

One final point on lecture notes

➤ These notes are ‘evolving’. You can help imorove them – report errors and provide feedback on content.

➤ Occasionally I will repost lecture notes with changes/additions [clearly indicated in red in the web-page]

➤ There will be much more going on in the classroom - so the notes are not enough for studying! Sometimes they are used as a summary.

- How to study for this course:

1) Rely primarily on lecture notes as a starting point. Use other sources [e.g., (online) books] to get a deeper understanding.

2) Do the practice exercises indicated in lecture notes + those occasionally posted in HW page.

3) Ask questions!

- Time to start!

GENERAL INTRODUCTION

- Background: Linear algebra and numerical linear algebra
- Types of problems to be seen in this course
- Mathematical background - matrices, eigenvalues, rank, ...
- Types of matrices, structutred matrices,
- Quick review of Matlab
- Vector norms, matrix norms

Introduction

- This course is about *Matrix algorithms* or "matrix computations"

- It involves: algorithms for standard matrix computations (e.g. solving linear systems) - and their analysis (e.g., their cost, numerical behavior, ..)

- Matrix algorithms pervade most areas of science and engineering.

- In computer science: recent increase of interest in matrix algorithms for data mining, information retrieval, search engines, pattern recognition, graphics, ...

Examples

➤ Modern version of an old problem

A set of 12 coins containing nickels (5c each), dimes (10c each) and quarters (25c each) totals to \$1.45. In addition, the total without the nickels amounts to \$1.25. How many of each coin are there?

Solution: The system you get is

$$\begin{pmatrix} 5 & 10 & 25 \\ 1 & 1 & 1 \\ 0 & 10 & 25 \end{pmatrix} \begin{pmatrix} x_n \\ x_d \\ x_q \end{pmatrix} = \begin{pmatrix} 145 \\ 12 \\ 125 \end{pmatrix}$$

where $x_n = \#$ nickels, $x_d = \#$ dimes, $x_q = \#$ quarters

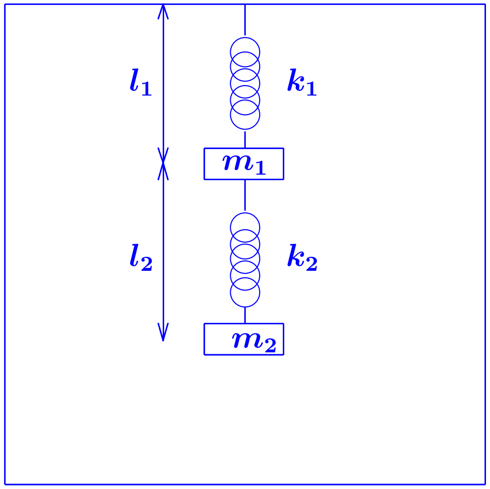
✍1 And the solution is: ?

- Pagerank of Webpages (21st cent AD)

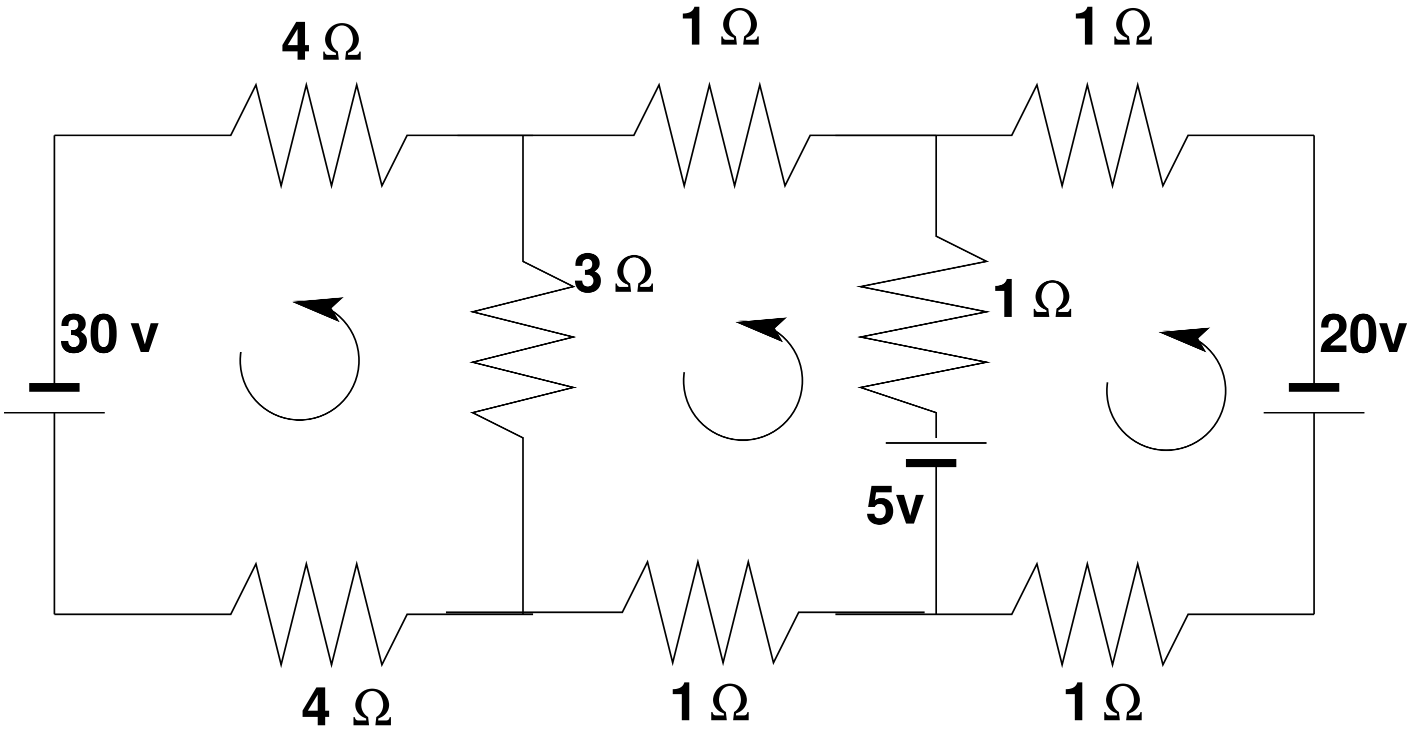
If one were to do a random walk from web page to web page, following each link on a given web page at random with equal likelihood, which are the pages to be encountered this way most often?

- Vibrations in mechanical systems. See: `www.cs.umn.edu/~saad/eig_book_2ndEd.pdf`

Problem: Determine the vibration modes of the mechanical system [to avoid resonance]. See details in Chapter 10 (sec. 10.2) of above reference.



➤ Electrical circuits / Power networks, .. [Kirchhiff's voltage Law]



Problem: Determine the loop currents in a an electrical circuit - using Kirchhoff's Law $(\boldsymbol{V} = \boldsymbol{RI})$

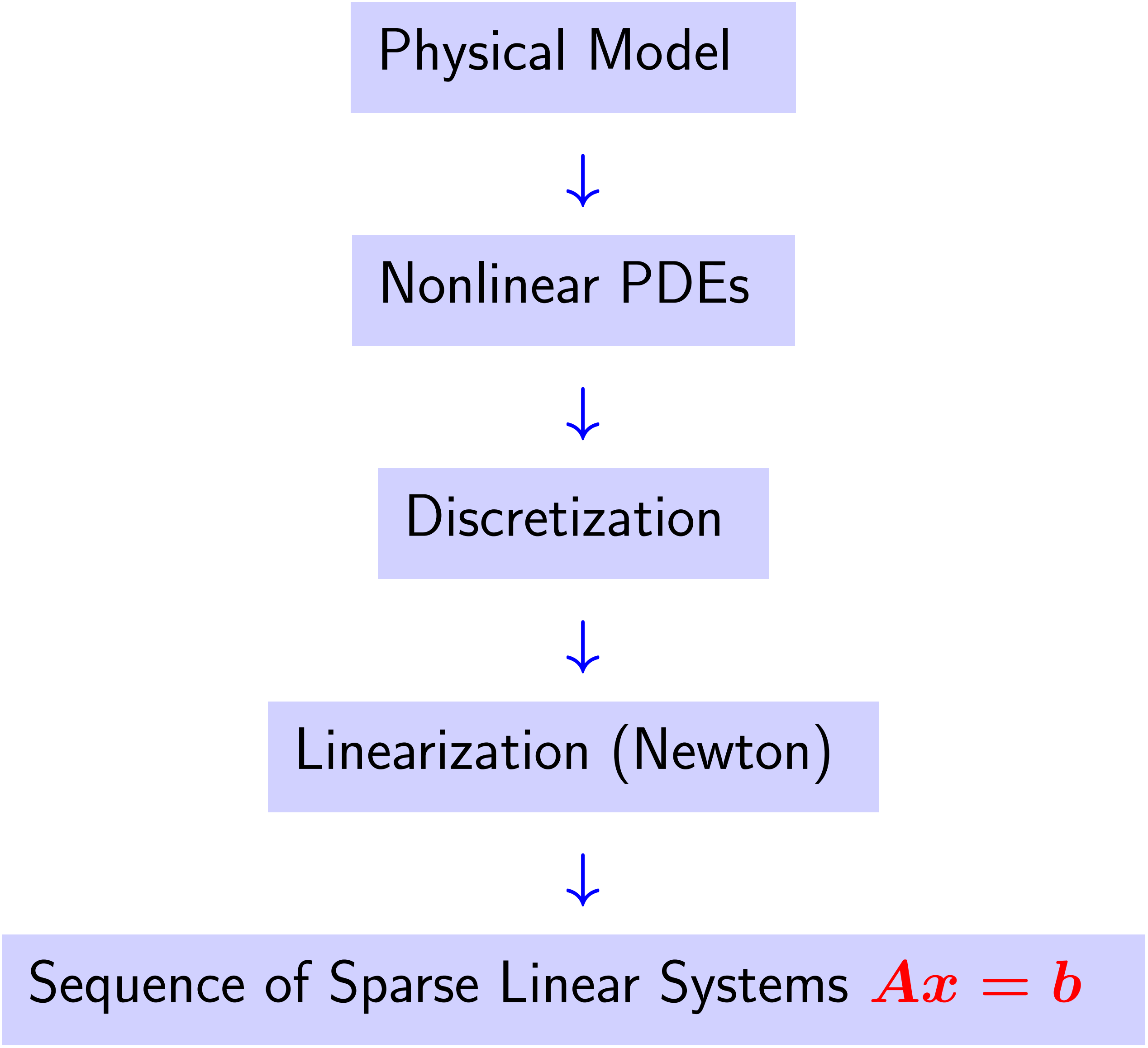
Examples (cont.)

- ➤ Method of least-squares (inspired by first use of least squares ever, by Gauss around 1801)

A planet follows an elliptical orbit according to $ay^2 + bxy + cx + dy + e = x^2$ in cartesian coordinates. Given a set of noisy observations of (x, y) positions, compute a, b, c, d, e, and use to predict future positions of the planet. This least squares problem is nearly rank-deficient and hence very sensitive to perturbations in the observations.

Read Wikipedia's article on planet ceres:
`http://en.wikipedia.org/wiki/Ceres_(dwarf_planet)`

Typical Large-scale problem (e.g. Fluid flow)



Physical Model

↓

Nonlinear PDEs

↓

Discretization

↓

Linearization (Newton)

↓

Sequence of Sparse Linear Systems $\boldsymbol{Ax = b}$

Background in linear algebra

- Review vector spaces.

- A vector subspace of $\mathbb{R}^n$ is a subset of $\mathbb{R}^n$ that is also a real vector space. The set of all linear combinations of a set of vectors $G = \{a_1, a_2, \ldots, a_q\}$ of $\mathbb{R}^n$ is a vector subspace called the linear span of G,

- If the a_i's are linearly independent, then each vector of $\mathbf{span}\{G\}$ admits a unique expression as a linear combination of the a_i's. The set G is then called a *basis*.

✍2 Recommended reading: Sections 1.1 – 1.6 of

`www.cs.umn.edu/~saad/eig_book_2ndEd.pdf`

Matrices

➤ A real $m \times n$ matrix A is an $m \times n$ array of real numbers

$$a_{ij}, \;\; i = 1, \ldots, m, \; j = 1, \ldots, n.$$

The set of all $m \times n$ matrices is a real vector space denoted by $\mathbb{R}^{m \times n}$.

➤ Complex matrices defined similarly.

➤ A matrix represents a linear mapping between two vector spaces of finite dimension n and m.

Operations:

Addition: $\boldsymbol{C = A + B}$, where $\boldsymbol{A, B, C} \in \mathbb{R}^{\boldsymbol{m \times n}}$ and

$$\boldsymbol{c_{ij} = a_{ij} + b_{ij}, \quad i = 1, 2, \ldots m, \quad j = 1, 2, \ldots n.}$$

Multiplication by a scalar: $\boldsymbol{C = \alpha A}$, where

$$\boldsymbol{c_{ij} = \alpha \; a_{ij}, \quad i = 1, 2, \ldots m, \quad j = 1, 2, \ldots n.}$$

Multiplication by another matrix:

$$\boldsymbol{C = AB,}$$

where $\boldsymbol{A} \in \mathbb{R}^{\boldsymbol{m \times n}}, \boldsymbol{B} \in \mathbb{R}^{\boldsymbol{n \times p}}, \boldsymbol{C} \in \mathbb{R}^{\boldsymbol{m \times p}}$, and

$$\boldsymbol{c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}.}$$

Transposition: If $A \in \mathbb{R}^{m\times n}$ then its transpose is a matrix $C \in \mathbb{R}^{n\times m}$ with entries

$$c_{ij} = a_{ji}, i = 1, \ldots, n, \ j = 1, \ldots, m$$

Notation : A^T.

Transpose Conjugate: for complex matrices, the **transpose conjugate** matrix denoted by A^H is more relevant: $A^H = \bar{A}^T = \overline{A^T}$.

✍3 $(A^T)^T = ??$

✍4 $(AB)^T = ??$

✍5 $(A^H)^H = ??$

✍6 $(A^H)^T = ??$

✍7 $(ABC)^T = ??$

✍8 True/False: $(AB)C = A(BC)$

✍9 True/False: $AB = BA$

✍10 True/False: $AA^T = A^TA$

Review: Matrix-matrix and Matrix-vector producs

- Recall definition of $\boldsymbol{C} = \boldsymbol{A} \times \boldsymbol{B}$.
- Recall what $\boldsymbol{C}$ represents [in terms of mappings]..
- Can do the product column-wise [Matlab notation used]:

$$\boldsymbol{C_{:,j} = \sum_{k=1}^{n} b_{kj} A_{:,k}}$$

- Can do it row-wise:

$$\boldsymbol{C_{i,:} = \sum_{k=1}^{n} a_{ik} B_{k,:}}$$

- Can do it as a sum of ‘outer-product’ matrices:

$$C = \sum_{k=1}^{n} A_{:,k} B_{k,:}$$

✍11 Verify (prove) all 3 formulas above..

✍12 Complexity? [number of multiplications and additions]

✍13 What happens to these 3 different approaches when B has one column $(p = 1)$?

✍14 Characterize the matrices AA^T and A^TA when A is of dimension $n \times 1$.

Range and null space (for $A \in \mathbb{R}^{m\times n}$)

- Range: $\mathbf{Ran}(A) = \{Ax \mid x \in \mathbb{R}^n\}$ $\subseteq \mathbb{R}^m$
- Null Space: $\mathbf{Null(A)} = \{x \in \mathbb{R}^n \mid Ax = \mathbf{0}\ \}$ $\subseteq \mathbb{R}^n$
- Range $=$ linear span of the columns of A
- Rank of a matrix $\mathbf{rank}(A) = \mathbf{dim}(\mathbf{Ran}(A))$ $\leq n$
- Ran$(A) \subseteq \mathbb{R}^m$ $\rightarrow$ rank $(A) \leq m \rightarrow$

$$\boxed{\text{rank } (A) \leq \min\{m, n\}}$$

- rank (A) $=$ number of linearly independent columns of A $=$ number of linearly independent rows of A
- A is of full rank if $\mathbf{rank}(A) = \min\{m, n\}$. Otherwise it is rank-deficient.

Rank+Nullity theorem for an $m \times n$ matrix:

$$dim(Ran(A)) + dim(Null(A)) = n$$

Apply to A^T: $dim(Ran(A^T)) + dim(Null(A^T)) = m \rightarrow$

$$\text{rank}(A) + dim(Null(A^T)) = m$$

- Terminology:
  - $dim(Null(A))$ is the Nullity of A

✍15 Show that $A \in \mathbb{R}^{n\times n}$ is of rank one iff [if and only if] there exist two nonzero vectors u and v such that

$$A = uv^T.$$

What are the eigenvalues and eigenvectors of A?

✍16 Is it true that

$$\mathbf{rank}(A) = \mathbf{rank}(\bar{A}) = \mathbf{rank}(A^T) = \mathbf{rank}(A^H)\ ?$$

✍17 Matlab exercise: explore the matlab function `rank`.

✍18 Matlab exercise: explore the matlab function `rref`.

✍19 Find the range and null space of the following matrix:

$$\begin{pmatrix} -1 & 1 & 0 \\ 1 & 2 & 3 \\ 1 & -2 & -1 \\ 2 & -1 & 1 \end{pmatrix}$$

Then verify your result with matlab.

Square matrices, matrix inversion, eigenvalues

- Square matrix: $n = m$, i.e., $A \in \mathbb{R}^{n\times n}$
- Identity matrix: square matrix with

$$a_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- Notation: I.
- Property: $AI = IA = A$
- Inverse of A (when it exists) is a matrix C such that

$$AC = CA = I$$

Notation: A^{-1} .

Eigenvalues and eigenvectors

A complex scalar λ is called an eigenvalue of a square matrix A if there exists a nonzero vector u in $\mathbb{C}^n$ such that $Au = \lambda u$. The vector u is called an eigenvector of A associated with λ. The set of all eigenvalues of A is the 'spectrum' of A. Notation: $\Lambda(A)$.

➤ λ is an eigenvalue iff the columns of $A - \lambda I$ are linearly dependent.

➤ ... equivalent to saying that its rows are linearly dependent. So: there is a nonzero vector w such that

$$w^H(A - \lambda I) = 0$$

➤ w is a left eigenvector of A (u= right eigenvector)

➤ λ is an eigenvalue iff $\boxed{\det(A - \lambda I) = 0}$

Eigenvalues/vectors

- An eigenvalue is a root of the Characteristic polynomial: $$p_A(\lambda) = \det(A - \lambda I)$$

- So there are n eigenvalues (counted with their multiplicities).

- The multiplicity of these eigenvalues as roots of p_A are called algebraic multiplicities.

- The geometric multiplicity of an eigenvalue λ_i is the number of linearly independent eigenvectors associated with λ_i.

- Geometric multiplicity is $\leq$ algebraic multiplicity.

- An eigenvalue is simple if its (algebraic) multiplicity is one. It is semi-simple if its geometric and algebraic multiplicities are equal.

➤ Two matrices A and B are similar if there exists a nonsingular matrix X such that $\boxed{A = XBX^{-1}}$

✍21 Eigenvalues of A and B are the same. What about eigenvectors?

➤ Note: A and B represent the same mapping using 2 different bases.

Fundamental Problem: Given A, find X so that B has a simpler structure (e.g., diagonal) $\longrightarrow$ Eigenvalues of B easier to compute

Definition: A is diagonalizable if it is similar to a diagonal matrix

➤ We will revisit these notions later in the semester

✍22 Given a polynomial $p(t)$ how would you define $p(A)$?

✍23 Given a smooth function $f(t)$ (e.g., e^t) how would you define $f(A)$? [Consider only the case when A is diagonalizable]

✍24 If A is nonsingular what are the eigenvalues/eigenvectors of A^{-1}?

✍25 What are the eigenvalues/eigenvectors of A^k for a given integer power k?

✍26 What are the eigenvalues/eigenvectors of $p(A)$ for a polynomial p?

✍27 What are the eigenvalues/eigenvectors of $f(A)$ for a function f? [Diagonalizable case]

✍28 For two $n \times n$ matrices A and B are the eigenvalues of AB and BA the same?

✍29 Review the Jordan canonical form. Define the eigenvalues, and eigenvectors from the Jordan form.

- ➤ Spectral radius = The maximum modulus of the eigenvalues

$$\boxed{\rho(A) = \max_{\lambda \in \lambda(A)} \ |\lambda|.}$$

- ➤ Trace of A = sum of diagonal elements of A.

$$\boxed{\mathbf{tr}(A) = \sum_{i=1}^{n} a_{ii}.}$$

- ➤ $\mathbf{tr}(A)$ = sum of all the eigenvalues of A counted with their multiplicities.

- ➤ Recall that $\mathbf{det}(A)$ = product of all the eigenvalues of A counted with their multiplicities.

✍30 Trace, spectral radius, and determinant of

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

Types of (square) matrices

- Symmetric $A^T = A$. • Skew-symmetric $A^T = -A$.
- Hermitian $A^H = A$. • Skew-Hermitian $A^H = -A$.

- Normal $A^H A = AA^H$.

- Nonnegative $a_{ij} \geq 0,\ i, j = 1, \ldots, n$

- Similarly for nonpositive, positive, and negative matrices

- Unitary $Q^H Q = I$. (for complex matrices)

[Note: Common useage restricts this definition to complex matrices. An orthogonal matrix is a unitary real matrix – not very natural]

- Orthogonal $Q^T Q = I$ [orthonormal columns]

[I will sometimes call unitary matrix a square matrix with orthonormal columns, regardless on whether it is real or complex]

➤ The term “orthonormal” matrix is rarely used.

✍31 What is the inverse of a unitary (complex) or orthogonal (real) matrix?

✍32 What can you say about the diagonal entries of a skew-symmetric (real) matrix?

✍33 What can you say about the diagonal entries of a Hermitian (complex) matrix?

✍34 What can you say about the diagonal entries of a skew-Hermitian (complex) matrix?

✍35 The following types of matrices are normal [true-false]: real symmetric, real skew-symmetric, complex Hermitian, complex skew-Hermitian.

✍36 Find all real $\mathbf{2} \times \mathbf{2}$ matrices that are normal.

✍37 Show that a triangular matrix that is normal is diagonal.

Matrices with structure

- Diagonal $a_{ij} = 0$ for $j \neq i$. Notation :

$$A = \mathrm{diag}\left(a_{11}, a_{22}, \ldots, a_{nn}\right).$$

- Upper triangular $a_{ij} = 0$ for $i > j$.
- Lower triangular $a_{ij} = 0$ for $i < j$.
- Upper bidiagonal $a_{ij} = 0$ for $j \neq i$ or $j \neq i + 1$.
- Lower bidiagonal $a_{ij} = 0$ for $j \neq i$ or $j \neq i - 1$.
- Tridiagonal $a_{ij} = 0$ when $|i - j| > 1$.

- Banded $a_{ij} \neq 0$ only when $i - m_l \leq j \leq i + m_u$, 'Bandwidth' $= m_l + m_u + 1$.

- Upper Hessenberg $a_{ij} = 0$ when $i > j + 1$. Lower Hessenberg matrices can be defined similarly.

- Outer product $A = uv^T$, where both u and v are vectors.

- Block tridiagonal generalizes tridiagonal matrices by replacing each nonzero entry by a square matrix.

Special matrices

Vandermonde :

➤ Given a column of entries $[x_0, x_1, \cdots, x_n]^T$ put its (component-wise) powers into the columns of a matrix V:

$$V = \begin{pmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^2 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{pmatrix}$$

✍38 Try the matlab function *vander*

✍39 What does the matrix-vector product Va represent?

✍40 Interpret the solution of the linear system $Va = y$ where a is the unknown. Sketch a ‘fast’ solution method based on this.

Toeplitz :

- Entries are constant along diagonals, i.e., $a_{ij} = r_{j-i}$.
- Determined by $m + n - 1$ values r_{j-i}.

$$T = \underbrace{\begin{pmatrix} r_0 & r_1 & r_2 & r_3 & r_4 \\ r_{-1} & r_0 & r_1 & r_2 & r_3 \\ r_{-2} & r_{-1} & r_0 & r_1 & r_2 \\ r_{-3} & r_{-2} & r_{-1} & r_0 & r_1 \\ r_{-4} & r_{-3} & r_{-2} & r_{-1} & r_0 \end{pmatrix}}_{Toeplitz}$$

- Toeplitz systems ($m = n$) can be solved in $O(n^2)$ ops.
- The whole inverse (!) can be determined in $O(n^2)$ ops.

✍41 Explore *toeplitz(c,r)* in matlab.

Hankel : Entries are constant along anti-diagonals, i.e., $a_{ij} = h_{j+i-1}$. Determined by $m + n - 1$ values h_{j+i-1}.

$$H = \underbrace{\begin{pmatrix} h_1 & h_2 & h_3 & h_4 & h_5 \\ h_2 & h_3 & h_4 & h_5 & h_6 \\ h_3 & h_4 & h_5 & h_6 & h_7 \\ h_4 & h_5 & h_6 & h_7 & h_8 \\ h_5 & h_6 & h_7 & h_8 & h_9 \end{pmatrix}}_{Hankel}$$

✍42 Explore *hankel(c,r)* in matlab.

Circulant : Entries in a row are cyclically right-shifted to form next row. Determined by n values.

$$C = \underbrace{\begin{pmatrix} v_1 & v_2 & v_3 & v_4 & v_5 \\ v_5 & v_1 & v_2 & v_3 & v_4 \\ v_4 & v_5 & v_1 & v_2 & v_3 \\ v_3 & v_4 & v_5 & v_1 & v_2 \\ v_2 & v_3 & v_4 & v_5 & v_1 \end{pmatrix}}_{Circulant}$$

✍43 How can you generate a circulant matrix in matlab?

✍44 If C is circulant (real) and symmetric, what can be said about the v_i's?

Sparse matrices

- Matrices with very few nonzero entries – so few that this can be exploited.

- Many of the large matrices encountered in applications are sparse.

- Main idea of “sparse matrix techniques” is not to represent the zeros.

- This will be covered in some detail at the end of the course.