UNIVERSITY OF MINNESOTA TWIN CITIES

CSCI 5304 Fall 2022

COMPUTATIONAL ASPECTS OF MATRIX THEORY

Class time	:	TTh 8:15 – 9:30 am
Room	:	Keller H. 3-125
Instructor	:	Yousef Saad

Lecture notes: `http://www-users.cse.umn.edu/~saad/csci5304/`

September 12, 2022

About this class. Instructor and Teaching Assistant

- Me: Yousef Saad
- TA: Zechen Zhang

– Course title:

"Computational Aspects of Matrix Theory"

What you will learn and why material is important

– Alternative title:

"Theoretical Aspects of Matrix Computations"

... a longer title:

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

➤ Subject is at the core of *most* disciplines requiring numerical computing..

➤ .. and gaining importance in Computer Science (machine learning, robotics, graphics, ...)

Who is in this class today?

➤ Out of ≈ 60 [excluding Unite]

- 27 in Computer Science [all levels]
- 19 Mechanical Engineering
- 6 Electrical Eng.
- 2 Computer Engineering
- 2 Aerospace Eng.
- 2 Statistics
- 1 each in: Math, Neuroscience, Data Science
- 14 Undergraduate students
- 21 PhD students + 25 MS $\longrightarrow$ 46 Grad.

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:

- Lecture notes, syllabus, schedule, a matlab/Python folder, and some basic information, can be found here:

  `http://www-users.cse.umn.edu/~saad/csci5304`

- Everything else will be found on Canvas: Homeworks, exam/quizzes info, your grades, etc..

➤ The two sites have links to each other

Please Note:

➤ Homeworks, tests, and their solutions are copyrighted

- *Solutions of HWs and tests are provided to you [Canvas] 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 web-sites.*

About lecture notes:

- Lecture notes (like this first set) will be posted on the class web-site – usually before the lecture. Note: format of notes used in class may be slightly different from the one posted – but contents are identical.

- 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 sometimes solved in class. Each set will have a supplement which includes solutions to some of these exercises + possibly additional notes/comments.

Occasional in-class practice exercises

- Posted in advance – [Canvas]
- Do them before class. No need to turn in anything.
- ... will be discussed - typically at beginning of class

Matlab and Python

- You will need to use matlab for testing algorithms.
- New this year: for those interested you can turn in your codes for assignments in Python+numpy. + demos often in both
- Some documentation is posted in the (class) matlab folder – No documentation for Python
- Important: I post the matlab diaries used for the demos (if any)...
- .. working on something similar for Python [under IPython]

- If you do not know matlab at all and have difficulties with it - and you do not know python - talk to me or the TA at office hours. All you may need is some initial help to get you started with matlab.

Final remarks on lecture notes

- Please do not hesitate to report errors and/or provide feedback on content.
- On occasion I will repost lecture notes with changes/additions

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 + the occasional practice exercise sets before class.

3) Ask questions! Participate in discussions (office hours, canvas, ...)

Covid, Zoom, Canvas, etc

- We are no longer required to wear masks but ...
- ... you are still encougared to wear one - especially in class
- If you are sick *please* do not come to class [there is really no need] !!
- Read syllabus info on rules for Covid/ Masks/ etc.
- If I get sick - I will schedule the class on Zoom [If I can!] –
- Office hours: Mixed mode both for instructor and TA – latest info in syllabus.

YS: First 30mn zoom - then in person, *ZZ:* Mon. via zoom - Fri. in person

- Office hours open to all (No “waiting room” for the Zoom parts). W’ll see how this works and adjusts as needed.

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,

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?

➤ Problem type: Linear system

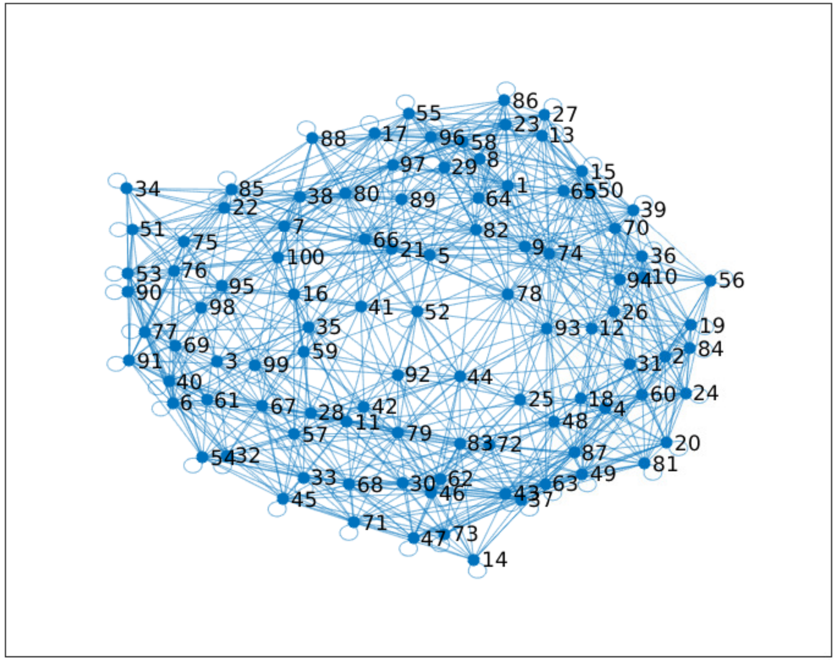
Solution: The system you get is: $$\begin{pmatrix} 5 & 10 & 25 \\ 1 & 1 & 1 \\ 0 & 10 & 25 \end{pmatrix} \begin{pmatrix} x_n \\ x_d \\ x_q \end{pmatrix} = \begin{pmatrix} 145 \\ 12 \\ 125 \end{pmatrix}$$

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?

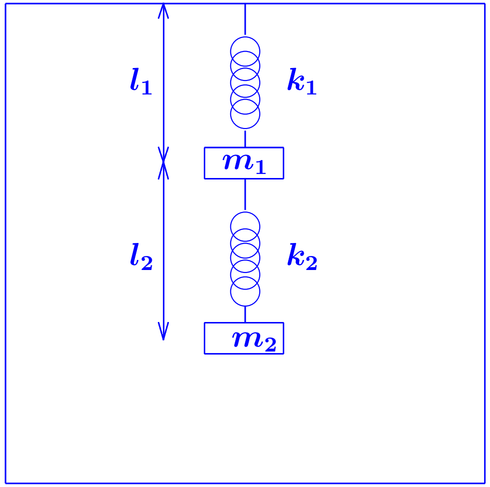


➤ Problem type: (homogeneous) Linear system. Eigenvector problem.

- Vibrations in mechanical systems. See:

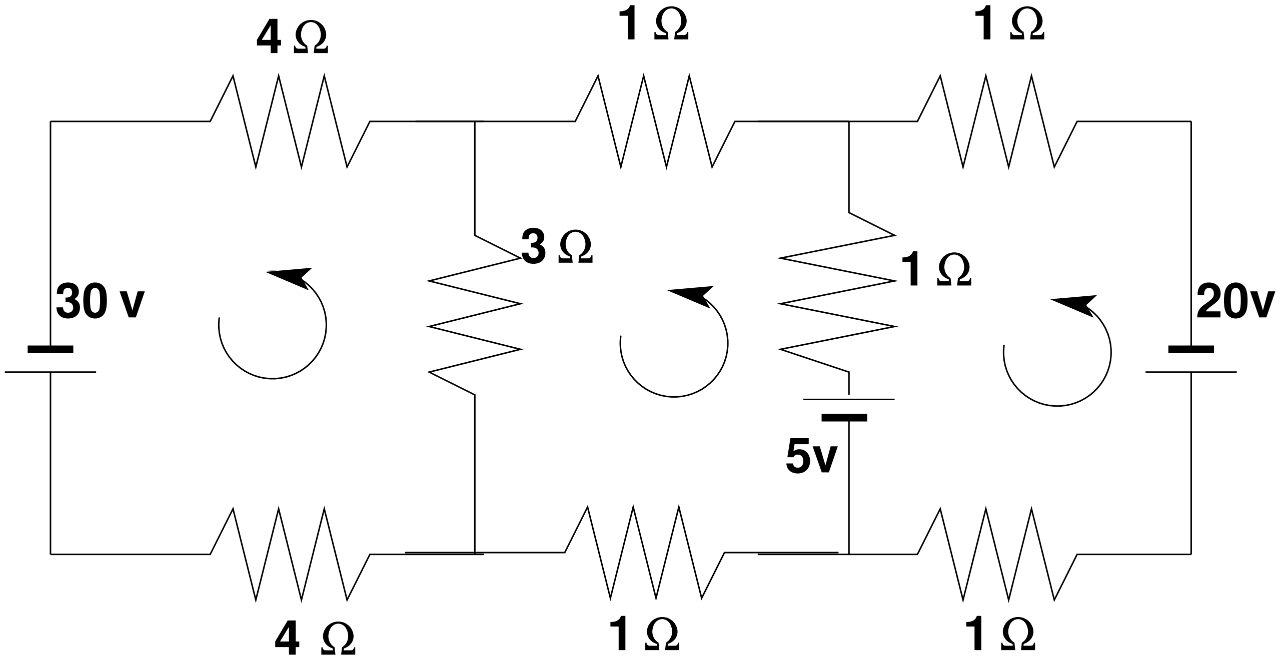
www.cs.umn.edu/~saad/eig_book_2ndEd.pdf

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



- Problem type: Eigenvalue Problem

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



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

➤ Problem type: Linear System

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.

➤ Problem type: Least-Squares system

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

Dynamical systems and epidemiology

A set of variables that fill a vector y are governed by the equation

$$\frac{dy}{dt} = Ay$$

Determine $y(t)$ for $t > 0$, given $y(0)$ [called 'orbit' of y]

➤ Problem type: (Linear) system of ordinary differential equations.

Solution:

$$y(t) = e^{tA}y(0)$$

➤ Involves exponential of A [think Taylor series], i.e., a matrix function

- This is the simplest form of dynamical systems (linear).
- Consider the slightly more complex system:

$$\frac{dy}{dt} = A(y)y$$

- Nonlinear. Requires 'integration scheme'.
- Next: a little digression into our interesting times...

Example: The SIR model in epidemiology

A population of N individuals, with $N = S + I + R$ where:

S Susceptible population. These are susecptible to being contaminated by others (not immune).

I Infectious population: will contaminate susceptible individuals.

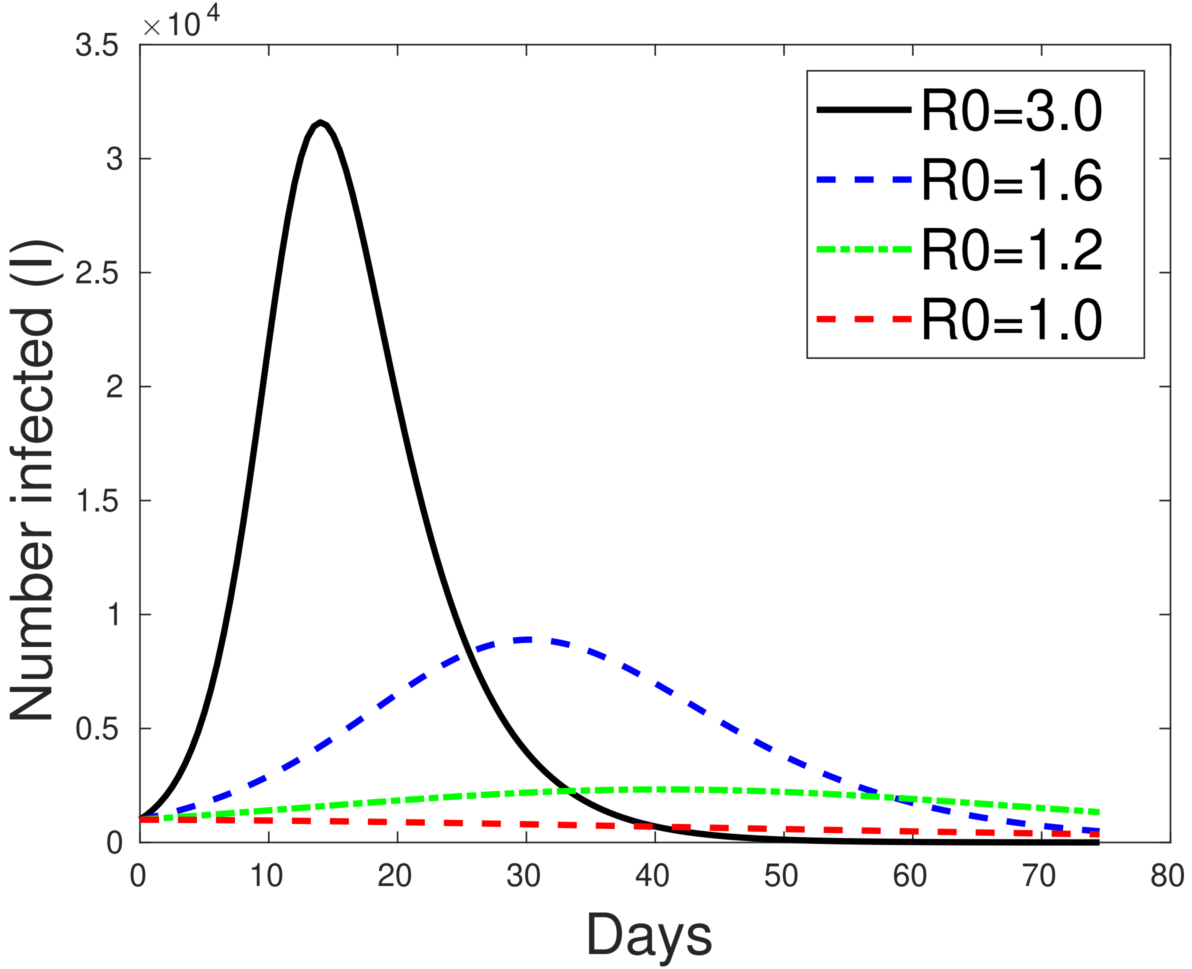
R 'Removed' population: either deceased or recovered. These will no longer contaminate others.

Three equations:

$$\frac{dS}{dt} = -\beta IS; \quad \frac{dI}{dt} = (\beta S - \mu)I; \quad \frac{dR}{dt} = \mu I$$

$1/\mu$ = infection period [e.g. 5 days].
$\beta = \mu R_0/N$ where R_0 = reproduction number.

- The importance of reducing R_0 (a.k.a. “social distancing”):



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

Physical Model

↓

Nonlinear PDEs

↓

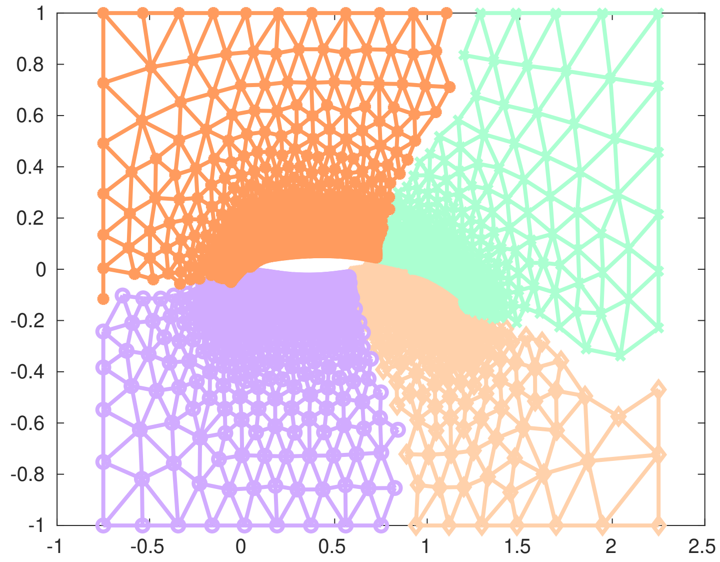
Discretization

↓

Linearization (Newton)

↓

Sparse Linear Systems $Ax = b$



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

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

Set of $m \times n$ 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:

$$\boxed{x \in \mathbb{R}^n \quad \longrightarrow \quad y = Ax \in \mathbb{R}^m}$$

➤ Recall: this mapping is linear [what does it mean?]

➤ Recall: Any linear mapping from $\mathbb{R}^n$ to $\mathbb{R}^m$ *is* a matrix vector product

Operations:

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

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

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

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

Multiplication by another matrix: $C = AB$,

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

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

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 $C = A \times B$: $c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$.
- Recall what C represents [in terms of mappings]..
- Can do the product column-wise [Matlab notation used]:

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

- Can do it row-wise:

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

➤ Can do it as a sum of 'outer-product' matrices:

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

✍11 Verify all 3 formulas above..

✍12 Complexity? [number of multiplications and additions]

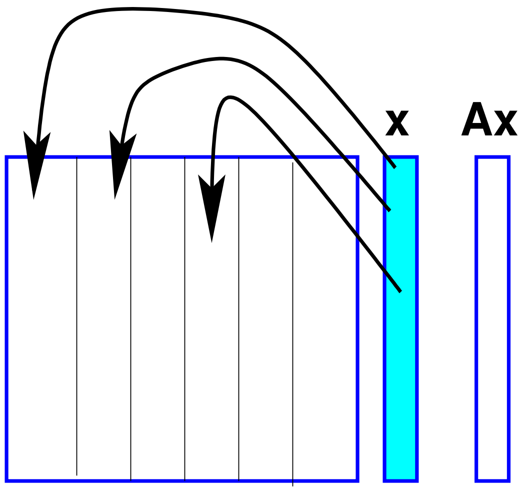
✍13 What happens to these 3 different approches to matrix-matrix multiplication when B has one column $(p = 1)$?

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

Matrix-vector product: computing $y = Ax$

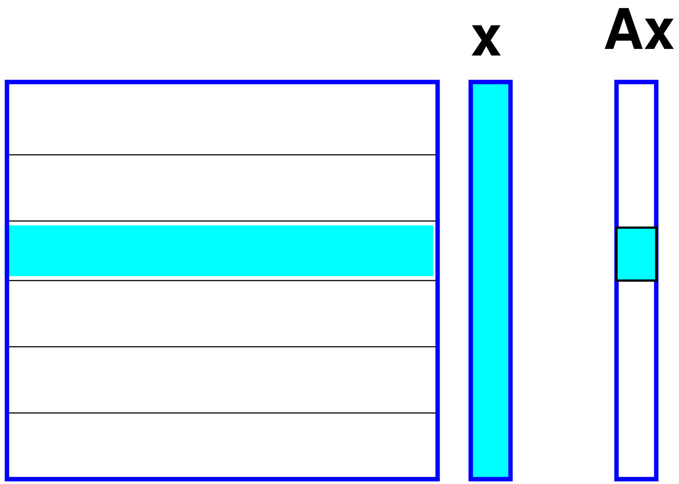
Column-form:

Linear combination of columns $A(:,j)$ with coefficients x_j yields y



Row-form:

Dot product of $A(i,:)$ and x gives y_i



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

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

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

- rank (A) = number of linearly independent columns of A = number of linearly independent rows of A
- A is of full rank if $\mathrm{rank}(A) = \min\{m, n\}$. 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 [Another term: co-rank]

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

$$A = uv^T.$$

What are the eigenvalues and eigenvectors of A?

✍16 Is it true that

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

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

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

- No `rref` function in numpy – [see sympy]

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

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

Verify your result with matlab [hint: use `null`, `rank`, `rref`]

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 $A = XBX^{-1}$

✍20 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) $\rightarrow$ 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

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

✍22 Given a function $f(t)$ (e.g., e^t) how would you define $f(A)$? [Leave the full justification for next chapter]

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

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

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

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

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

✍28 Review the Jordan canonical form. [Short description in sec. 1.8.2 of `http://www.cs.umn.edu/~saad/eig_book_2ndEd.pdf`

Define the eigenvalues, and eigenvectors from the Jordan form.

➤ Spectral radius = The maximum modulus of the eigenvalues

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

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

$$\mathrm{Tr}\,(A) = \sum_{i=1}^{n} a_{ii}.$$

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

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

✍29 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 $A^H A = A A^H$.

- 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 $Q^TQ = I$ [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.

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

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

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

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

✍34 Which matrices of the following type are also normal: real symmetric, real skew-symmetric, Hermitian, skew-Hermitian, complex symmetric, complex skew-symmetric matrices.

✍35 Find all real 2×2 matrices that are normal.

✍36 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 $j \neq i$ and $j \neq i + 1$.
- Lower bidiagonal $a_{ij} = 0$ for $j \neq i$ and $j \neq i - 1$.
- 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:

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

✍37 Try the matlab function *vander*

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

✍39 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.

✍40 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}.

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

✍41 Explore *hankel(c,r)* in matlab.

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

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

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

✍43 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.