CSE 392: Matrix and Tensor Algorithms for Data

Instructor: Shashanka Ubaru

University of Texas, Austin Spring 2024 Lecture 1: Introduction and Overview

Outline

- Class Topics and Logistics
- 2 Introduction Vector spaces and matrices
- 3 Eigenvalues and singular values
- 4 Vector and matrix norms

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Data Deluge

- Modern applications involve large dimensional datasets (matrices and beyond!).
- New technologies generation and collection of large volumes of scientific data.
- Algorithms Inexpensive, scalable; parallel and online/streaming.





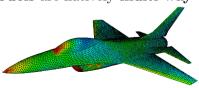
A Multi-Dimensional World

• Much of real-world data is inherently multidimensional





• Many operators and models are natively multi-way



Algorithms for Data

- Growing demands of data science and artificial intelligence and the need to handle large and high dimensional data have ushered in a "new era" for algorithms research.
- Today's data problems are two folds:
 - ▶ Computational issues in handling large and high dimensional data.
 - Representational challenges in order to capture multi-dimensional correlation structure.
- Typical data applications require combining a diverse set of algorithmic tools. Most are not heavily covered in traditional algorithms curriculum.

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Class topics

- The class topics are divided into two parts:
 - Randomized matrix computations
 - 2 Tensor algebraic methods
- Randomized linear algebra Approximate computational paradigm through the interplay between statistics, algebra and geometry.
- Tensor algebra algebraic constructs that represent and manipulate natively high-dimensional entities, while preserving their multi-dimensional integrity.
- We will cover theory, matlab/Python implementations, and applications.
- Focus on the tools to design new algorithms.
- Will need strong background in *linear algebra* and *probability*.

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Course Logistics

Course webpage:

https://shashankaubaru.github.io/Teaching/CSE392-2024.html You will find all information related to the course.

Instructor: Shashanka Ubaru

- Email: shashanka.ubaru@austin.utexas.edu or @ibm.com
- \bullet Office hours: Wednesdays 3:00pm 4:00pm.
- Location: POB 3.134

Class time and Location:

Mondays and Wednesdays, 11:00am - 12:30pm, GDC 2.402.

Class Logistics II

- Syllabus, schedule, lecture notes and other information can all be found in the *class* webpage.
- Assignments are to be submitted through Canvas, and should be individual work. You can discuss the problems, but should submit individually. Preferably typewritten.
- The programming languages for the course will be Matlab and/or Python.
- Some of the assignments and exercises will involve programming and code submission.
- We will use *Canvas* for grades, submissions, etc.

Class Logistics III

Grading:

- Scribing 10%: Participation and scribed notes preparation. 1 2 lectures, depending on the class strength. LaTeX template is available in the webpage.
- Assignments 50%: Around 5 problem sets each contributing an equal amount to the grade. Will include programming exercises.
- Class Project 40%: Teams of two. There will be a final presentation of the projects during the last week of the semester.

Relevant resources will be posted on the webpage.

 ${\bf Questions?}$

This lecture

General Introduction

- Background: Linear algebra and numerical linear algebra.
- Mathematical background vector spaces, matrices, rank.
- Types of matrices, structured matrices.
- eigenvalues, singular values.
- Inner products, norms.

Vector spaces and matrices

- 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 $\mathbb{A} = \{a_1, a_2, \dots, a_q\}$ of \mathbb{R}^n is a vector subspace called the linear span of \mathbb{A} .
- If the a_i 's are linearly independent, then each vector of span(\mathbb{A}) admits a unique expression as a linear combination of the a_i 's. The set \mathbb{A} is then called a *basis*.

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- A matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ is an $m \times n$ array of real numbers

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

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

$$oldsymbol{x} \in \mathbb{R}^n \longrightarrow oldsymbol{y} = oldsymbol{A} oldsymbol{x} \in \mathbb{R}^m$$

Tensors

- Notation : $\mathcal{A}^{n_1 \times n_2 \dots, \times n_d}$ d^{th} order tensor
 - $ightharpoonup 0^{th}$ order tensor scalar
 - $ightharpoonup 1^{st}$ order tensor vector

 $ightharpoonup 2^{nd}$ order tensor - matrix

 $ightharpoonup 3^{rd}$ order tensor ...



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Matrix operations

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

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

• Scalar multiplication: $C = \alpha A$, where

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

• Matrix-matrix multiplication: C = AB, where $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, $C \in \mathbb{R}^{m \times p}$ with

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}, \quad i = 1, \dots, m, \quad j = 1, \dots, p.$$

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Matrix operations

• Transposition: $C = A^{\top}$, where $A \in \mathbb{R}^{m \times n}$, $C \in \mathbb{R}^{n \times m}$ with

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

• Transpose conjugate: for complex matrices

$$oldsymbol{A}^H = ar{oldsymbol{A}}^ op = ar{oldsymbol{A}}^ op.$$

• Kronecker product: For $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times q}$

$$m{A} \otimes m{B} = egin{bmatrix} a_{11}m{B} & a_{12}m{B} & \cdots & a_{1n}m{B} \ a_{21}m{B} & a_{22}m{B} & \cdots & a_{2n}m{B} \ dots & \ddots & \ddots & dots \ a_{m1}m{B} & a_{m2}m{B} & \cdots & a_{mn}m{B} \end{bmatrix}$$

In Matlab and Numpy: kron(A,B). Size = ??

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Questions and Exercises

- $\bullet (A^{\top})^{\top} = ? (AB)^{\top} = ? (A^{H})^{H} = ?$ $(\mathbf{A}^H)^{\top} = ? \quad (\mathbf{A}\mathbf{B}\mathbf{C})^{\top} = ?$
- When is $AA^{\top} = A^{\top}A$?
- What are the computational complexity of (a) matrix addition, (b)matrix-vector product (matvec), and (c) matrix-matrix product?
- If $u, v \in \mathbb{R}^n$, then what are the sizes of $u^\top v$ and uv^\top ? What are these called?
- Exercise 1: Show that for $u, v \in \mathbb{R}^n$, we have $v^{\top} \otimes u = uv^{\top}$.

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Range, rank, and null space

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

$$rank(\mathbf{A}) \le \min\{m, n\}.$$

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

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Rank - Nullity Theorem

• For $\mathbf{A} \in \mathbb{R}^{m \times n}$:

$$\dim(\operatorname{Ran}(\boldsymbol{A})) + \dim(\operatorname{Null}(\boldsymbol{A})) = n$$

Also

$$\dim(\operatorname{Ran}(\boldsymbol{A}^{\top})) + \dim(\operatorname{Null}(\boldsymbol{A}^{\top})) = m$$

- $\dim(\text{Null}(A))$ is called the **nullity** or **co-rank** of A.
- $rank(\mathbf{A}) + nullity(\mathbf{A}) = n$.

Question: If $rank(\mathbf{A}) = r$, what are $rank(\mathbf{A}^{\top})$, $rank(\bar{\mathbf{A}})$, $rank(\mathbf{A}^{H})$. Explore rank function in Matlab or numpy.

Types of matrices

- Orthonormal : $U \in \mathbb{R}^{m \times n}$ is orthonormal if $U^{\top}U = I$.
- If U is square, then it is orthogonal (or unitary if complex), and $UU^{\top} = I$.
- A square matrix $A \in \mathbb{C}^{n \times n}$ is, Symmetric: $A^{\top} = A$, Skew-symmetric: $A^{\top} = -A$, Hermitian: $A^{H} = A$, Skew-Hermitian: $A^{H} = -A$, Normal: $A^{H}A = AA^{H}$.
- Matrix is non-negative if $a_{ij} \geq 0, i, j = 1, \ldots, n$.
- A symmetric matrix P of the form $P = UU^{\top}$ is a projection matrix, and PP = P.
- Structured matrices: Diagonal, Upper (U) and Lower (L) triangular, U & L bidiagonal, tridiagonal, and U & L Hessenberg.
- Special matrices: Toeplitz, Hankel, and circulant matrices.
- Sparse matrices Many of the large matrices encountered in applications are sparse. Sparse matrix computations can be a separate course.

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Reference

Recommended reading:

If these topics are not familiar, refer to sections 1.1 to 1.6 in Dr. Yousef Saad's text book:

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

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Eigenvalues and Eigenvectors

A complex scalar λ is called an *eigenvalue* of a square matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ if there exists a nonzero vector $\mathbf{u} \in \mathbb{C}^n$ such that

$$\mathbf{A}\mathbf{u} = \lambda \mathbf{u}$$
.

The vector \boldsymbol{u} is called an *eigenvector* of \boldsymbol{A} associated with λ .

- The set of all eigenvalues of A, denoted $\Lambda(A)$, is the spectrum of A.
- An eigenvalue is a root of the *characteristic polynomial*:

$$p_{\mathbf{A}}(\lambda) = \det(\mathbf{A} - \lambda \mathbf{I})$$

• bf Diagonalization: Two matrices A, B are *similar* if there exists a nonsingular matrix X such that: $A = XBX^{-1}$.

 \boldsymbol{A} is diagonalizable if it is similar to a diagonal matrix

Eigenvalues and properties

• For every square symmetric matrix $A \in \mathbb{R}^{n \times n}$, we can compute eigendecomposition:

$$\boldsymbol{A} = \boldsymbol{U} \Lambda \boldsymbol{U}^{\top},$$

where U is an orthogonal matrix with eigenvectors u_i as columns, and Λ is diagonal matrix with eigenvalues λ_i on the diagonal.

• Spectral radius: The maximum modulus of the eigenvalues

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

• Trace of A is the sum of diagonal elements

$$Tr(\mathbf{A}) = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \lambda_i$$

sum of all the eigenvalues of A counted with their multiplicities.

• Note $det(\mathbf{A})$ = product of all the eigenvalues of \mathbf{A} counted with their multiplicities.

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Singular values

- Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ or $\mathbb{C}^{m \times n}$.
- The eigenvalues of $A^H A$ and $A A^H$ are real and ≤ 0 .
- Let $\sigma_i = \sqrt{\mathbf{A}^H \mathbf{A}}$ if $n \leq m$ else $\sigma_i = \sqrt{\mathbf{A} \mathbf{A}^H}$ for $i = 1, \dots, \min\{n, m\}$.
- These σ_i 's are called the singular values of A.

Singular value decomposition: For every matrix $A \in \mathbb{R}^{m \times n}$, m we have

$$\boldsymbol{A} = \boldsymbol{U} \boldsymbol{\Sigma} \boldsymbol{V}^{\top},$$

where $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{m \times n}$ are an orthogonal matrices, and $\Sigma \in \mathbb{R}^{m \times n}$ is diagonal matrix with singular values σ_i on the diagonal ordered nonincreasingly: $\sigma_1 > \sigma_2 > \cdots > \sigma_m > 0$.

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Questions and Exercises

- Given a symmetric matrix A with eigen-decomposition $A = U\Lambda U^{\top}$, then
 - **1** What are the eigenvalues/eigenvectors of A^q for a given integer power q?
 - ② If A is nonsingular what are the eigenvalues/eigenvectors of A^{-1} ?
 - **3** What are the eigenvalues/eigenvectors of p(A) for a polynomial $p(\cdot)$?
- Similarly, for a general matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$, with SVD $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^{\top}$, what are the eigen-values of $\mathbf{A}^{\top} \mathbf{A}$?

Inner products and norms

• Inner product of two vectors $u, v \in \mathbb{R}^n$:

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \boldsymbol{u}^{\top} \boldsymbol{v} = \sum_{i=1}^{n} u_i v_i$$

- For complex numbers?
- Given $\mathbf{A} \in \mathbb{C}^{m \times n}$ then,

$$\langle \boldsymbol{A}\boldsymbol{u}, \boldsymbol{v} \rangle = \langle \boldsymbol{u}, \boldsymbol{A}^H \boldsymbol{v} \rangle.$$

- **Vector norm** on a vector space X is a real-valued function on X, which satisfies the following three conditions:
 - 1. $\|x\| \le 0, \forall x \in X$, and $\|x\| = 0$ iff x = 0.
 - 2. $\|\alpha \boldsymbol{x}\| = |\alpha|\|\boldsymbol{x}\|, \forall \boldsymbol{x} \in \mathbb{X}, \forall \alpha \in \mathbb{C}.$
 - 3. $\|x + y\| \le |x\| + |y|, \forall x, y \in X$.

Vector norms

• Euclidean norm on $\mathbb{X} = \mathbb{C}^n$,

$$\|\boldsymbol{x}\|_2 = \langle \boldsymbol{x}, \boldsymbol{x} \rangle^{1/2} = \sqrt{\sum_{i=1}^n |x_i|^2}$$

• Most common vector norms in numerical linear algebra: for $p \ge 1$ (Hölder norms)

$$\|oldsymbol{x}\|_p = \left(\sum_i |x_i|^2\right)^{1/p}$$

• Cauchy-Schwartz inequality:

$$|\langle \boldsymbol{x}, \boldsymbol{y} \rangle| \le \|\boldsymbol{x}\|_2 \|\boldsymbol{y}\|_2$$

• Hölder inequality:

$$|\langle \boldsymbol{x}, \boldsymbol{y} \rangle| \le \|\boldsymbol{x}\|_p \|\boldsymbol{y}\|_q, \operatorname{with} \frac{1}{p} + \frac{1}{q} = 1$$

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Matrix norms

- Matrix norm by treating $m \times n$ matrices as vectors in \mathbb{C}^{mn} :
 - 1. $\|\mathbf{A}\| \le 0, \forall \mathbf{A} \in \mathbb{C}^{m \times n}$, and $\|\mathbf{A}\| = 0$ iff $\mathbf{A} = 0$.
 - 2. $\|\alpha \mathbf{A}\| = |\alpha| \|\mathbf{A}\|, \forall \mathbf{x} \in \mathbb{C}^{m \times n}, \forall \alpha \in \mathbb{C}.$
 - 3. $\|A + B\| \le \|A\| + \|B\|, \forall A, B \in \mathbb{C}^{m \times n}$.
- Given $\mathbf{A} \in \mathbb{C}^{m \times n}$, we define a set of matrix norms:

$$\|oldsymbol{A}\|_p = \max_{oldsymbol{x} \in \mathbb{C}^m, oldsymbol{x}
eq 0} rac{\|oldsymbol{A} oldsymbol{x}\|_p}{\|oldsymbol{x}\|_p}$$

• Consistency / sub-mutiplicativity of matrix norms:

$$\|oldsymbol{A}oldsymbol{B}\|_p \leq \|oldsymbol{A}\|_p \|oldsymbol{B}\|_p$$

• Frobenius norm of a matrix:

$$\|\mathbf{A}\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2}.$$

Expressions of standard matrix norms

• Recall for a square matrix, we have $\rho(\mathbf{A}) = \max_{\lambda \in \Lambda(\mathbf{A})} |\lambda|$ and $\operatorname{Tr}(\mathbf{A}) = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \lambda_{i}$.

• Then the matrix norms are:

$$\begin{aligned} \|\boldsymbol{A}\|_{1} &= \max_{j} \sum_{i=1}^{m} |a_{ij}|, \\ \|\boldsymbol{A}\|_{\infty} &= \max_{i} \sum_{j=1}^{n} |a_{ij}|, \\ \|\boldsymbol{A}\|_{2} &= [\rho(\boldsymbol{A}^{H}\boldsymbol{A})]^{1/2} = [\rho(\boldsymbol{A}^{H}\boldsymbol{A})]^{1/2}. \\ \|\boldsymbol{A}\|_{F} &= [\operatorname{Tr}(\boldsymbol{A}^{H}\boldsymbol{A})]^{1/2} = [\operatorname{Tr}(\boldsymbol{A}^{H}\boldsymbol{A})]^{1/2}. \end{aligned}$$

In terms of singular values

• For A, assume we have r nonzero singular values (with $r \leq \min\{m, n\}$):

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0.$$

• Then, we have

$$\|\boldsymbol{A}\|_2 = \sigma_1$$
 and $\|\boldsymbol{A}\|_F = \sqrt{\sum_{i=1}^r \sigma_i^2}$

• Schatten p-norms for $p \ge 1$

$$\|oldsymbol{A}\|_{*,p} = \left[\sum_{i=1}^r \sigma_i^p
ight]^{1/p}$$

• In particular: $\|A\|_{*,1} = \sum_{i=1}^r \sigma_i$ is called the **nuclear norm** and is denoted by $\|A\|_*$.

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Questions and Exercises

- For an orthogonal matrix U, show that $||Ux||_2 = ||x||_2$.
- Exercise 2: Show that for any x: $\frac{1}{\sqrt{n}} \|x\|_1 \le \|x\|_2 \le \|x\|_1$.
- Exercise 3: Prove that the Frobenius norm is consistent [Hint: Use Cauchy-Schwartz]
- Let $\mathbf{A} = \mathbf{u}\mathbf{v}^{\top}$. Then, $\|\mathbf{A}\|_{2} = \|\mathbf{u}\|_{2}\|\mathbf{v}\|_{2}$.
- Exercise 4: Prove the above. What is $||A||_F = ?$