Announcements

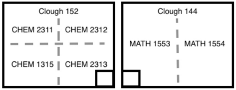
Thursday, April 19

- Please fill out the CIOS form online. *Current response: 15%*
  - If we *get an 80% response rate* before the final, I'll drop the *two* lowest quiz grades instead of one.

- **Optional Assignment:** due by email on April 20th (midnight)
- **Resources**
  - Office hours: posted on the website.
  - Math Lab at Clough is also a good place to visit.
  - Materials to review:
    `https://people.math.gatech.edu/~leslava3/1718S-2802.html`
  - Reading day Wednesday, April 25th:

Organic Chemistry & Linear Algebra

3:00 PM - 5:00 PM



CHEM 1315 - CHEM 2311 - CHEM 2312 (solutions) - CHEM 2313 - MATH 1553 - MATH 1554

- **Final Exam:**
  - Date: Thursday, April 26th
  - Location: This lecture room, College of Comp. 017
  - Time: 2:50-5:40 pm

Section 7.4

Singular Values Decomposition

Singular values of a matrix

What is important for this section:

- A constrained optimization problem where singular values appear
- How to find decomposition of A using singular values
- Condition number (avoid error-prone matrices)

Linear Transformation: Constrained optimization

EXAMPLE 1 If $A = \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix}$, then the linear transformation $\mathbf{x} \mapsto A\mathbf{x}$ maps the unit sphere $\{\mathbf{x} : \|\mathbf{x}\| = 1\}$ in $\mathbb{R}^3$ onto an ellipse in $\mathbb{R}^2$, shown in Fig. 1. Find a unit vector $\mathbf{x}$ at which the length $\|A\mathbf{x}\|$ is maximized, and compute this maximum length.

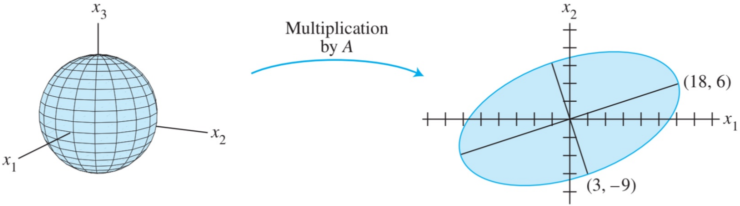


FIGURE 1 A transformation from $\mathbb{R}^3$ to $\mathbb{R}^2$.

Want to maximize $||Ax||^2$ subject to $||x|| = 1$.

This yields a quadratic function, as in section 7.3!

Linear Transformation: Constrained optimization
continued

Computing $||Ax||^2$ to obtain the quadratic function:

$$||Ax||^2 = (Ax)^T(Ax) = x^T(A^TA)x$$

where A^TA **is symmetric!**

$$A^TA = \begin{bmatrix} 4 & 8 \\ 11 & 7 \\ 14 & -2 \end{bmatrix} \begin{bmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{bmatrix} = \begin{bmatrix} 80 & 100 & 40 \\ 100 & 170 & 140 \\ 40 & 140 & 200 \end{bmatrix}$$

Solution. Look at eigenvalues of A^TA and find the largest one.

Properties for $A^T A$

If A is an $m \times n$ matrix then

- $A^T A$ is symmetric
- All eigenvalues of $A^T A$ are real
- There is orthonormal basis $\{v_1, \dots v_n\}$ where v_i's are eigenvectors of $A^T A$.
- All eigenvalues are non-negative

$$\begin{aligned} \|A\mathbf{v}_i\|^2 &= (A\mathbf{v}_i)^T A\mathbf{v}_i = \mathbf{v}_i^T A^T A\mathbf{v}_i \\ &= \mathbf{v}_i^T(\lambda_i \mathbf{v}_i) && \text{Since } \mathbf{v}_i \text{ is an eigenvector of } A^T A \\ &= \lambda_i && \text{Since } \mathbf{v}_i \text{ is a unit vector} \end{aligned}$$

Warning:

- Eigenvalues of $A^T A$ may be zero.
- Eigenvectors of $A^T A$ may not be eigenvectors of A.
- *but...* if $A^T A v = 0$ then $Av = 0$

In Fact:

- $NulA$ has an orthogonal basis consisting of v_i's which have $\sigma_i = 0$

Singular Values for $m \times n$ matrix

Let A be an $m \times n$ matrix. Order the eigenvalues of $A^T A$:
$\lambda_1 \geq \lambda_2 \geq \ldots \lambda_n \geq 0$.

- The **singular values of** A are square roots:

$$\sigma_1 = \sqrt{\lambda_1}, \qquad \sigma_2 = \sqrt{\lambda_2}, \qquad \ldots \qquad \sigma_n = \sqrt{\lambda_n}$$

- If $\{v_1, \ldots, v_n\}$ is orthonormal basis consisting of eigenvectors of $A^T A$, then singular values are *lengths* of vectors Av_i.

$$\begin{aligned} \|A\mathbf{v}_i\|^2 &= (A\mathbf{v}_i)^T A\mathbf{v}_i = \mathbf{v}_i^T A^T A\mathbf{v}_i \\ &= \mathbf{v}_i^T(\lambda_i \mathbf{v}_i) && \text{Since } \mathbf{v}_i \text{ is an eigenvector of } A^TA \\ &= \lambda_i && \text{Since } \mathbf{v}_i \text{ is a unit vector} \end{aligned}$$

- **Condition number of** A is σ_1/σ_n

  Rule of thumb: Condition number is close to 1 then matrix A is less computational-error prone.

An old problem with a twist

Example

Find an **orthogonal** basis for *Col A*

Old Procedure

- Select columns of A corresponding to pivot columns in row reduction.
- Apply Gram-Schmidt if necessary.

New Approach: Use $\{Av_1, \ldots Av_r\}$, where v_i are eigenvectors of $A^T A$

(details follow)

Orthogonal Basis for *Col A*

Theorem

Suppose $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is an orthonormal basis of $\mathbb{R}^n$ consisting of eigenvectors of A^TA, arranged so that the corresponding eigenvalues of A^TA satisfy $\lambda_1 \geq \cdots \geq \lambda_n$, and suppose A has r nonzero singular values. Then $\{A\mathbf{v}_1, \dots, A\mathbf{v}_r\}$ is an orthogonal basis for Col A, and rank $A = r$.

Why?

- The vectors $v_1, \dots, v_r$ are orthogonal:

$$(Av_i)^T(Av_j) = v_i^T(A^TA)v_j = \lambda_j(v_i^Tv_j) = 0$$

- Same argument is true for all collection $v_1, \dots, v_n$,
- **but** take only vectors v_i corresponding to $\lambda_i > 0$ because otherwise:

$$\begin{aligned}
\|A\mathbf{v}_i\|^2 &= (A\mathbf{v}_i)^TA\mathbf{v}_i = \mathbf{v}_i^TA^TA\mathbf{v}_i \\
&= \mathbf{v}_i^T(\lambda_i\mathbf{v}_i) && \text{Since } \mathbf{v}_i \text{ is an eigenvector of } A^TA \\
&= \lambda_i && \text{Since } \mathbf{v}_i \text{ is a unit vector}
\end{aligned}$$

The SVD decomposition theorem

The Singular Value Decomposition

Let A be an $m \times n$ matrix with rank r. Then there exists an $m \times n$ matrix Σ as in (3) for which the diagonal entries in D are the first r singular values of A, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, and there exist an $m \times m$ orthogonal matrix U and an $n \times n$ orthogonal matrix V such that

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

The matrix Σ has same number of rows/columns as A.

$$\Sigma = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} \leftarrow m - r \text{ rows}$$

$\uparrow$ $n - r$ columns

The only non-zero entries correspond to non-zero singular values

The SVD decomposition theorem
cont.

The Singular Value Decomposition

Let A be an $m \times n$ matrix with rank r. Then there exists an $m \times n$ matrix Σ as in (3) for which the diagonal entries in D are the first r singular values of A, $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, and there exist an $m \times m$ orthogonal matrix U and an $n \times n$ orthogonal matrix V such that

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

1. The matrix V has the orthonormal basis found in the decomposition $A^T A = PDP^T$.
   - That is, P has vector columns $v_1, v_2, \ldots, v_n$
2. Matrix D has diagonal entries $\sigma_1^2 \geq \sigma_2^2, \ldots, \sigma_n^2$
3. For matrix U:
   - For all indices with $\sigma_i \neq 0$, write $u_i = \frac{1}{\sigma_i} A v_i$

     extend $\{\mathbf{u}_1, \ldots, \mathbf{u}_r\}$ to an orthonormal basis $\{\mathbf{u}_1, \ldots, \mathbf{u}_m\}$ of $\mathbb{R}^m$, and let
   - $$U = [\, \mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_m \,] \quad \text{and} \quad V = [\, \mathbf{v}_1 \quad \mathbf{v}_2 \quad \cdots \quad \mathbf{v}_n \,]$$

Example: SVD decomposition of an $m \times n$ matrix

Example

Construct an SDV decomposition for $A = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix}$

1. Find an orthogonal diagonalization of $A^T A = PDP^T$.
   Entries in D are in decreasing order: $\lambda_1 = 360, \lambda_2 = 90, \lambda_3 = 0$.
2. Let $V = P$

$$V = [\,\mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3\,] = \begin{bmatrix} 1/3 & -2/3 & 2/3 \\ 2/3 & -1/3 & -2/3 \\ 2/3 & 2/3 & 1/3 \end{bmatrix}$$

3. Non-singular values $\sigma_1 = 6\sqrt{10}, \sigma_2 = 3\sqrt{10}$ define first columns of U

$$\mathbf{u}_1 = \frac{1}{\sigma_1} A\mathbf{v}_1 = \frac{1}{6\sqrt{10}} \begin{bmatrix} 18 \\ 6 \end{bmatrix} = \begin{bmatrix} 3/\sqrt{10} \\ 1/\sqrt{10} \end{bmatrix}$$

$$\mathbf{u}_2 = \frac{1}{\sigma_2} A\mathbf{v}_2 = \frac{1}{3\sqrt{10}} \begin{bmatrix} 3 \\ -9 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{10} \\ -3/\sqrt{10} \end{bmatrix}$$

4. If necessary, complete $\{u_1, \ldots, u_m\}$ to an orthonormal basis of $\mathbf{R}^m$.
   (Extra columns correspond to a basis of $Nul\,A$)
5. Σ is has entries σ_1, σ_2 on 'diagonal'.

Example: SVD decomposition of an $m \times n$ matrix

Continued

Example

Construct an SDV decomposition for $A = \begin{pmatrix} 4 & 11 & 14 \\ 8 & 7 & -2 \end{pmatrix}$

- The non-zero singular values are $\sigma_1 = 6\sqrt{10}, \sigma_2 = 3\sqrt{10}$
- Let $V = P$

$$V = [\, \mathbf{v}_1 \quad \mathbf{v}_2 \quad \mathbf{v}_3 \,] = \begin{bmatrix} 1/3 & -2/3 & 2/3 \\ 2/3 & -1/3 & -2/3 \\ 2/3 & 2/3 & 1/3 \end{bmatrix}$$

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- Decomposition:

$$A = \underbrace{\begin{bmatrix} 3/\sqrt{10} & 1/\sqrt{10} \\ 1/\sqrt{10} & -3/\sqrt{10} \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 6\sqrt{10} & 0 & 0 \\ 0 & 3\sqrt{10} & 0 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} 1/3 & 2/3 & 2/3 \\ -2/3 & -1/3 & 2/3 \\ 2/3 & -2/3 & 1/3 \end{bmatrix}}_{V^T}$$