### Summer Class: Machine Learning and Data Science

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June & July 2025

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Any matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  transforms a vector  $\mathbf{x} \in \mathbb{R}^n$  into a new vector  $\mathbf{y} \in \mathbb{R}^m$ :

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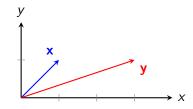
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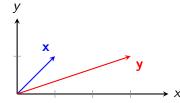


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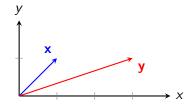
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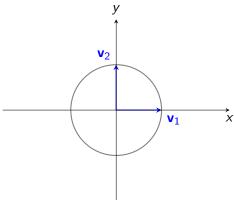
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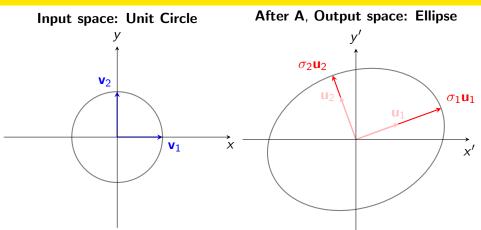
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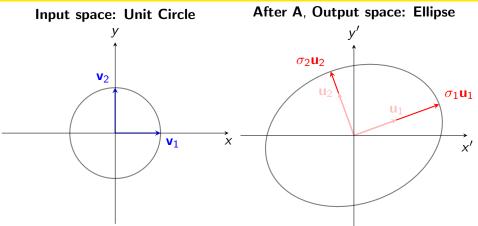
- Changes length (scaling).
- Changes direction (rotation/skewing).
- May collapse dimensions.

#### Input space: Unit Circle



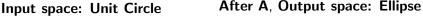
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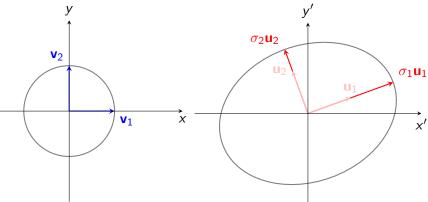




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$$Av_i = \sigma_i u_i \Rightarrow AV = U\Sigma \Rightarrow A = U\Sigma V^*.$$

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# What is Singular Value Decomposition?

• The Singular Value Decomposition (SVD) is a fundamental matrix factorization in linear algebra. It asserts that any real or complex matrix  $A \in \mathbb{C}^{m \times n}$  can be decomposed into the product of three specific matrices.

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- $U \in \mathbb{C}^{m \times m}$ : An orthogonal (or unitary for complex) matrix whose columns are the left singular vectors.
- $\Sigma \in \mathbb{C}^{m \times n}$ : A diagonal matrix (with non-negative real numbers in decreasing order on the diagonal) containing the singular values  $\sigma$ .
- $V \in \mathbb{C}^{n \times n}$ : An orthogonal (or unitary for complex) matrix whose columns are the right singular vectors.

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  - If m > n,  $\Sigma = \begin{bmatrix} \hat{\Sigma} \in \mathbb{C}^{n \times n} \\ 0 \end{bmatrix}$ . If m < n,  $\Sigma = [\hat{\Sigma} \in \mathbb{C}^{m \times m}, 0]$ . If m = n,  $\Sigma = \hat{\Sigma} \in \mathbb{C}^{m \times n}$ .

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Any linear transformation  $X_{new} = AX_0$  represented by a matrix A can be decomposed into a sequence of three fundamental geometric operations:

• Rotation by  $V^T$ :

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  - $V^T$  is an orthogonal matrix. It rotates the input vectors in the domain (input space  $\mathbb{R}^n$ ).
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  - ullet  $\Sigma$  is a diagonal matrix. It scales the rotated vectors along these new axes.
  - The scaling factor along each axis i is the singular value  $\sigma_i$ . Some axes might be stretched ( $\sigma_i > 1$ ), some shrunk ( $\sigma_i < 1$ ), and some collapsed ( $\sigma_i = 0$ ).

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- Scaling by Σ:
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- Rotation by U:
  - U is an orthogonal matrix. It rotates the scaled vectors into their final positions in the codomain (output space  $\mathbb{R}^m$ ).
  - It aligns the scaled vectors with the basis vectors of the range  $(u_i)$ .

Let's start with an ellipse and apply the transformation matrix:

$$A = \begin{pmatrix} 0.4330 & -0.7500 \\ 1.2500 & -0.4330 \end{pmatrix}$$

• Rotation ( $V^T$ ): Rotation by 30°.

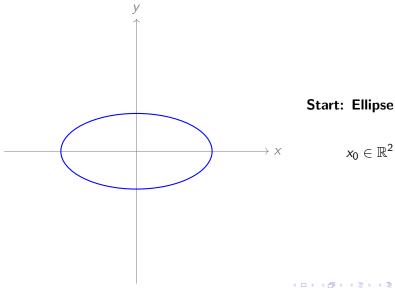
$$V^T = \begin{pmatrix} 0.866 & -0.5 \\ 0.5 & 0.866 \end{pmatrix} \approx R(30^\circ)$$

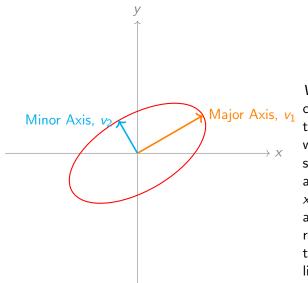
• Scaling  $(\Sigma)$ :

$$\Sigma = \begin{pmatrix} 1.5 & 0 \\ 0 & 0.5 \end{pmatrix}$$

• **Rotation** (*U*): Rotation by 60°.

$$U = \begin{pmatrix} 0.5 & -0.866 \\ 0.866 & 0.5 \end{pmatrix} \approx R(60^{\circ})$$

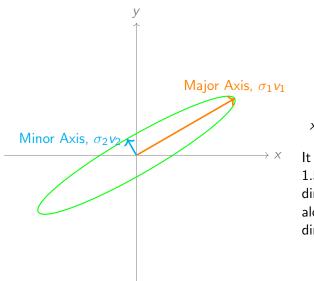




#### Step 1: Apply $V^{\top}$

$$x_1 = V^{\top} x_0$$

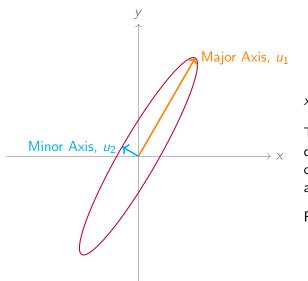
 $V^{\top}$  rotates the entire coordinate system so that the directions we want to stretch and shrink are perfectly aligned with the main x and y axes (major and minor axes are rotated to lie along the  $30^{\circ}$  and  $120^{\circ}$ lines).



#### Step 2: Apply $\Sigma$

$$x_2 = \Sigma x_1 = \Sigma V^{\top} x_0$$

It scales everything by 1.5 along the new 30° direction and by 0.5 along the new 120° direction.



#### Step 3: Apply U

$$x_{\text{new}} = Ux_2 = U\Sigma V^{\top}x_0$$

The columns of the *U* define the directions of the final ellipse's axes.

Final rotation gives:

$$x_{\text{new}} = Ax_0$$

### Full vs Economy (Reduced) SVD

• Full SVD:  $U \in \mathbb{C}^{m \times m}$ ,  $\Sigma \in \mathbb{C}^{m \times n}$ ,  $V \in \mathbb{C}^{n \times n}$ .

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- Economy SVD:
  - Case 1: Tall-and-Skinny Matrix (m > n)

$$A_{m \times n} = \underbrace{\begin{bmatrix} & & & & & \\ & u_1 & \cdots & u_n \\ & & & & \end{bmatrix}}_{U \in \mathbb{C}^{m \times n}} \underbrace{\begin{bmatrix} & \sigma_1 & & 0 \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}}_{\Sigma \in \mathbb{C}^{n \times n}} \underbrace{\begin{bmatrix} & - & v_1^\top & - \\ & \vdots & \\ & - & v_n^\top & - \end{bmatrix}}_{V^\top \in \mathbb{C}^{n \times n}}$$

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• Case 2: Short-and-Fat Matrix (m < n)

$$A_{m \times n} = \underbrace{\left[ \begin{array}{ccc} | & & | \\ u_1 & \cdots & u_m \\ | & & | \end{array} \right]}_{U \in \mathbb{C}^{m \times m}} \underbrace{\left[ \begin{array}{ccc} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_m \end{array} \right]}_{\mathbf{\Sigma} \in \mathbb{C}^{m \times m}} \underbrace{\left[ \begin{array}{ccc} - & v_1^\top & - \\ & \cdots & \\ - & v_m^\top & - \end{array} \right]}_{V^\top \in \mathbb{C}^{m \times n}}$$

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### How to Compute SVD

• Let  $A = U\Sigma V^T$ .

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# How to Compute SVD

- Let  $A = U\Sigma V^T$ .
- Then:
  - Row-space correlation matrix:

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Column-space correlation matrix:

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• Eigenvalues:  $\Sigma^2$ 



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- For "Big Data" scenarios where m and n are in the tens of thousands, millions, or more, computing the full SVD becomes impractical in terms of time and memory.
- However, many large real-world matrices are approximately low-rank, or we are only interested in a low-rank approximation (e.g., top k singular values/vectors).

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  - How:
    - **1** Generate a random matrix  $\Omega \in \mathbb{R}^{n \times l}$ .
    - ② Form the "sketch" or "sample" matrix  $Y = A\Omega \in \mathbb{R}^{m \times l}$ . Multiplying A by random vectors effectively samples its range.
    - **3** Compute an orthonormal basis for the columns of Y, typically via QR decomposition: Y=QR. The matrix  $Q\in\mathbb{R}^{m\times l}$  is our approximate basis

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The insight here is that random projections can preserve the essential geometric structure of the original matrix A, particularly its dominant components, allowing us to work with a much smaller sketch Y.

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    - **③** The final SVD approximation for A is then  $A \approx (Q\tilde{U})\Sigma V^T$ . Let  $U_{rSVD} = Q\tilde{U}$  and then  $A \approx U_{rSVD}\Sigma V^T$ .

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Approximate the top k singular values/vectors of a large matrix  $A \in \mathbb{R}^{m \times n}$ 

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$$Y = QR \quad \Rightarrow \quad Q \in \mathbb{R}^{m \times (k+p)}$$

- **o** Project *A* into lower dimension:  $B = Q^T A \in \mathbb{R}^{(k+p) \times n}$
- **6** Compute SVD on small matrix:  $B = \tilde{U} \Sigma V^T$
- **•** Form approximate SVD of *A*:

$$A \approx (Q\tilde{U})\Sigma V^T \quad \Rightarrow \quad A_{rSVD} = A_k = U_k \Sigma_k V_k^T$$



Approximate the top k singular values/vectors of a large matrix  $A \in \mathbb{R}^{m \times n}$ 

- **①** Generate random test matrix:  $\Omega \in \mathbb{R}^{n \times (k+p)}$  (l = k + p)
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MATLAB Demonstration.



SVD as a Sum of Rank-One Matrices:

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- $\sigma_i$  is the *i*-th singular value.
- $u_i$  is the *i*-th left singular vector (column of U).
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This means any matrix A can be expressed as a weighted sum of r rank-one matrices. The weights are the singular values  $\sigma_i$ . Since  $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0$ , the first few terms in this sum capture the most "significant" parts of the matrix A.

Low-Rank Approximation:

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#### Low-Rank Approximation:

If we truncate the sum of rank-one matrices after k terms (k < r):

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- $A_k$  is constructed using the k largest singular values and their corresponding singular vectors.
- This process effectively filters out information associated with smaller singular values, which often corresponds to noise or less significant details.

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Frobenius norm

$$||A||_F = \left(\sum_{i=1}^n \sum_{j=1}^p |a_{ij}|^2\right)^{\frac{1}{2}} = (\operatorname{tr} A^T A)^{\frac{1}{2}}, ||A||_F = \left(\sum_{i=1}^r \sigma_i^2\right)^{\frac{1}{2}}$$

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p-norms

$$||A||_p = \sup_{x \neq 0} \frac{||Ax||_p}{||x||_p} = \sup_{x:||x||_p = 1} ||Ax||_p, ||A||_2 = \sigma_1$$

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#### Theorem (Eckart-Young-Mirsky)

For either  $\|\cdot\|_2$  or  $\|\cdot\|_F$ ,

$$||A - A_k|| \le ||A - B||$$
 for all rank-k matrices B.

Moreover,

$$||A - A_k|| = \begin{cases} \sigma_{k+1}, ||\cdot||_2 \text{ norm} \\ \left(\sum_{i=k+1}^r \sigma_i^2\right)^{\frac{1}{2}}, ||\cdot||_F \text{ norm.} \end{cases}$$

• Every image can be seen as a large matrix of pixel intensity values.

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- MATLAB Demonstration (SVD and rSVD).

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Can we predict the values of the '?' cells?

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#### • Why is Low Rank?

- The columns (and rows) are not independent; they are combinations of a few "basis" vectors.
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#### • How does SVD help?

- SVD finds the best low-rank approximation of any matrix.
- It decomposes a matrix A into:

$$A = USV^T$$

• By keeping only the top k singular values in S and setting others to zero  $(S_k)$ , we get the best rank-k approximation:  $A_k = US_kV^T$ .

We can't apply SVD directly to a matrix with holes. So, we:

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- Repeat: Go back to Step 2 and repeat. The guesses for the missing values will converge.

Recommender Systems.

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#### Recommender Systems.

- Matrix: Rows are users, columns are movies, and entries are ratings (1-5 stars).
- **Problem:** This matrix is extremely sparse—most users have rated only a tiny fraction of the available movies.
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|   | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| 9 | 5 |   | 1 | 1 |   | 2 |
| Ь |   | 2 |   | 4 |   | 4 |
| 9 | 4 | 5 |   | 1 | 1 | 2 |
| d |   |   | 3 | 5 | 2 |   |
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Recovering corrupted or missing parts of an image.

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Recovering corrupted or missing parts of an image.

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- y: vector of observed outcomes  $(m \times 1)$ .
- X: design matrix of features ( $m \times n$ , where each row is an observation and each column is a feature).
- $\beta$ : vector of unknown regression coefficients ( $n \times 1$ ).
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Standard Solution:  $\beta = (X^T X)^{-1} X^T y (X^T X \text{ is invertible}).$ 

Challenges: Multicollinearity. This occurs when two or more feature columns in the data matrix X are highly correlated. This means they are nearly linearly dependent.

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- If columns are nearly linearly dependent (high multicollinearity),  $X^TX$  is ill-conditioned, leading to the numerical instability.

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The regression coefficients are found by:

$$\beta = X^+ y = V \Sigma^+ U^T y$$

This solution minimizes the least-squares error  $||y - X\beta||_2^2$ .

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#### MATLAB Demonstration.

$$\begin{bmatrix} | & | & \cdots & | \\ 1 & x_1 & \cdots & x_n \\ | & | & \cdots & | \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$$

# Summary of What You've Learned Today

- Properties of SVD, U, Σ, V.
- Computation of SVD: Conventional method and randomized SVD.
- Geometric Interpretation of SVD
- Applications
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See you on Wednesday (7/2) for Lecture 3 on Singular Value Decomposition (PCA, POD, LSA).