

Linear Algebra for Computer Science

Lecture 29

Low-rank Approximation Principal Component Analysis

Low-rank matrices



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$$A \quad \text{rank}(A) = r < \min(m, n)$$

LA29(I)

$$A = U \begin{bmatrix} \sigma_1 & & \\ & \sigma_r & \\ & & 0 \end{bmatrix} V^T$$

$$A = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \dots & a_n \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{200 \times n}$$

Near-low-rank matrices



$A \in \mathbb{R}^{m \times n}$ is of rank $r < \min(m, n)$

VIII

what we have is

$$\tilde{A} = A + N \rightarrow \text{small noise matrix}$$

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

$$A \in \mathbb{R}^{100 \times 10}$$

$$\underline{\text{rank}(A) = 4}$$

$$\text{rank}(\tilde{A}) = 10$$

$$\tilde{A} = U \begin{bmatrix} 20.1 & & & & & & & & & & \\ & 15 & & & & & & & & & \\ & & 9 & & & & & & & & \\ & & & 4 & & & & & & & \\ & & & & 10^{-8} & & & & & & \\ & & & & & 10^{-9} & & & & & \\ & & & & & & 10^{-9} & & & & \end{bmatrix}$$

~~the~~ threshold $\sigma_i < T$

better: $\frac{\sigma_i}{\sigma_1} < T$

Near-low-rank matrices



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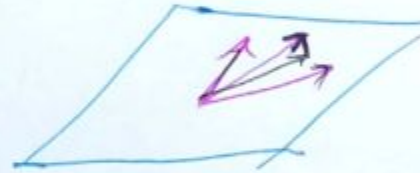
Example



$$A = [a_1 \ a_2 \ a_3] \in \mathbb{R}^{3 \times 3}$$

$$\begin{bmatrix} \sigma_1 & & \\ & \sigma_2 & \\ & & \sigma_3 \end{bmatrix}$$

σ_3
 σ_1



Matrix Norms



$$\begin{aligned} \circled{\|A - \tilde{A}\|_F} &= \sqrt{\sum_{i=1}^m \sum_{j=1}^n (a_{ij} - \tilde{a}_{ij})^2} \\ \|M\|_F &= \sqrt{\sum_{i=1}^m \sum_{j=1}^n m_{ij}^2} = \sqrt{\sum_{i=1}^{\min(m,n)} \sigma_i^2} \\ \circled{\|M\|_2} &= \max_{\|x\|_2=1} \|Mx\|_2 \\ &= \sigma_{\max} = \sigma_1 \end{aligned}$$

Low-rank Approximation



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find A s.t. $A - \tilde{A}$

$$\min_A \|A - \tilde{A}\|_F \quad \text{s.t.} \quad \text{rank}(A) \leq r$$

$$\|X\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n x_{ij}^2}$$

low rank approximation (Eckart-Young-Mirsky)
Lemma/Theorem

$$\tilde{A} = U \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \\ & & & & 0 \end{bmatrix} V^T$$

$$\text{or } A = U \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \sigma_r & \\ & & & 0 \end{bmatrix} V^T$$

Low-rank Approximation



$$\tilde{A} = U \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & \sigma \end{bmatrix} V^T$$
$$A = U \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_r & \\ & & & \emptyset \end{bmatrix} V^T$$

Application: Reduce memory/computation



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$10^3 \times 10^5 \left\{ \begin{matrix} \overbrace{A}^{100 \times 5} \\ = 10G \end{matrix} \right. \quad A = \begin{bmatrix} u_1 & \dots & u_n \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \dots & \\ & & \sigma_{100} \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_n^T \end{bmatrix}$

Low-rank Matrix Approximation

$$\approx \begin{bmatrix} u_1 & \dots & u_{100} \end{bmatrix} \begin{bmatrix} \sigma_1 & & \\ & \dots & \\ & & \sigma_{100} \end{bmatrix} \begin{bmatrix} v_1^T \\ \vdots \\ v_{100}^T \end{bmatrix}$$

$100 \times 10^5 \quad \quad \quad 100 \quad \quad \quad 100 \times 10^5$

$\approx 20M$

Application: Reduce memory/computation



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$$\tilde{A} = \begin{bmatrix} \\ \\ \end{bmatrix} \approx A = \begin{bmatrix} U \\ \Sigma \\ V^T \end{bmatrix}$$

Application: Computing the Fundamental Matrix in computer vision



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$x = \begin{bmatrix} m_1 \\ m_2 \\ 1 \end{bmatrix}$

$y = \begin{bmatrix} y_1 \\ y_2 \\ 1 \end{bmatrix}$

$x^T F y = 0$

→ Fundamental matrix.

$\text{rank}(F) = 2$

Eigen-decomposition as an optimization problem



A symmetric MA

$$\max_x \frac{x^T A x}{x^T x} = \max_x \frac{x^T A x}{\|x\|^2} \quad x^T x = 1$$
$$\max \quad x^T A x$$
$$\min \quad x^T A x \quad \text{subject to } \|x\| = 1$$

$\vec{v}_1, \vec{v}_2, \dots, \vec{v}_n$
 $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$
 $\lambda_{\max} \quad \lambda_{\min}$

$$\lambda_{\min} \leq \frac{x^T A x}{\|x\|^2} \leq \lambda_{\max}$$
$$A = \sum_{i=1}^n \lambda_i v_i v_i^T$$
$$\lambda_{\max} = \max_x \frac{x^T A x}{x^T x} \quad v_{\max} = \operatorname{argmax}_x \frac{x^T A x}{x^T x}$$
$$\lambda_{\min} = \min_x \frac{x^T A x}{x^T x}$$

Eigen-decomposition as an optimization problem



~~max~~
 A symmetric \rightarrow ~~eigen~~ n real eigenvector

Eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} \geq \lambda_n$
 Corresponding Eigenvector $v_1 \quad v_2 \quad \dots \quad v_{n-1} \quad v_n$

$x_{\max} = v_1$
 $x_{\min} = v_n$

$\vec{v}_1 = \operatorname{argmax}_x x^T A x$ subject to $\|x\|=1$
 $\vec{v}_2 = \operatorname{argmax}_x x^T A x$ s.t. $x^T x = 1, x \perp v_1$
 $\vec{v}_3 = \operatorname{argmax}_x x^T A x$ s.t. $x^T x = 1, x \perp v_1, x \perp v_2$

$A = V \Lambda V^T = \lambda_1 v_1 v_1^T + \lambda_2 v_2 v_2^T + \dots + \lambda_n v_n v_n^T$
 $Ax = \lambda_1 v_1 v_1^T x + \lambda_2 v_2 v_2^T x + \dots + \lambda_n v_n v_n^T x$

SVD as an optimization problem



$$\begin{aligned} & \max_x \|Ax\| \quad \text{subject to } \|x\|=1 \\ & \max_x \frac{\|Ax\|}{\|x\|} = ? \\ & \max_x \frac{\|Ax\|^2}{\|x\|^2} = \frac{(Ax)^T(Ax)}{x^T x} = \frac{x^T(A^T A)x}{x^T x} \\ & \max_x \frac{\|Ax\|^2}{\|x\|^2} = \lambda_{\max}(A^T A) = \sigma_{\max}^2 = \sigma_1^2 \\ & \max_x \frac{\|Ax\|}{\|x\|} = \sigma_1 = \sigma_{\max} \\ & \operatorname{argmax}_x \frac{\|Ax\|}{\|x\|} = \vec{v}_1 \quad A = U \Sigma \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix} \end{aligned}$$

Handwritten notes in a box:
$$\frac{v_i^T A v_i}{v_i^T v_i} = \frac{v_i^T (\lambda_i v_i)}{1}$$
$$\lambda_i v_i^T v_i = \lambda_i$$

SVD as an optimization problem



$$\begin{array}{l} \vec{y} = Ax \in \mathbb{R}^m \\ \swarrow \quad \searrow \\ m \times n \quad x \in \mathbb{R}^n \end{array}$$

LA29 (IV)

$$\begin{aligned} x_{\max} &= \operatorname{argmax}_x \|Ax\|_2 && \text{subject to } \|x\|=1 \\ &= \operatorname{argmax}_x \|Ax\|_2^2 && \text{subject to } x^T x = 1 \\ &= \operatorname{argmax}_x (Ax)^T (Ax) && \text{" " "} \\ &= \operatorname{argmax}_x \underbrace{x^T A^T A x}_{\text{}} && \text{s. t. } x^T x = 1 \end{aligned}$$

x_{\max} is the eigenvector of $A^T A$ corresponding to the largest eigenvalue.

$A^T A$ symmetric & Positive Semidefinite

$\Rightarrow x_{\max} = v_1$ = the right singular vector of A correspond to largest singular value.

SVD as an optimization problem



$$\begin{aligned} \min_x \|Ax\| \quad \text{s.t.} \quad \|x\|=1 &= \sigma_{\min} \\ \operatorname{argmin}_x \|Ax\| \quad \text{s.t.} \quad \|x\|=1 &= v_{\min} \end{aligned}$$
$$A = U \begin{bmatrix} \sigma_{\max} & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_{\min} \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_{\min}^T \end{bmatrix}$$

SVD as an optimization problem



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$A \in \mathbb{R}^{m \times n}$

$x_{\min} = v_i$

$A = \begin{bmatrix} u_1 & u_2 & \dots & u_m \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_{\min(m,n)} \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$

$x = v_i \Rightarrow \|Ax\| = \|\sigma_i u_i\| = \sigma_i$

x_{\max}

x_{\min}

Remember: Solving Homogeneous Equations



$$\begin{cases} 2x + 3y + z = 0 \\ -4x + y - z = 0 \\ x - y = 0 \end{cases}$$

homogeneous
equations

\mathbb{R}^3

if $\begin{bmatrix} x \\ y \\ z \end{bmatrix}$ is a solution, so is $\begin{bmatrix} \alpha x \\ \alpha y \\ \alpha z \end{bmatrix}$ for all $\alpha \in \mathbb{R}$

$$\begin{bmatrix} 2 & 3 & 1 \\ -4 & 1 & -1 \\ 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$A \vec{x} = \vec{0}$$

find $N(A)$ $\vec{x} \in N(A)$

$$\begin{bmatrix} x_i \\ y_i \\ 1 \end{bmatrix} = \begin{bmatrix} h_1 & h_2 & h_3 \\ h_4 & h_5 & h_6 \\ h_7 & h_8 & h_9 \end{bmatrix} \begin{bmatrix} x_i \\ y_i \\ 1 \end{bmatrix}$$

homography transform

Example)

Application: Noisy Homogeneous Equations



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In practice A has full rank, $N(A) = \{0\}$

$$A = \begin{matrix} & n \\ \begin{matrix} \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \end{matrix} & \end{matrix}$$

$m \gg n$ in most situations.
 $r = \text{rank}(A) = n$

$Ax = 0 \Rightarrow$ no solution!

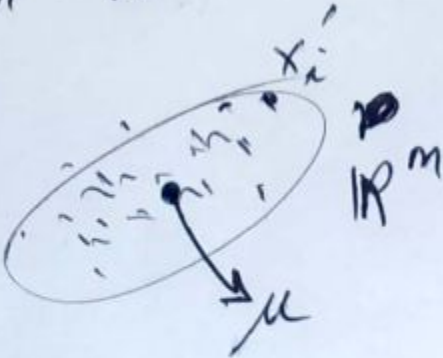
find $x_* = \arg \min_x \|Ax\|$ subject to $\|x\| = 1$

$$= \arg \min \frac{\|Ax\|}{\|x\|} = \arg \min \frac{\|Ax\|^2}{\|x\|^2} = \frac{x^T A^T A x}{x^T x}$$

$$A = U \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$$

$x_* = v_n$
singular vector corr. to smallest σ_i

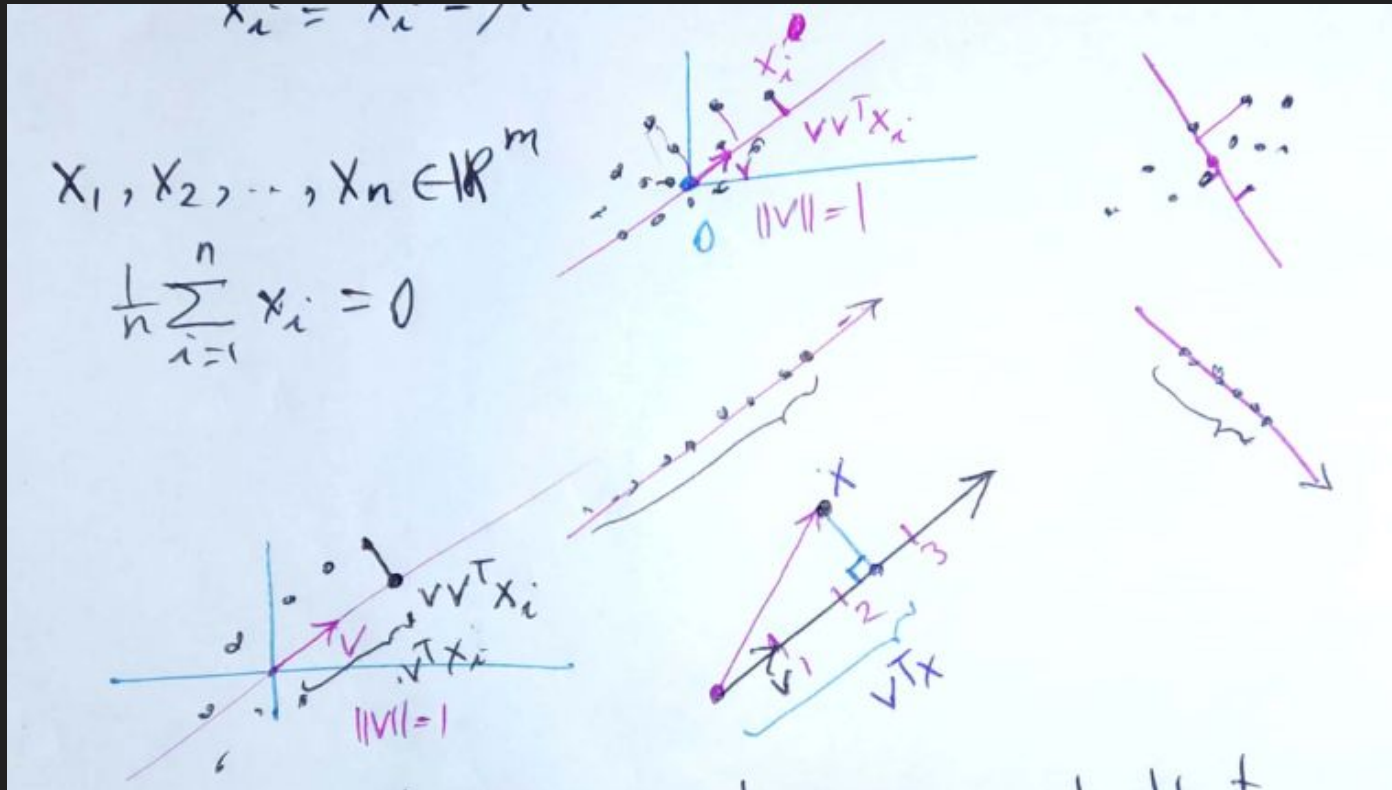
Zero centering data


$$x_1', x_2', \dots, x_n' \in \mathbb{R}^m$$
$$X' = [x_1' \ x_2' \ \dots \ x_n']$$

$$\mu = \frac{1}{n} \sum_{i=1}^n x_i'$$

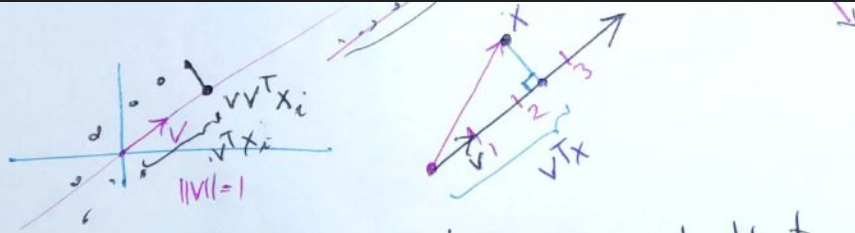
~~x_i~~

$$x_i = x_i' - \mu$$

Projecting points on a line



Find direction maximizing variance



Find the direction v such that the variance of the projected points is maximized

$$v = \arg \max_v \sum_{i=1}^n (v^T x_i)^2 \quad \text{s.t. } \|v\|=1$$


$$\begin{aligned} \sum_{i=1}^n (v^T x_i)^2 &= \sum_{i=1}^n \cancel{x_i^T v} (v^T x_i) (x_i^T v) \\ &= \sum_{i=1}^n v^T (x_i x_i^T) v \\ &= v^T \left(\sum_{i=1}^n x_i x_i^T \right) v \end{aligned}$$

Covariance matrix

Find direction maximizing variance



LA29 (VI)


$$\text{Var}(x_1, \dots, x_n)$$
$$\text{Var} = v^T \left(\sum_{i=1}^n x_i x_i^T \right) v$$

$n \times 1$ $1 \times n$
 $n \times n$

Covariance

$$v^T \sum_{i=1}^n (x_i' - \mu)(x_i' - \mu)^T v$$
$$X = [x_1, x_2, \dots, x_n]$$
$$C = X X^T = [x_1, \dots, x_n] \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} = \sum_{i=1}^n x_i x_i^T$$

Covariance matrix

Find direction maximizing variance


$$X = [x_1, x_2, \dots, x_n]$$
$$C = XX^T = [x_1 \dots x_n] \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} = \sum_{i=1}^n x_i x_i^T$$

Covariance matrix

$$v_{\max} = \arg \max_v v^T (XX^T) v \quad \text{s.t.} \quad \|v\| = 1$$

v_{\max} = the eigenvector of XX^T corresponding to the largest eigenvalue
= the first ~~left~~ right singular vector of X^T
= the first left singular vector of $X = u_1$

Principal Component Analysis (PCA)



max 0 V

V_{\max} = the eigenvector of XX^T ~~corresponding~~
corresponding to the largest eigenvalue
= the first ~~left~~ right singular vector
of X^T
= the first left singular vector
of $X = u_1$

u_1, u_2, u_3 Principal Components
Principal Component Analysis (PCA)