More on SVD and PCA

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Outline

- More on SVD
- Low rank approximation
- SVD and PCA

More on SVD

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$$\mathbb{A} \begin{bmatrix} v_i \\ u_i \end{bmatrix} = \sigma_i \begin{bmatrix} v_i \\ u_i \end{bmatrix} \quad \text{and} \quad \mathbb{A} \begin{bmatrix} v_i \\ -u_i \end{bmatrix} = -\sigma_i \begin{bmatrix} v_i \\ -u_i \end{bmatrix} \quad \text{for } i = 1:r.$$

Extreme singular values

Let $A \in \mathbb{C}^{m\times n}$. Consider the SVD $A = U\Sigma V^*$. Let $\sigma_{\max}(A)$ and $\sigma_{\min}(A)$, respectively, denote the largest and the smallest nonzero singular values of A. Then

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Recall that the condition number of A is given by

$$\mathrm{cond}_2(A) := \|A\|_2\|A^+\|_2 = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}.$$

Properties of singular values

Theorem: Let $A \in \mathbb{C}^{m\times n}$. Let $\sigma_1(A) \geq \cdots \geq \sigma_p(A)$ be the singular values of A, where $p := \min(m, n)$. Then, for $k = 1 : p$, we have

$$\sigma_k(A) = \max_{\dim(S)=k} \min \left\{ \frac{\|Ax\|_2}{\|x\|_2} : x \in S \text{ and } x \neq 0 \right\}.$$

Let $E \in \mathbb{C}^{m\times n}$ and let $\sigma_1(A+E) \geq \cdots \geq \sigma_p(A+E)$ be the singular values of $A+E$. Then, for $k = 1 : p$, we have

$$|\sigma_k(A+E) - \sigma_k(A)| \leq \|E\|_2.$$

Singular values and singular vectors

Let $A \in \mathbb{C}^{m\times n}$ and $\mathrm{rank}(A) = r$. Then $A = U\Sigma V^* = \sum_{j=1}^{r} \sigma_j u_j v_j^*$, where

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v_1 = \arg\max\limits_{\|x\|_2=1} \{\|Ax\|_2 : x \in \mathbb{R}^n\} & \sigma_1 := \|Av_1\|_2 & u_1 := Av_1/\sigma_1 \\
v_2 = \arg\max\limits_{\|x\|_2=1} \{\|Ax\|_2 : x \perp v_1\} & \sigma_2 := \|Av_2\|_2 & u_2 := Av_2/\sigma_2 \\
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Also note that for $j = 1 : r$, we have

$$v_j = \arg\max_{\|x\|_2=1} \{\|Ax\|_2 : x \perp \{v_1, \ldots, v_{j-1}\}\} = \arg\max_{\|x\|_2=1} \{x^* A^* Ax : x \perp \{v_1, \ldots, v_{j-1}\}\}.$$

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Consider the subspace $S := \mathrm{span}(v_1, \cdots, v_{\ell+1})$. Then $S \cap N(X) \neq \{0\}$ (Why?). Hence there exists a nonzero $u \in S \cap N(X)$ such that $\|u\|_2 = 1$.

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which contradicts that $\|Au\|_2 < \sigma_{\ell+1}$ for any $u \in N(X)$ such that $\|u\|_2 = 1$. ■

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Remark: The proof for the Frobenius norm follows from the fact that

$$\|A - A_\ell\|_F = \sqrt{\sigma_{\ell+1}^2 + \cdots + \sigma_r^2} \text{ and } \|Au\|_2 \leq \|A\|_F \|u\|_2.$$

Further, $A_\ell = \mathrm{argmin}_{\mathrm{rank}(X)=\ell} \|A - X\|_F$ is unique.

Consequences of Eckart-Young theorem

Suppose $A \in \mathbb{C}^{n\times n}$ is nonsingular. Consider the SVD $A = U\mathrm{diag}(\sigma_1, \cdots, \sigma_n)V^*$. Set $A_{n-1} := U\mathrm{diag}(\sigma_1, \cdots, \sigma_{n-1}, 0)V^*$. Then A_{n-1} is singular and

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$$A := \begin{bmatrix} 1 & -1 & -1 & \cdots & -1 & -1 \\ 0 & 1 & -1 & \cdots & -1 & -1 \\ 0 & 0 & 1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}, B := \begin{bmatrix} 1 & -1 & -1 & \cdots & -1 & -1 \\ 0 & 1 & -1 & \cdots & -1 & -1 \\ 0 & 0 & 1 & \cdots & -1 & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ \frac{-1}{2^{n-2}} & 0 & 0 & \cdots & 0 & 1 \end{bmatrix}$$

Consequences of Eckart-Young theorem

Then $\det(A) = 1$ and $Bx = 0$, where $x := \begin{bmatrix} 2^{n-2} & 2^{n-3} & \cdots & 2^0 & 1 \end{bmatrix}^\top$. Hence

$$\det(B) = 0 \text{ and } \sigma_n = \min\{\|A - X\|_2 : X \text{ singular}\} \leq \|A - B\|_2 = \frac{1}{2^{n-2}}.$$

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Numerical rank: If $A \in \mathbb{C}^{m \times n}$ is close enough to a matrix of rank r, where $r < \min(m, n)$, then A will behave like a rank r matrix in finite precision arithmetic. More precisely, the numerical rank of A is the number of singular values of A that are greater than $\max(m, n)\sigma_1 \mathbf{eps}$.

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Example: Suppose that A is a 5×5 matrix with singular values

$$\sigma_1 = 4, \sigma_2 = 1, \sigma_3 = 10^{-12}, \sigma_4 = 3.1 \times 10^{-14}, \sigma_5 = 2.6 \times 10^{-15}.$$

Assume that **eps** $= 5 \times 10^{-15}$. Then $\sigma_1 \max(m, n)$**eps** $= 4 \times 5 \times 5 \times 10^{-15} = 10^{-13}$. Since three singular values of A are greater than 10^{-13}, the numerical rank of A is 3. ■

Variance and covariance

Let $x \in \mathbb{R}^n$. Then $\mathbf{x} := x - \mathrm{mean}(x)\mathbf{e}$ is the vector of deviations from $\mathrm{mean}(x) := \dfrac{1}{n}\sum_{j=1}^{n} x_j$,

where $\mathbf{e} := [1, \cdots, 1]^\top$. The variance σ^2 is defined by

$$\sigma^2 := \frac{1}{n-1}\sum_{j=1}^{n}(x_j - \mathrm{mean}(\mathrm{x}))^2 = \frac{\mathbf{x}^\top \mathbf{x}}{n-1}.$$

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More generally, let $X = \begin{bmatrix} \mathbf{x}_1 & \cdots & \mathbf{x}_n \end{bmatrix} \in \mathbb{R}^{m \times n}$ be such that $\mathrm{mean}(\mathbf{x}_j) = 0$ for $j = 1 : n$. Then

$$S = \frac{1}{n-1} X^\top X = \frac{1}{n-1}\begin{bmatrix} \mathrm{cov}(\mathbf{x}_1, \mathbf{x}_1) & \mathrm{cov}(\mathbf{x}_1, \mathbf{x}_2) & \cdots & \mathrm{cov}(\mathbf{x}_1, \mathbf{x}_n) \\ \mathrm{cov}(\mathbf{x}_1, \mathbf{x}_2) & \mathrm{cov}(\mathbf{x}_2, \mathbf{x}_2) & \cdots & \mathrm{cov}(\mathbf{x}_2, \mathbf{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{cov}(\mathbf{x}_1, \mathbf{x}_n) & \mathrm{cov}(\mathbf{x}_2, \mathbf{x}_n) & \cdots & \mathrm{cov}(\mathbf{x}_n, \mathbf{x}_n) \end{bmatrix}$$

is called the covariance matrix.

Principal component analysis (PCA)

A Statistical view of PCA: Let $\mathbf{x} \in \mathbb{R}^m$ a zero-mean multivariate random variable and $\mathbf{u} \in \mathbb{R}^m$. Then the variance of $\mathbf{u}^\top \mathbf{x} \in \mathbb{R}$ is given by

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Given a natural number $n < m$, the n principal components $\mathbf{y} := \begin{bmatrix} y_1 & \cdots & y_n \end{bmatrix}^\top \in \mathbb{R}^n$ of $\mathbf{x}$ are defined as n uncorrelated linear components of $\mathbf{x}$,

$$y_i := \mathbf{u}_i^\top \mathbf{x} \in \mathbb{R}, \ \mathbf{u}_i \in \mathbb{R}^m, \ \mathbf{u}_i^\top \mathbf{u}_i = 1, \ i = 1:n,$$

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$$\mathrm{Var}(y_1) \geq \mathrm{Var}(y_2) \geq \cdots \geq \mathrm{Var}(y_n) > 0.$$

The vectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$ are called principal component directions.

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For example, the first principal component y_1 seeks to determine $\mathbf{u}_1$ such that

$$\begin{aligned}\mathbf{u}_1 &= \arg\max\{\mathrm{Var}(\mathbf{u}^\top \mathbf{x}) : \mathbf{u} \in \mathbb{R}^m, \mathbf{u}^\top \mathbf{u} = 1\} \\ &= \arg\max\{\mathbf{u}^\top \mathbb{E}(\mathbf{x}\mathbf{x}^\top)\mathbf{u} : \mathbf{u} \in \mathbb{R}^m, \mathbf{u}^\top \mathbf{u} = 1\}.\end{aligned}$$

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Theorem: Assume that $\mathrm{rank}(\mathbb{E}(\mathbf{x}\mathbf{x}^\top)) \geq n$. Then the first n principal components $y_1, \ldots, y_n$ of a zero-mean multivariate random variable $\mathbf{x} \in \mathbb{R}^n$ are given by

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A Statistical view of PCA and SVD

Sample Principal Components: The covariance matrix $\mathbb{E}(\mathbf{x}\mathbf{x}^\top)$ of a zero-mean multivariate random variable $\mathbf{x} \in \mathbb{R}^m$ may not be known in practice. Instead, we may be given N i.i.d. samples $\mathbf{x}_1, \ldots, \mathbf{x}_N$ of the random variable $\mathbf{x}$.

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As if X/sqrt(N-1) = USV*, then XX(T)/(N-1) = U[S^2, 0; 0, 0;]U*,
So XX(T)ui = sigma^2*ui

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PCA and SVD

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Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ and $\mathbf{v}_1, \ldots, \mathbf{v}_n$ be left and right singular vectors of $\mathtt{X}$ corresponding to the first n singular values $\sigma_1(\mathtt{X}), \ldots, \sigma_1(\mathtt{X})$. Then $\mathtt{X}\mathbf{v}_i = \sigma_i(\mathtt{X})\mathbf{u}_i$ and $\mathbf{u}_i^\top \mathtt{X} = \sigma_i(\mathtt{X})\mathbf{v}_i^\top$ for $i = 1 : n$.

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is the sample data of the principal component $y_i := \mathbf{u}_i^\top \mathbf{x}$ for $i = 1 : n$.

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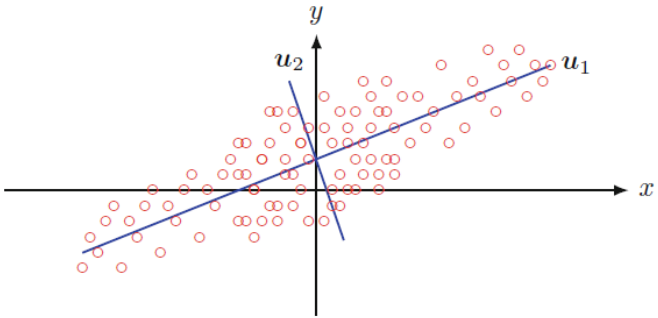
$$\mathrm{Var}(\mathbf{y}_i) = \frac{1}{N-1}\mathbf{y}_i^\top \mathbf{y}_i = \frac{\sigma_i(X)^2}{N-1}\mathbf{v}_i^\top \mathbf{v}_i = \frac{\sigma_i(X)^2}{N-1} = \sigma_i^2.$$

A Statistical view of PCA



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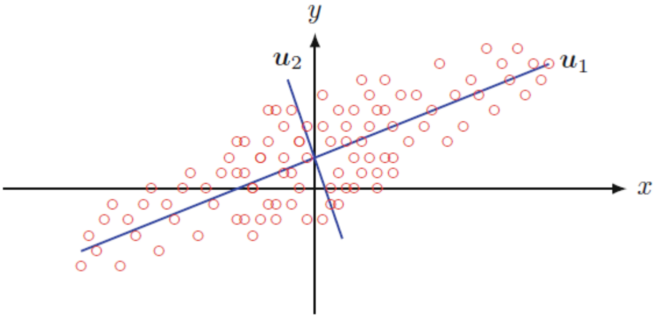

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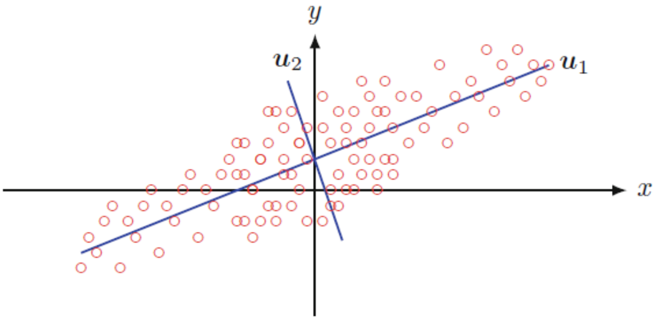
A Statistical view of PCA



Remark: Computation of SVD of $\mathtt{X}$ is preferred over spectral decomposition of $\mathtt{X}\mathtt{X}^\top \in \mathbb{R}^{m\times m}$ due to finite precision arithmetic. If $N < m$ then we can compute orthonormal eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of $\mathtt{X}^\top\mathtt{X} \in \mathbb{R}^{N\times N}$ corresponding to n largest eigenvalues $\sigma_1^2 \geq \cdots \geq \sigma_n^2 > 0$ and set $\mathbf{u}_j := \mathtt{X}\mathbf{v}_j/\sigma_j$ for $j = 1 : n$. For stable computation, it is advisable to compute SVD of $\mathtt{X}$.

PCA Summary

PCA of a Random Variable: Let $\mathbf{x} \in \mathbb{R}^m$ be a zero-mean multivariate random variable. Assume that $\mathrm{rank}(\mathbb{E}(\mathbf{x}\mathbf{x}^\top)) \geq n$. Then the first n principal components $y_1, \ldots, y_n$ of $\mathbf{x}$ are given by

$$y_i := \mathbf{u}_i^\top \mathbf{x} \quad \text{for} \quad i = 1 : n,$$

where $\mathbf{u}_1, \ldots, \mathbf{u}_n$ are orthonormal eigenvectors of the covariance matrix $\mathbb{E}(\mathbf{x}\mathbf{x}^\top)$ corresponding to the n largest eigenvalues $\sigma_1^2 \geq \cdots \geq \sigma_n^2 > 0$.

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