Introduction to Machine Learning

Principal Component Analysis

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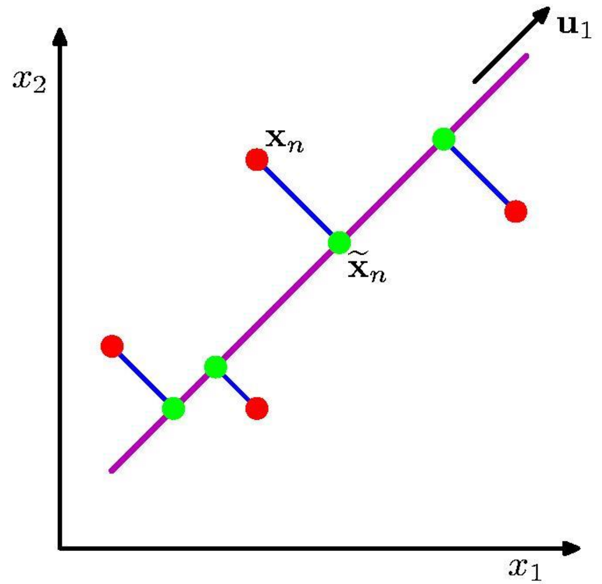
Principal Component Analysis



PCA:

Orthogonal projection of the data onto a lower-dimension linear space that...

- maximizes variance of projected data (purple line)

- minimizes the mean squared distance between
  - data point and
  - projections (sum of blue lines)

Principal Component Analysis

Idea:

- Given data points in a d-dimensional space, project them into a lower dimensional space while preserving as much information as possible.
  - Find best 2D approximation of 3D data
  - Find best 12-D approximation of 10^4-D data

- In particular, choose projection that minimizes *squared error* in reconstructing the original data.

PCA algorithm II (sample covariance matrix)

- Given data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, compute covariance matrix $\boldsymbol{\Sigma}$

$$\Sigma = \frac{1}{m}\sum_{i=1}^{m}(\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^T$$

where

$$\bar{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m}\mathbf{x}_i$$

- **PCA** basis vectors = the eigenvectors of Σ

- Larger eigenvalue $\Rightarrow$ more important eigenvectors

PCA algorithm II (sample covariance matrix)

PCA algorithm($\mathbf{X}$, k): top k eigenvalues/eigenvectors

% $\underline{\mathbf{X}}$ = N × m data matrix,
% … each data point $\mathbf{x}_i$ = column vector, i=1..m

- $\underline{\mathbf{x}} = \frac{1}{m}\sum_{i=1}^{m} \mathbf{x}_i$
- $\mathbf{X} \leftarrow$ subtract mean $\underline{\mathbf{x}}$ from each column vector $\mathbf{x}_i$ in $\underline{\mathbf{X}}$
- $\Sigma \leftarrow \mathbf{X}\mathbf{X}^T$ … covariance matrix of $\mathbf{X}$
- $\{ \lambda_i, \mathbf{u}_i \}_{i=1..N}$ = eigenvectors/eigenvalues of Σ
  … $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$
- Return $\{ \lambda_i, \mathbf{u}_i \}_{i=1..k}$
  % top k PCA components

PCA algorithm III (SVD of the data matrix)

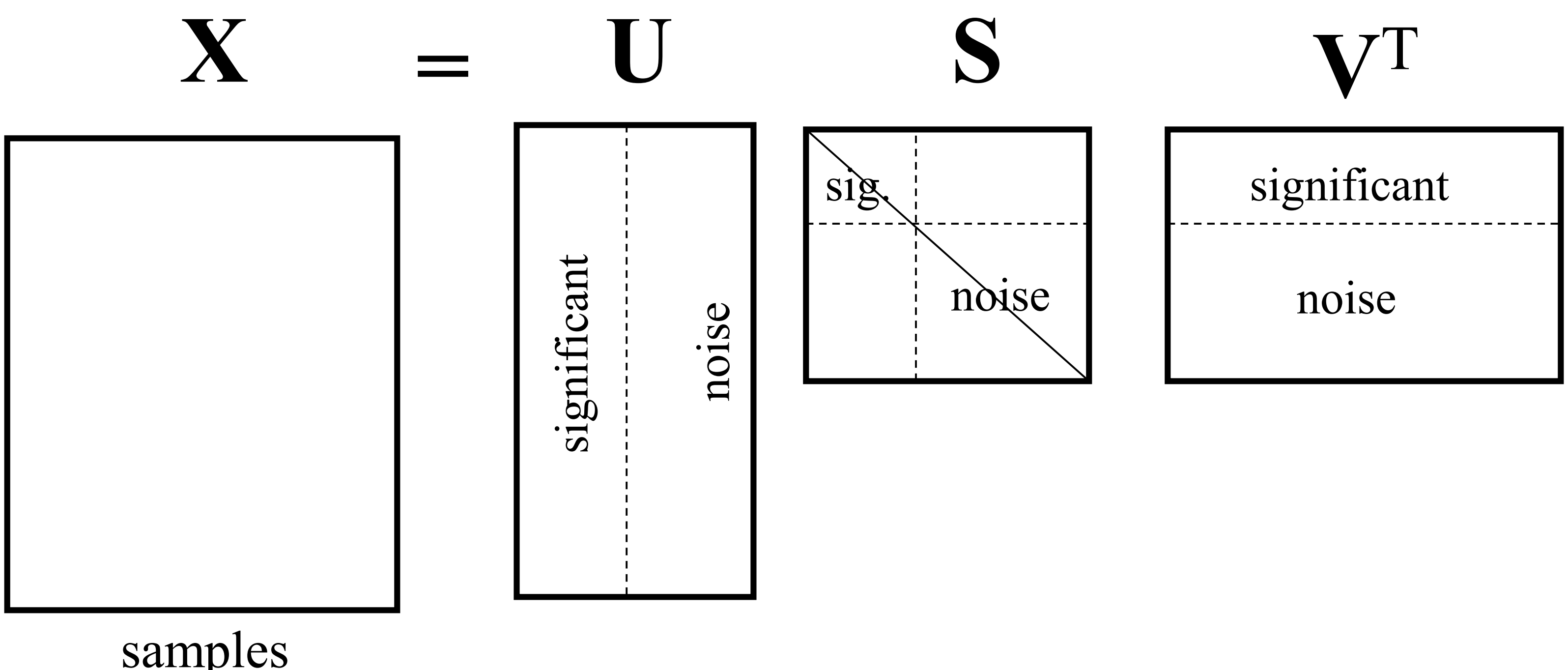
Singular Value Decomposition of the **centered** data matrix **X**.

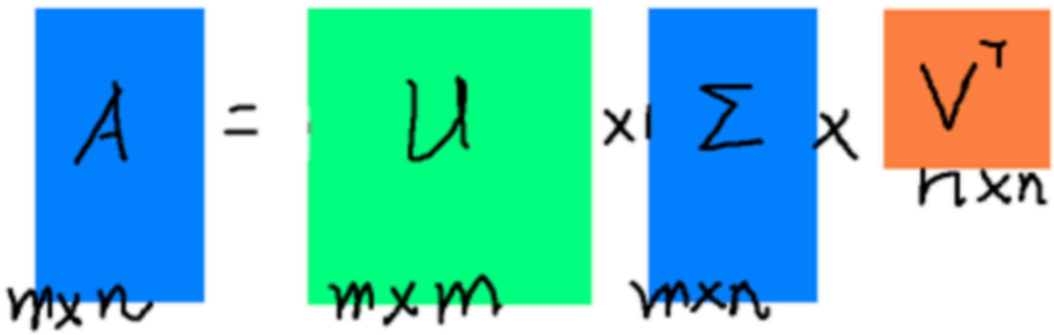
$$\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_m] \in \mathbb{R}^{N \times m},$$

m: number of instances,

N: dimension

$$\mathbf{X}_{\text{features} \times \text{samples}} = \mathbf{USV}^{T}$$





那么奇异值和特征值是怎么对应起来的呢？首先，我们将一个矩阵A的转置 * A，将会得到一个方阵，我们用这个方阵求特征值可以得到：

$$(A^T A)v_i = \lambda_i v_i$$

这里得到的v，就是我们上面的右奇异向量。此外我们还可以得到：

$$\sigma_i = \sqrt{\lambda_i}$$

$$u_i = \frac{1}{\sigma_i} A v_i$$

PCA algorithm III

- **Columns of U**
  - the principal vectors, $\{ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)} \}$
  - orthogonal and has unit norm – so $U^T U = I$
  - Can reconstruct the data using linear combinations of $\{ \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(k)} \}$
- **Matrix S**
  - Diagonal
  - Shows importance of each eigenvector
- **Columns of $\mathbf{V}^T$**
  - The coefficients for reconstructing the samples

PCA algorithm I (sequential)

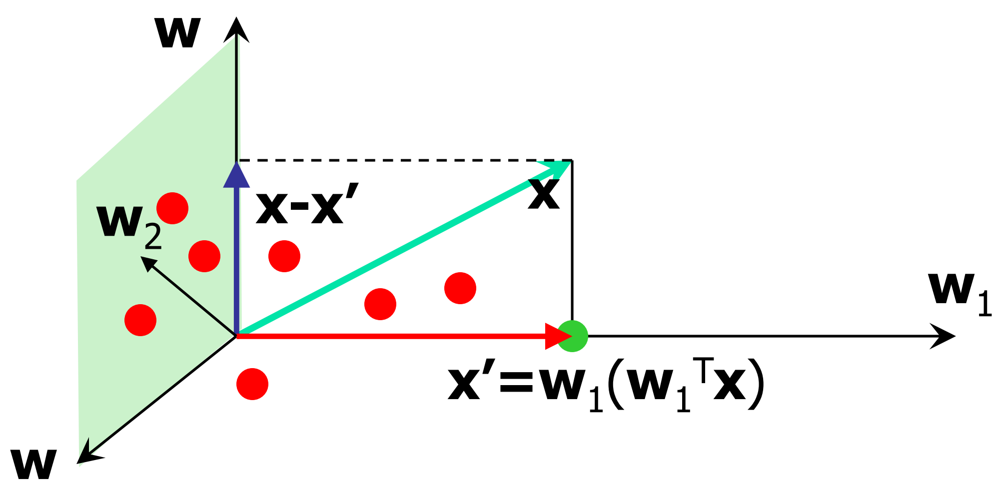
Given the **centered** data $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, compute the principal vectors:

$$\mathbf{w}_1 = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m}\sum_{i=1}^{m}\{(\mathbf{w}^T\mathbf{x}_i)^2\} \qquad \text{1}^{\text{st}} \text{ PCA vector}$$

To find $\mathbf{w}_1$, maximize the variance of projection of $\mathbf{x}$

$$\mathbf{w}_2 = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m}\sum_{i=1}^{m}\{[\mathbf{w}^T(\mathbf{x}_i - \underbrace{\mathbf{w}_1\mathbf{w}_1^T\mathbf{x}_i}_{\mathbf{x}' \text{ PCA reconstruction}})]^2\} \qquad \text{2}^{\text{nd}} \text{ PCA vector}$$

To find $\mathbf{w}_2$, we maximize the **variance** of the projection in the **residual** subspace



PCA algorithm I (sequential)

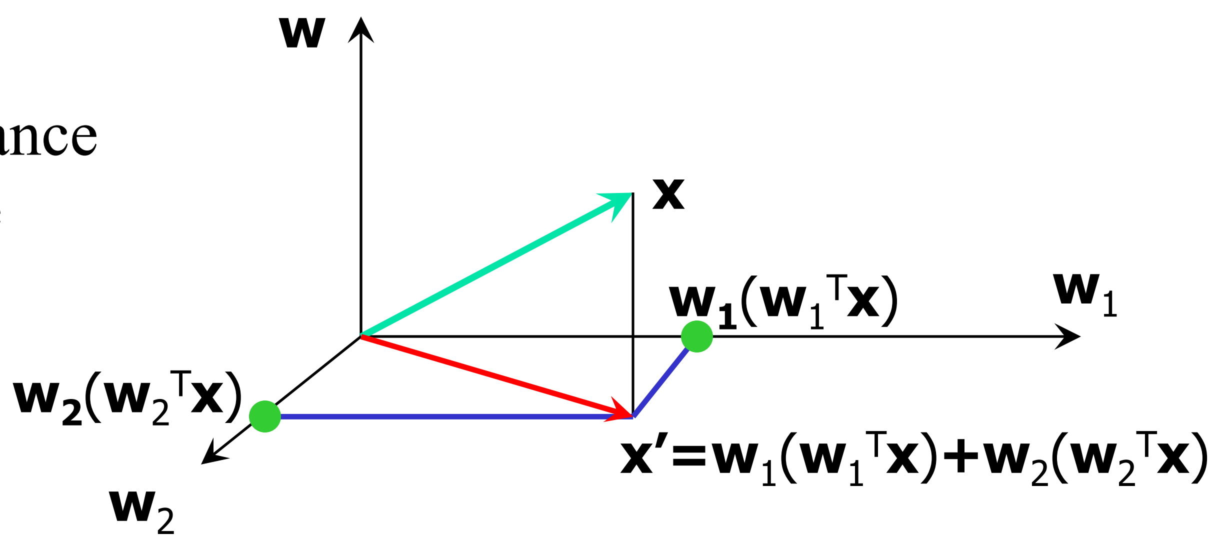
Given $\mathbf{w_1},\ldots,\mathbf{w_{k-1}}$, we calculate $\mathbf{w_k}$ principal vector as before:

Maximize the variance of projection of **x**

$$\mathbf{w}_k = \arg\max_{\|\mathbf{w}\|=1} \frac{1}{m}\sum_{i=1}^{m}\{[\mathbf{w}^T(\underbrace{\mathbf{x}_i - \sum_{j=1}^{k-1}\mathbf{w}_j\mathbf{w}_j^T\mathbf{x}_i}_{\mathbf{x}' \text{ PCA reconstruction}})]^2\}$$

k^{th} PCA vector

We maximize the variance of the projection in the residual subspace



Principal Component Analysis

Properties:

- **PCA Vectors** originate from the center of mass.
- Principal component #1: points in the direction of the **largest variance**.
- Each subsequent principal component
  - is **orthogonal** to the previous ones, and
  - points in the directions of the **largest variance of the residual subspace**