Linear Dimensionality Reduction: PCA

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Outline

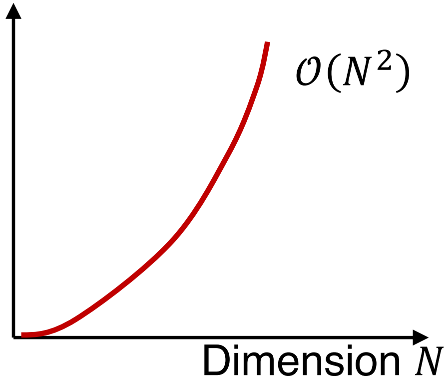
- Motivation
- Perspective 1: Minimizing Reconstruction Error
- Perspective 2: Maximizing Variance
- Perspective 3: SVD
- Other Applications of PCA

Motivation

- The dimensionality of many types of data is very high, *e.g.*, the dimension of images below is as high as

$$256\times256 = 65536$$

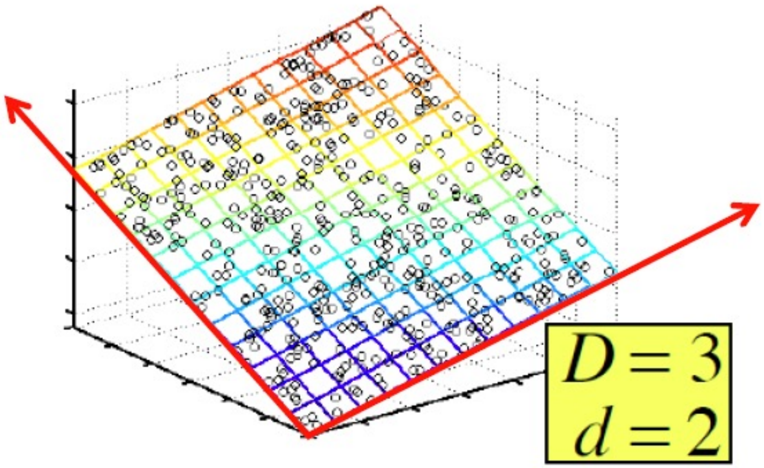
- If we work on the raw data directly, the complexity of subsequent tasks (*e.g.*, classification) could be extremely high



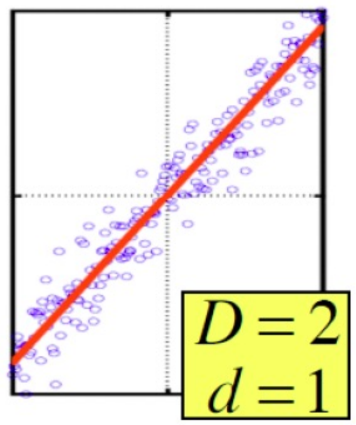
The complexity of logistic regression

Why the dimensionality could be reduced?

- The high-dimensional data often resides on a low-dimensional intrinsic space approximately



3-dimensional data lies on a 2-dimensional plane approximately

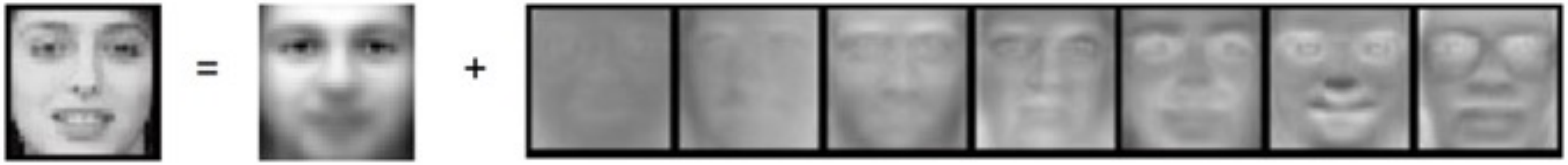


2-dimensional data lies on a 1-dimensional line approximately

The key is how to find *the principal directions* under which data samples could be represented with much fewer dimensions

- For the real-world data, it is also possible to find the low-dimensional space

  For instance, human faces can be well represented *with only several values* if appropriate directions can be found



$$\boldsymbol{x} \approx \boldsymbol{\mu}_0 + a_1\boldsymbol{\mu}_1 + \cdots + a_7\boldsymbol{\mu}_7$$

The raw image $\boldsymbol{x}$ that has 65536 values can be represented by only 7 values of $a_1, \cdots a_7$

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Re-representation under New Directions

- How to represent orthogonal directions in high dimensional space?

A set of vectors $\boldsymbol{u}_i$ satisfying

$$\boldsymbol{u}_i^T \boldsymbol{u}_j = \delta_{ij}$$

where $\delta_{ij} = 1$ if $i = j$; 0 otherwise

Theorem: Under the M given orthogonal directions $\{\boldsymbol{u}_i\}_{i=1}^{M}$, the *best approximation* to a data sample $\boldsymbol{x}$ is

$$\widetilde{\boldsymbol{x}} = \alpha_1 \boldsymbol{u}_1 + \alpha_2 \boldsymbol{u}_2 + \cdots + \alpha_M \boldsymbol{u}_M$$

with the α_i equal to

$$\alpha_i = \boldsymbol{u}_i^T \boldsymbol{x}$$

Proof:

$$\|\boldsymbol{x}-\tilde{\boldsymbol{x}}\|^2 = \left\|\boldsymbol{x}-\sum_{i=1}^{M}\alpha_i \boldsymbol{u}_i\right\|^2$$

$$= \|\boldsymbol{x}\|^2 - 2\sum_{i=1}^{M}\alpha_i \boldsymbol{u}_i^T \boldsymbol{x} + \sum_{i=1}^{M}\alpha_i^2$$

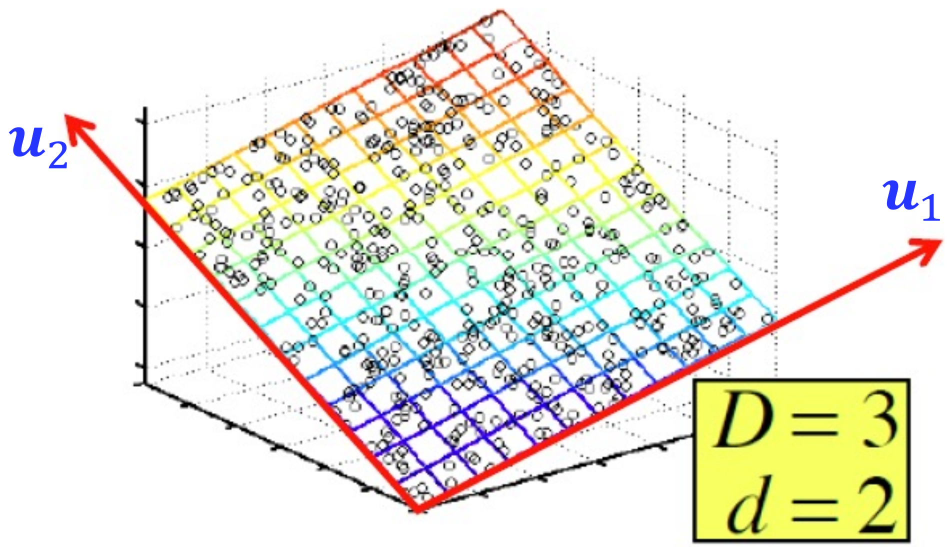
where we used $\boldsymbol{u}_i^T \boldsymbol{u}_j = 0$ for $i \neq j$ and 1 for $i = j$

This is a quadratic function, and can be minimized when $\alpha_i = \boldsymbol{u}_i^T \boldsymbol{x}$

Given the directions $\{\boldsymbol{u}_i\}_{i=1}^{M}$, the best coefficient is $\alpha_i = \boldsymbol{u}_i^T \boldsymbol{x}$.
But *how to find the best directions is still unknown*

Finding the Best Directions

- **Goal:** Given data samples $\{\boldsymbol{x}^{(n)}\}_{n=1}^{N}$ from $\mathbb{R}^D$, finding M orthogonal directions $\boldsymbol{u}_i$ such that the original data can be best represented under them



$$\boldsymbol{x}^{(n)} \approx \sum_{i=1}^{M} \alpha_i^{(n)} \boldsymbol{u}_i$$

- Suppose the best directions $\{\boldsymbol{u}_i\}_{i=1}^{M}$ are given, what are the best coefficients $\alpha_i^{(n)}$?

$$\alpha_i^{(n)} = \boldsymbol{u}_i^T \boldsymbol{x}^{(n)}$$

Instead of representing the data $\boldsymbol{x}^{(n)}$ directly, we first center the data to the origin, *i.e.*, subtracting each data point $\boldsymbol{x}^{(n)}$ by its mean

$$\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}, \quad \text{where } \overline{\boldsymbol{x}} = \frac{1}{N}\sum_{i=1}^{N} \boldsymbol{x}^{(n)}$$

- The objective can now be described as minimizing the error between $\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}$ and its best approximant $\widetilde{\boldsymbol{x}}^{(n)} = \sum_{i=1}^{M} \alpha_i^{(n)} \boldsymbol{u}_i$

$$Min_{\alpha_i^{(n)}, \boldsymbol{u}_i} \; E \qquad \text{with} \quad E \triangleq \frac{1}{N}\sum_{n=1}^{N} \left\| \left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right) - \sum_{i=1}^{M} \alpha_i^{(n)} \boldsymbol{u}_i \right\|^2$$

where the best coefficient $\alpha_i^{(n)}$ is known to be

$$\alpha_i^{(n)} = \boldsymbol{u}_i^T \left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)$$

- Reformulating the reconstruction error E

a) Rewriting $E = \frac{1}{N}\sum_{n=1}^{N}\left\|\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right) - \sum_{i=1}^{M}\alpha_i^{(n)}\boldsymbol{u}_i\right\|^2$ and noticing $\boldsymbol{u}_i^T\boldsymbol{u}_j = \delta_{ij}$ gives

$$E = \frac{1}{N}\left(\sum_{n=1}^{N}\left\|\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right\|^2 - 2\sum_{n=1}^{N}\sum_{i=1}^{M}\alpha_i^{(n)}\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)^T\boldsymbol{u}_i + \sum_{n=1}^{N}\sum_{i=1}^{M}\left(\alpha_i^{(n)}\right)^2\right)$$

b) Substituting $\alpha_i^{(n)} = \boldsymbol{u}_i^T\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)$ gives

$$E = \frac{1}{N}\sum_{n=1}^{N}\left\|\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right\|^2 - \sum_{i=1}^{M}\boldsymbol{u}_i^T\underbrace{\frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)^T}_{\triangleq \boldsymbol{S}}\boldsymbol{u}_i$$

c) Writing it into a matrix form gives

$$E = \frac{1}{N}\|\boldsymbol{X} - \overline{\boldsymbol{X}}\|_F^2 - \frac{1}{N}\sum_{i=1}^{M} \boldsymbol{u}_i^T \boldsymbol{S} \boldsymbol{u}_i$$

where $\boldsymbol{X} \triangleq \left[\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \cdots, \boldsymbol{x}^{(N)}\right]$ and $\|\cdot\|_F$ is the Frobenius norm

- Minimizing $E = \frac{1}{N}\|\boldsymbol{X} - \overline{\boldsymbol{X}}\|_F^2 - \frac{1}{\mathrm{N}}\sum_{i=1}^{M} \boldsymbol{u}_i^T \boldsymbol{S} \boldsymbol{u}_i$ under the constraint $\boldsymbol{u}_i^T \boldsymbol{u}_j = \delta_{ij}$ is equivalent to maximize

$$\boxed{\begin{gathered}\max_{\boldsymbol{u}_1 \cdots \boldsymbol{u}_M} \sum_{i=1}^{M} \boldsymbol{u}_i^T \boldsymbol{S} \boldsymbol{u}_i \\ s.t.: \boldsymbol{u}_i^T \boldsymbol{u}_j = \delta_{ij}\end{gathered}}$$

- Consider the simple case with $M = 1$. The problem is reduced to:

$$\max_{\boldsymbol{u}_1} \boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1$$
$$s.t.: \boldsymbol{u}_1^T \boldsymbol{u}_1 = 1$$

  - This is equivalent to maximize

$$\boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1 - \lambda(\boldsymbol{u}_1^T \boldsymbol{u}_1 - 1)$$

  - Taking the derivative *w.r.t.* $\boldsymbol{u}_1$ and setting it to 0 gives

$$\boldsymbol{S}\boldsymbol{u}_1 = \lambda \boldsymbol{u}_1,$$

  from which we can see that $\boldsymbol{u}_1$ should be the eigenvector of $\boldsymbol{S}$

  - It can be further checked that it is the eigenvector *w.r.t. to the largest eigenvalue that maximizes* $\boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1$

- For the case of $M = 2$, the problem becomes

$$\max_{\boldsymbol{u}_1, \boldsymbol{u}_2} \boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1 + \boldsymbol{u}_2^T \boldsymbol{S} \boldsymbol{u}_2$$

$$s.t.: \boldsymbol{u}_1^T \boldsymbol{u}_1 = 1, \boldsymbol{u}_2^T \boldsymbol{u}_2 = 1, \boldsymbol{u}_1^T \boldsymbol{u}_2 = 0$$

  - This is equivalent to maximize

$$\boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1 - \lambda_1(\boldsymbol{u}_1^T \boldsymbol{u}_1 - 1) + \boldsymbol{u}_2^T \boldsymbol{S} \boldsymbol{u}_2 - \lambda_2(\boldsymbol{u}_2^T \boldsymbol{u}_2 - 1)$$

    under the constraint $\boldsymbol{u}_1^T \boldsymbol{u}_2 = 0$

  - Taking the derivative *w.r.t.* $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ and setting it to 0 gives

$$\boldsymbol{S} \boldsymbol{u}_1 = \lambda_1 \boldsymbol{u}_1, \qquad \boldsymbol{S} \boldsymbol{u}_2 = \lambda_2 \boldsymbol{u}_2,$$

    $\Rightarrow$ $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ must be the eigenvectors of $\boldsymbol{S}$

    $\Rightarrow$ It can be seen that to maximize $\boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1 + \boldsymbol{u}_2^T \boldsymbol{S} \boldsymbol{u}_2$, $\boldsymbol{u}_1$ and $\boldsymbol{u}_2$ must be the eigenvectors *corresponding to the two largest eigenvalues*

For the case $M > 1$, the directions $\boldsymbol{u}_i$ are *the eigenvectors of $\boldsymbol{S}$ corresponding to the largest M eigenvalues*

$\boldsymbol{A} = \boldsymbol{X} - \overline{\boldsymbol{X}}$

Question: Will the eigenvectors $\boldsymbol{u}_i$ of $\boldsymbol{S}$ satisfy $\boldsymbol{u}_i^T \boldsymbol{u}_j = 0$ for $i \neq j$?

- For any $D \times D$ *real symmetric* matrix like $\boldsymbol{S} \triangleq \boldsymbol{A}\boldsymbol{A}^T$, it has D eigenvectors that are orthogonal to each other

- For every $\boldsymbol{S} \triangleq \boldsymbol{A}\boldsymbol{A}^T$, it can be decomposed as

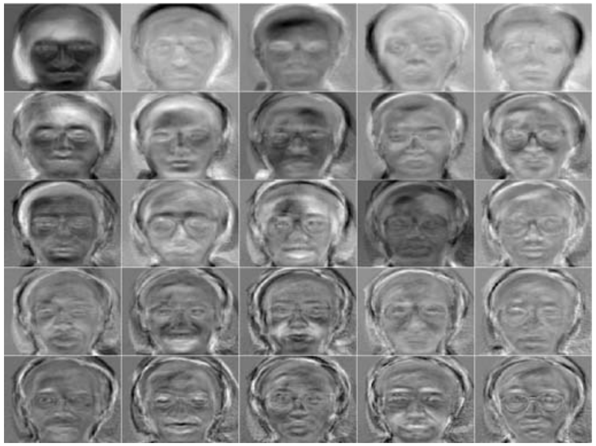
$$\boldsymbol{S} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$

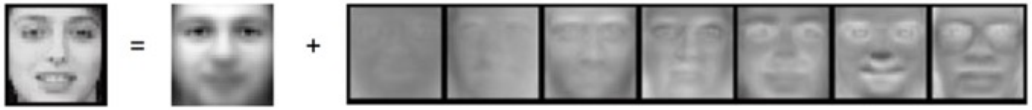
where $\boldsymbol{U}$ is comprised of the eigenvectors of $\boldsymbol{S}$ and $\boldsymbol{U}\boldsymbol{U}^T = I$; $\boldsymbol{\Lambda}$ is a diagonal matrix composed of eigenvalues of $\boldsymbol{S}$

Examples

Input data: each face image is a data point

Top 25 principal directions





$$\boldsymbol{x} \approx \overline{\boldsymbol{x}} + \alpha_1 \boldsymbol{u}_1 + \cdots + \alpha_7 \boldsymbol{u}_7$$

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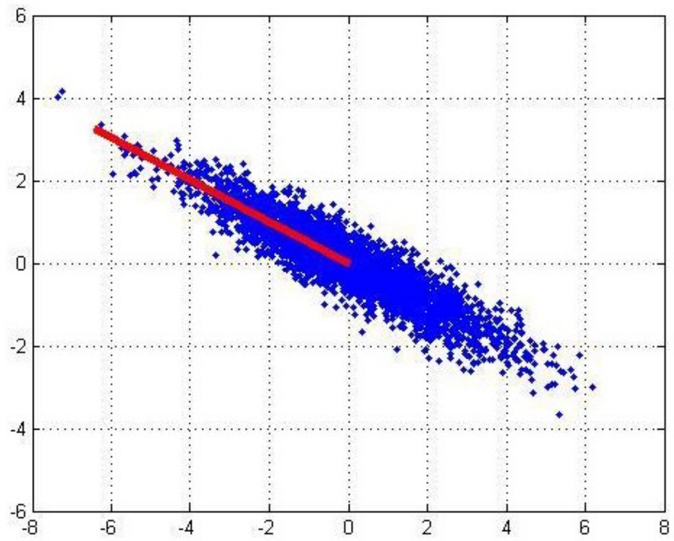
Problem Formulation

- **Goal:** Given a dataset $\{\boldsymbol{x}^{(n)}\}_{n=1}^{N}$, find orthogonal directions $\{\boldsymbol{u}_k\}_{k=1}^{M}$ such that the variance of data projected onto these directions are maximized



Maximizing the variance amounts to *preserve the information of original data as much as possible*

- For the first direction $\boldsymbol{u}_1$, we hope the variance of projected data along the direction $\boldsymbol{u}_1$, *i.e.*, $\{\boldsymbol{u}_1^T \boldsymbol{x}^{(n)}\}_{n=1}^{N}$, is maximized
  - The variance expression

$$var = \frac{1}{N} \sum_{n=1}^{N} \left(\boldsymbol{u}_1^T (\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}) \right)^2$$

$$= \boldsymbol{u}_1^T \frac{1}{N} \sum_{n=1}^{N} (\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}})(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}})^T \boldsymbol{u}_1$$

$$= \boldsymbol{u}_1^T \boldsymbol{S} \boldsymbol{u}_1$$

  - Subjecting to $\boldsymbol{u}_1^T \boldsymbol{u}_1 = 1$, as proved previously, the variance is maximized when $\boldsymbol{u}_1$ is *the eigenvector of $\boldsymbol{S}$ corresponding to the largest eigenvalue*

- For the second direction $\boldsymbol{u}_2$, it also should maximize the variance

$$var = \boldsymbol{u}_2^T \boldsymbol{S} \boldsymbol{u}_2,$$

but should subject to the constraints $\boldsymbol{u}_i^T \boldsymbol{u}_j = \delta_{ij}$, that is,

$$\boldsymbol{u}_2^T \boldsymbol{u}_2 = 1 \qquad \boldsymbol{u}_1^T \boldsymbol{u}_2 = 0$$

- Due to $\boldsymbol{u}_1$ being the eigenvector *w.r.t.* the largest eigenvalue, it can be proved that ***$\boldsymbol{u}_2$* is the eigenvector of $\boldsymbol{S}$ corresponding the second largest eigenvalue**

$\boldsymbol{u}_i$ *is the eigenvector of* $\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)^T$ *corresponding the i-th largest eigenvalue*

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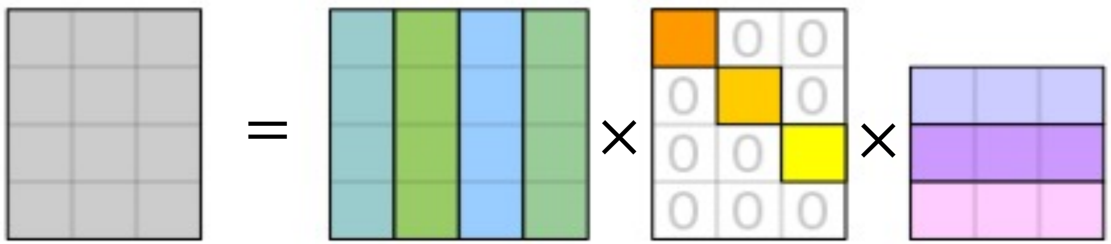
Singular Value Decomposition (SVD)

- For any $M \times N$ matrix $\boldsymbol{A}$, it can always be decomposed as

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T$$



$\boldsymbol{A}$	$\boldsymbol{U}$	$\boldsymbol{\Sigma}$	$\boldsymbol{V}^T$
$M \times N$	$M \times M$	$M \times N$	$N \times N$

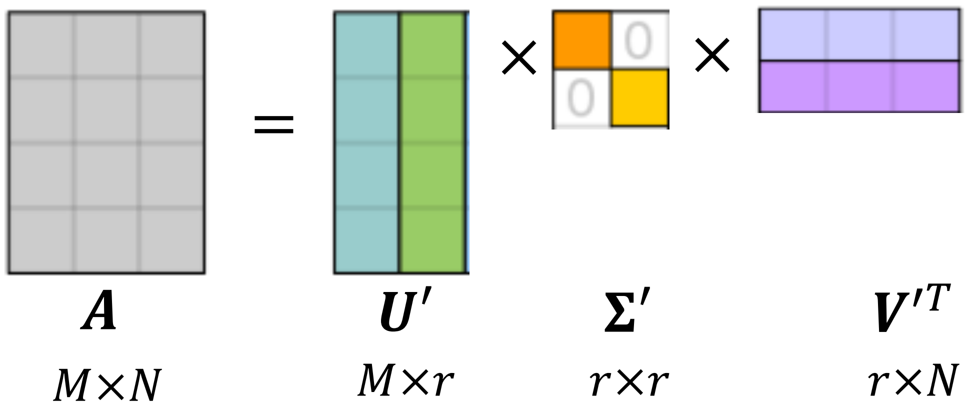
  - $\boldsymbol{U} = [\boldsymbol{u}_1, \cdots, \boldsymbol{u}_M]$ and $\boldsymbol{V} = [\boldsymbol{v}_1, \cdots, \boldsymbol{v}_N]$, with $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ being the i-th eigenvector of $\boldsymbol{A}\boldsymbol{A}^T$ and $\boldsymbol{A}^T\boldsymbol{A}$, *and* $\boldsymbol{u}_i^T\boldsymbol{u}_j = \delta_{ij}$ and $\boldsymbol{v}_i^T\boldsymbol{v}_j = \delta_{ij}$
  - $\boldsymbol{\Sigma}$ *only* has nonzero values on the diagonal, which are the squared root of eigenvalues of $\boldsymbol{A}\boldsymbol{A}^T$ or $\boldsymbol{A}^T\boldsymbol{A}$ *(Nonzero eigenvalues of $\boldsymbol{A}\boldsymbol{A}^T$ and $\boldsymbol{A}^T\boldsymbol{A}$ are the same)*

    Σ_{ii} is called *singular values* and are stored in a descending order

- Because $\mathbf{\Sigma}$ only has nonzero values on the diagonal, $\boldsymbol{A}$ can be expressed as

$$\boldsymbol{A} = \sum_{i=1}^{r} \Sigma_{ii}\boldsymbol{u}_i\boldsymbol{v}_i^T = \boldsymbol{U}'\mathbf{\Sigma}'\boldsymbol{V}'^T$$

where $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ are the i-th column of $\boldsymbol{U}$ and $\boldsymbol{V}$; r is the number of nonzero diagonal elements in $\mathbf{\Sigma}$



$$\begin{bmatrix} \mathbf{1} & \mathbf{1} & \mathbf{1} & 0 & 0 \\ \mathbf{3} & \mathbf{3} & \mathbf{3} & 0 & 0 \\ \mathbf{4} & \mathbf{4} & \mathbf{4} & 0 & 0 \\ \mathbf{5} & \mathbf{5} & \mathbf{5} & 0 & 0 \\ 0 & \mathbf{2} & 0 & \mathbf{4} & \mathbf{4} \\ 0 & 0 & 0 & \mathbf{5} & \mathbf{5} \\ 0 & \mathbf{1} & 0 & \mathbf{2} & \mathbf{2} \end{bmatrix} = \begin{bmatrix} \mathbf{0.13} & 0.02 & -0.01 \\ \mathbf{0.41} & 0.07 & -0.03 \\ \mathbf{0.55} & 0.09 & -0.04 \\ \mathbf{0.68} & 0.11 & -0.05 \\ 0.15 & \mathbf{-0.59} & \mathbf{0.65} \\ 0.07 & \mathbf{-0.73} & \mathbf{-0.67} \\ 0.07 & \mathbf{-0.29} & \mathbf{0.32} \end{bmatrix} \begin{bmatrix} \mathbf{12.4} & 0 & 0 \\ 0 & \mathbf{9.5} & 0 \\ 0 & 0 & \mathbf{1.3} \end{bmatrix} \begin{bmatrix} \mathbf{0.56} & \mathbf{0.59} & \mathbf{0.56} & 0.09 & 0.09 \\ 0.12 & -0.02 & 0.12 & \mathbf{-0.69} & \mathbf{-0.69} \\ 0.40 & \mathbf{-0.80} & 0.40 & 0.09 & 0.09 \end{bmatrix}$$

- The vector $\boldsymbol{u}_i$ in the SVD decomposition of $\boldsymbol{A}$ is the eigenvector of $\boldsymbol{A}\boldsymbol{A}^T$ *w.r.t.* its i-th largest eigenvalues

- By setting $\boldsymbol{A} = \widetilde{\boldsymbol{X}}$ with $\widetilde{\boldsymbol{X}} \triangleq \left[\boldsymbol{x}^{(1)} - \overline{\boldsymbol{x}}, \boldsymbol{x}^{(2)} - \overline{\boldsymbol{x}}, \cdots, \boldsymbol{x}^{(N)} - \overline{\boldsymbol{x}}\right]$, we can see that

$$\widetilde{\boldsymbol{X}}\widetilde{\boldsymbol{X}}^T = \sum_{n=1}^{N}\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)\left(\boldsymbol{x}^{(n)} - \overline{\boldsymbol{x}}\right)^T$$

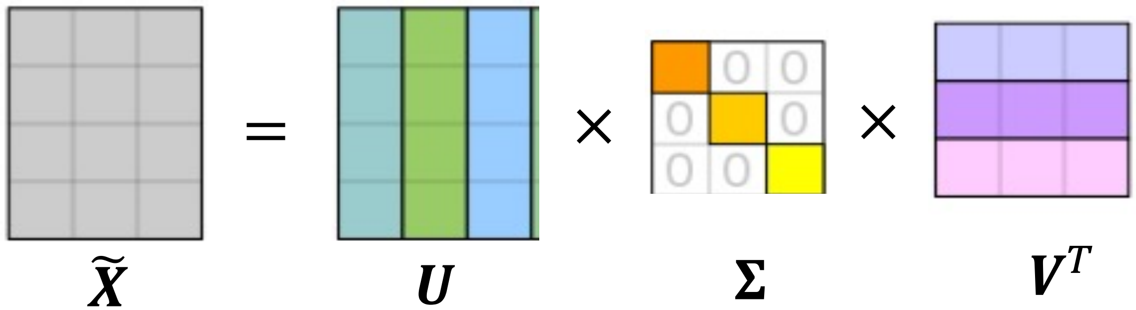
$$= N \cdot \boldsymbol{S}$$

$\Longrightarrow$ The eigenvectors of $\widetilde{\boldsymbol{X}}\widetilde{\boldsymbol{X}}^T$ are the same as the matrix $\boldsymbol{S}$

By performing SVD on $\widetilde{\boldsymbol{X}}$, principal directions of data $\left\{\boldsymbol{x}^{(n)}\right\}_{n=1}^{N}$ can be directly obtained, which are the columns of left SVD matrix $\boldsymbol{U}$

- Question:

Given the SVD decomposition of $\widetilde{\boldsymbol{X}}$ as shown below, what are the principle directions and the coefficients α_i's for $\widetilde{\boldsymbol{x}}^{(n)}$?



If only top two directions are kept, what are the coefficients α_i's?

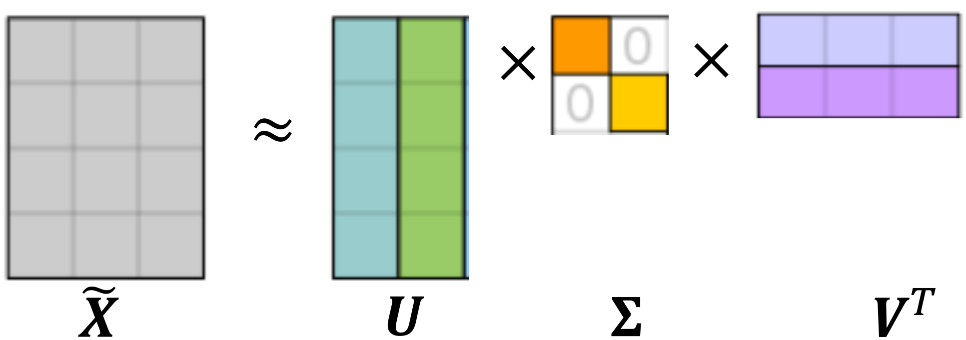


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Image Compression

Partition a 372×492 image below into many 12×12 patches

- Each patch is viewed as a data instance
- Performing PCA on the patches

Reconstruction Error vs # PCA components

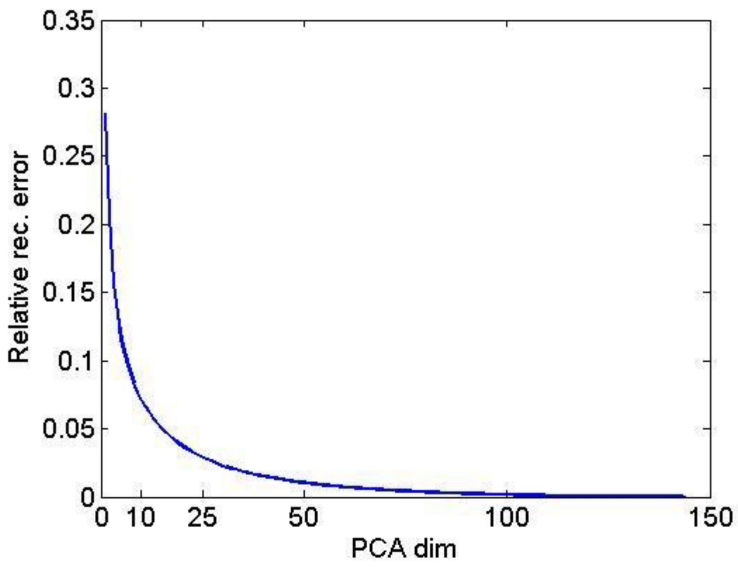
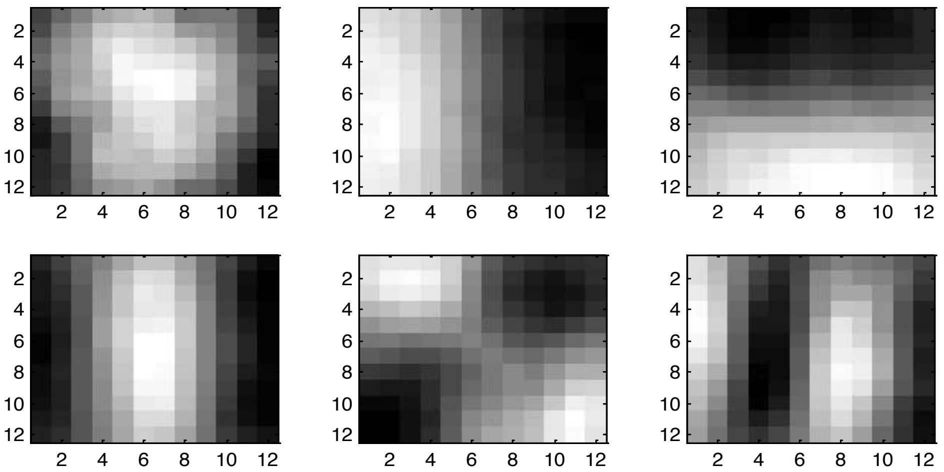


Illustration of the top 6 PCA components



Reconstruction with the top 60 components

Reconstruction with the top 16 components

Denoising

Noisy Image

Denoised Image

Reconstructed from the top 15 principal components