

Principal Component Analysis (PCA)

2IMM20 - Foundations of data mining
TU Eindhoven, Quartile 3, 2017-2018

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Why reduce the dimension?

Why reduce the dimension?

Representation of input data often is often high dimensional (images, documents, etc.)

There are two main reasons to reduce the dimension:

- some algorithms have **running time** exponential in the dimension
- we want to **visualize** inherent structure in the data

Overview of this lecture

- Principal Component Analysis (PCA)
- Interpretation of Principle Components
- Computing Principal Components
- Singular-Value Decomposition (SVD)
- Power Method
- Eigenvectors of the Sample Covariance Matrix
- Multidimensional scaling
- Isomap

Principal Component Analysis (PCA)

Principal components provide a sequence of best linear approximations to a data set

Given a data set $P = \{\mathbf{p}_1, \dots, \mathbf{p}_n\}$, we want to represent P using a k -dimensional linear model

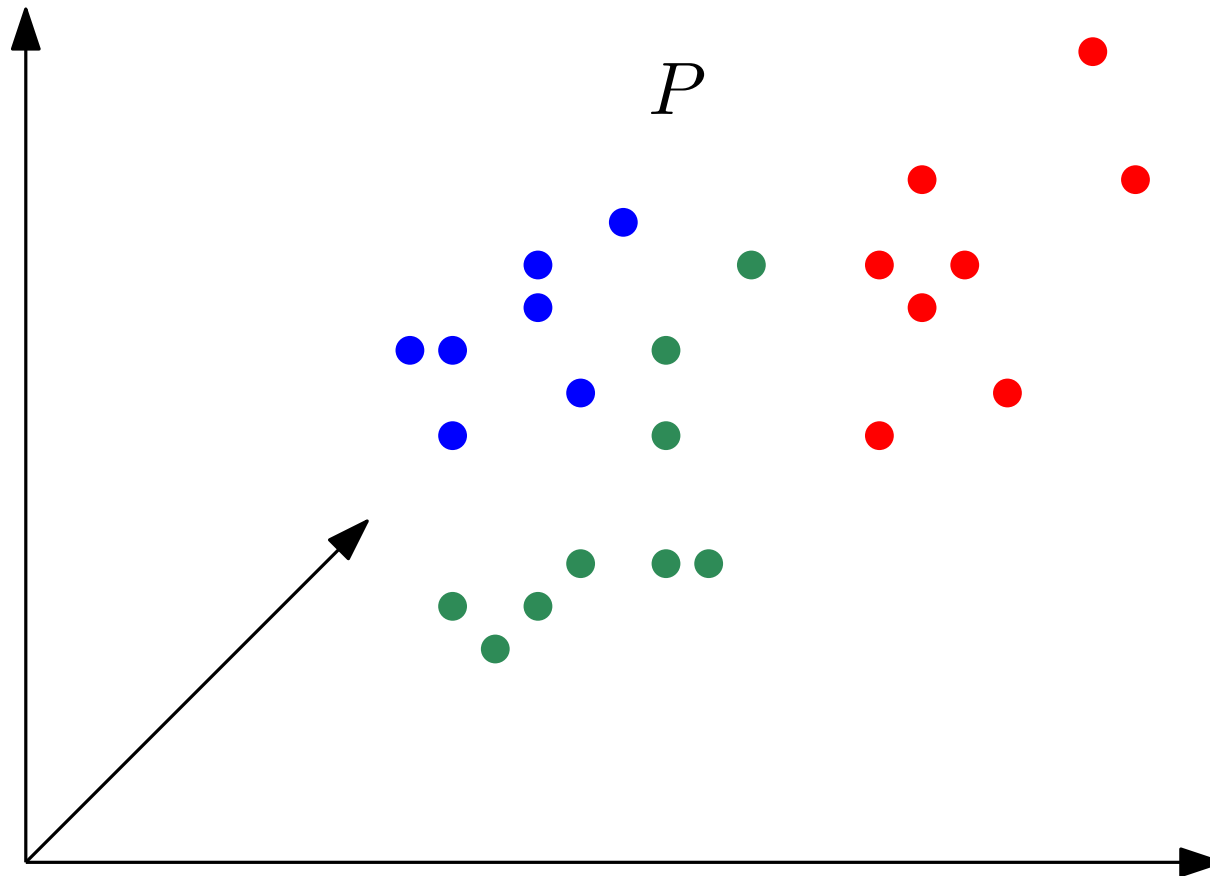
$$f(\lambda) = \mu + \mathbf{V}\lambda,$$

where

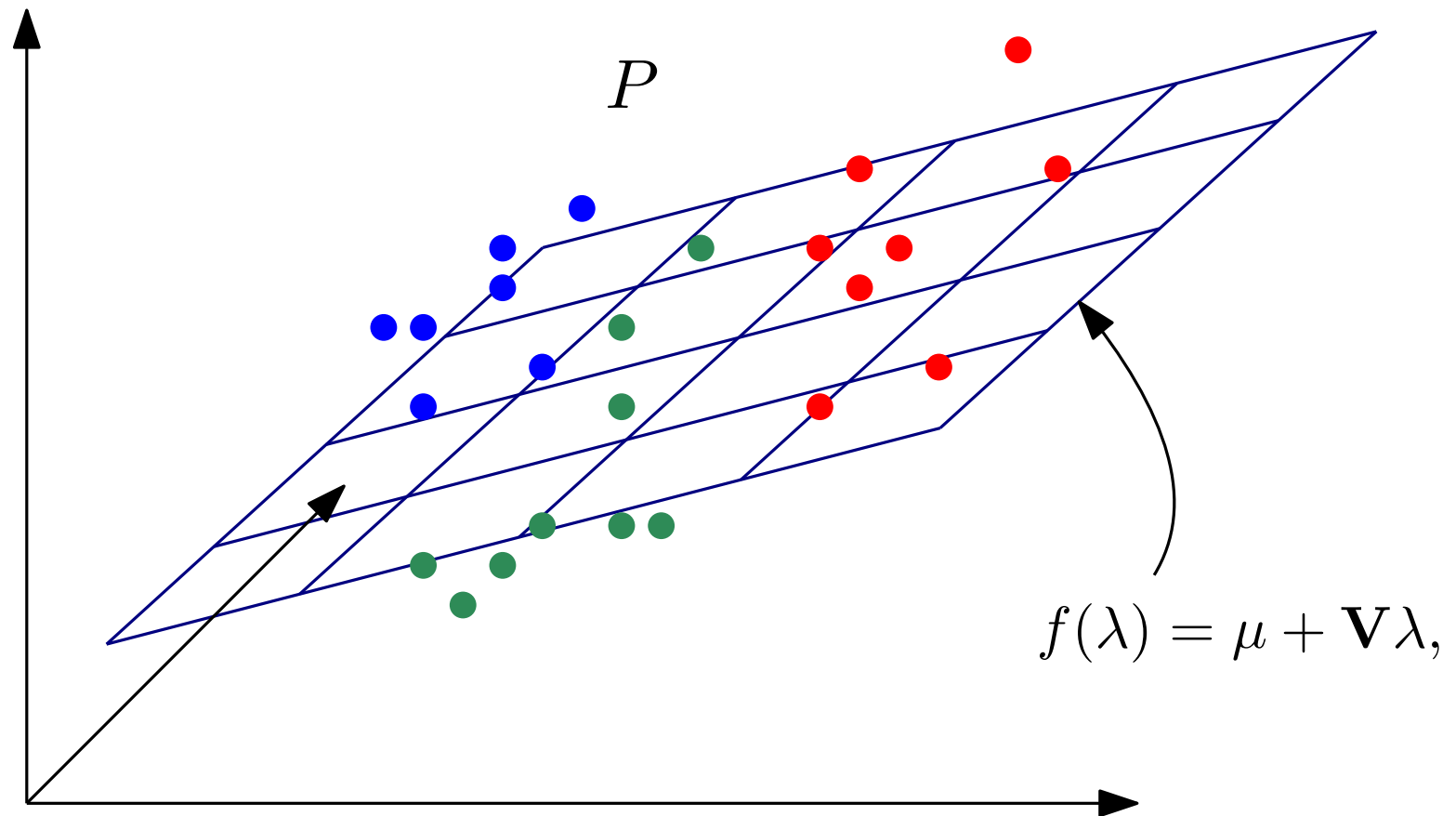
- μ is a location vector in \mathbb{R}^d
- \mathbf{V} is a $d \times k$ orthonormal matrix
- λ is a k vector of parameters

The above is a parametric representation of an affine hyperplane of dimension k

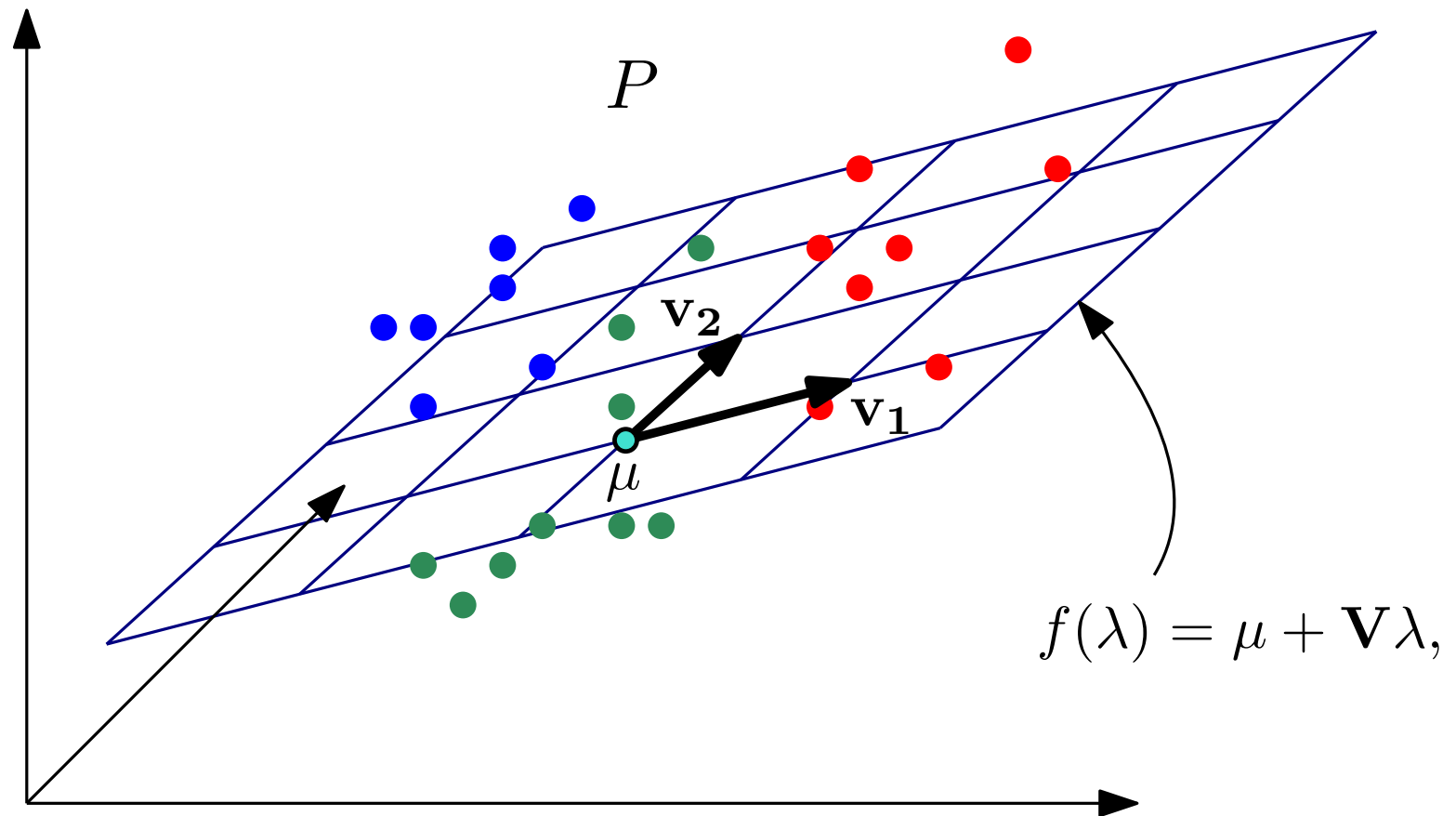
Principal Component Analysis (PCA)



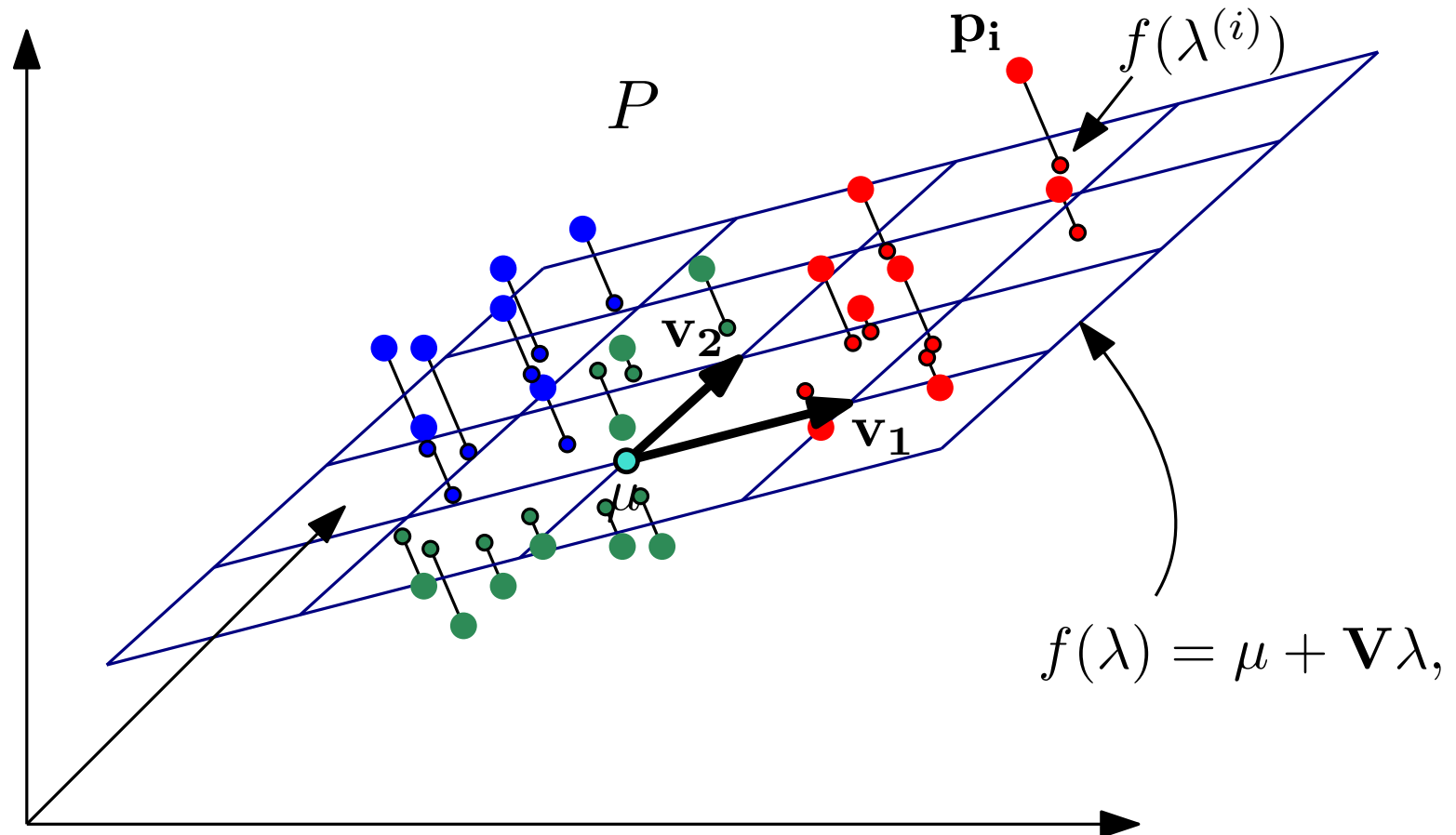
Principal Component Analysis (PCA)



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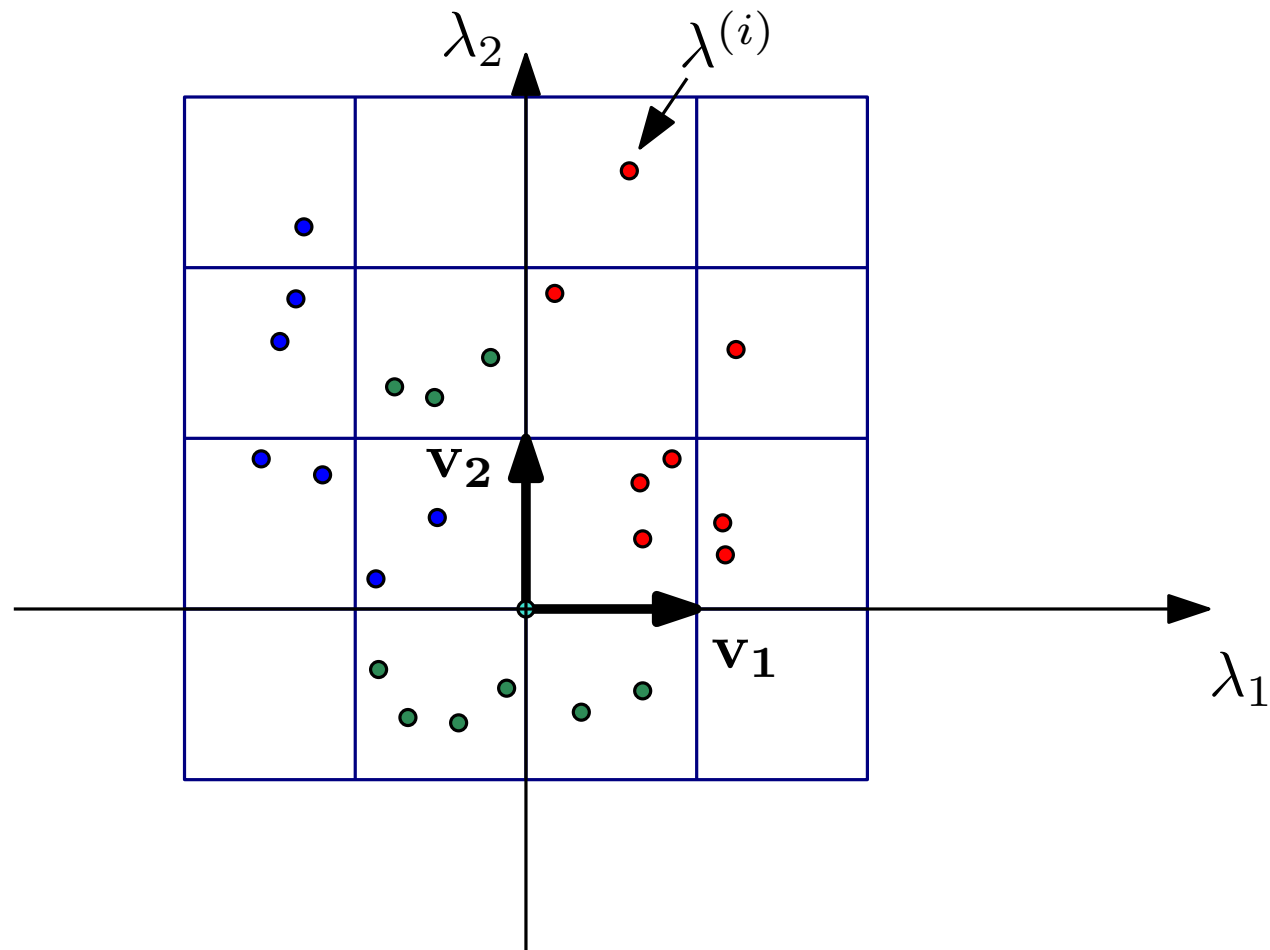


Want to find the hyperplane which minimizes sum of squared distances ("best fitting")

$$\sum_{1 \leq i \leq n} \|\mathbf{p}_i - f(\lambda^{(i)})\|^2$$

Principal Component Analysis (PCA)

We can visualize P in the subspace spanned by \mathbf{v}_1 and \mathbf{v}_2 by plotting the principle coordinates λ .



Principal Component Analysis (PCA)

We have our linear model

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We have a function that defines "best fitting"

$$\min_{\mu, \mathbf{V}_k, \lambda} \sum_{1 \leq i \leq n} \|\mathbf{p}_i - f(\lambda^{(i)})\|^2$$

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Optimizing for μ and λ gives

$$\mu = \frac{1}{n} \sum_{1 \leq i \leq n} \mathbf{p}_i \quad \text{and} \quad \lambda^{(i)} = \mathbf{V}^T (\mathbf{p}_i - \mu)$$

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... and we use the projection onto \mathbf{V} for λ

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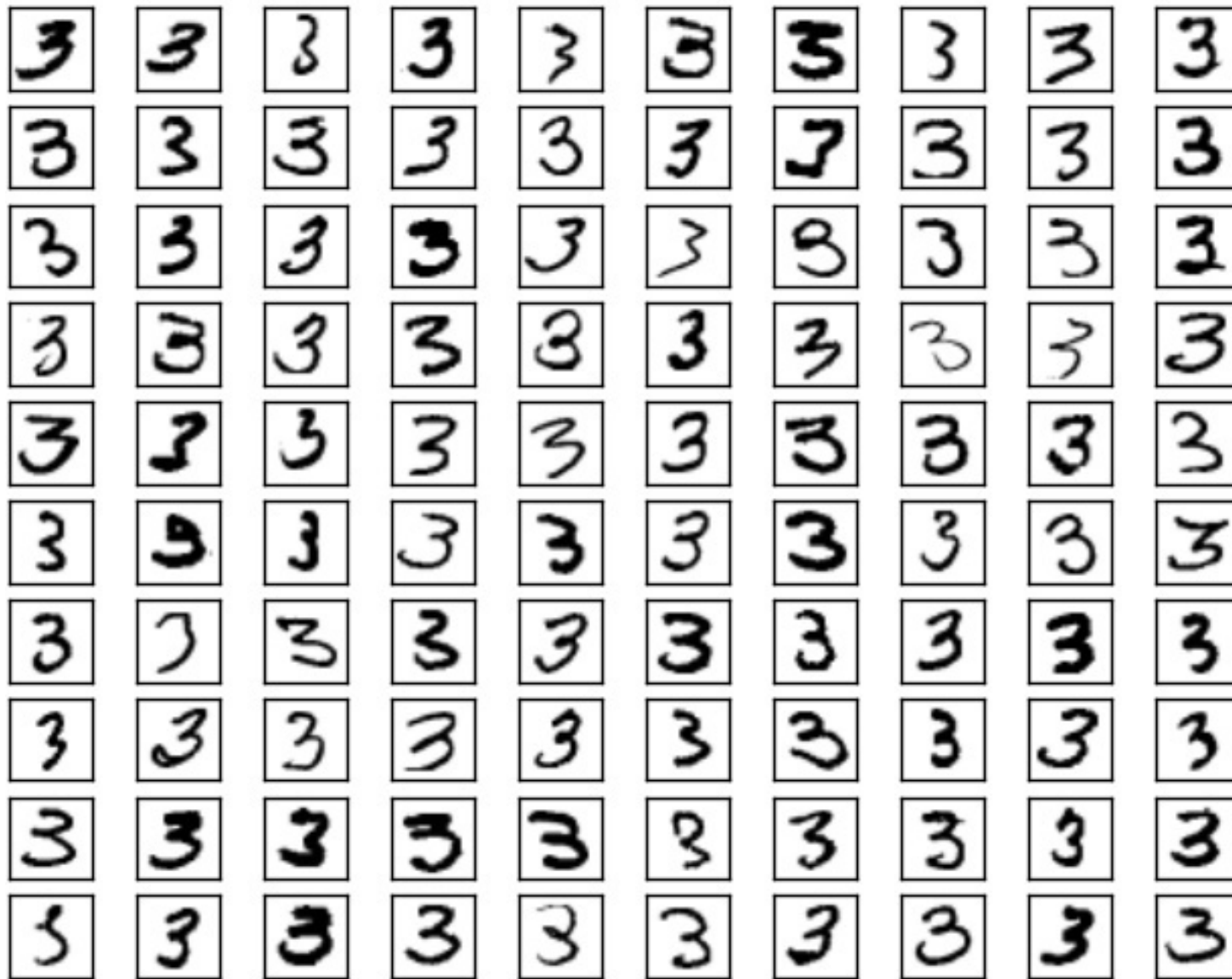
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Principal Component Analysis (PCA)

Example: handwritten digits



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Assume we computed the first two principal components

We obtain an interpretable representation

$$\hat{f}(\lambda) = \mu + \mathbf{V}\lambda,$$

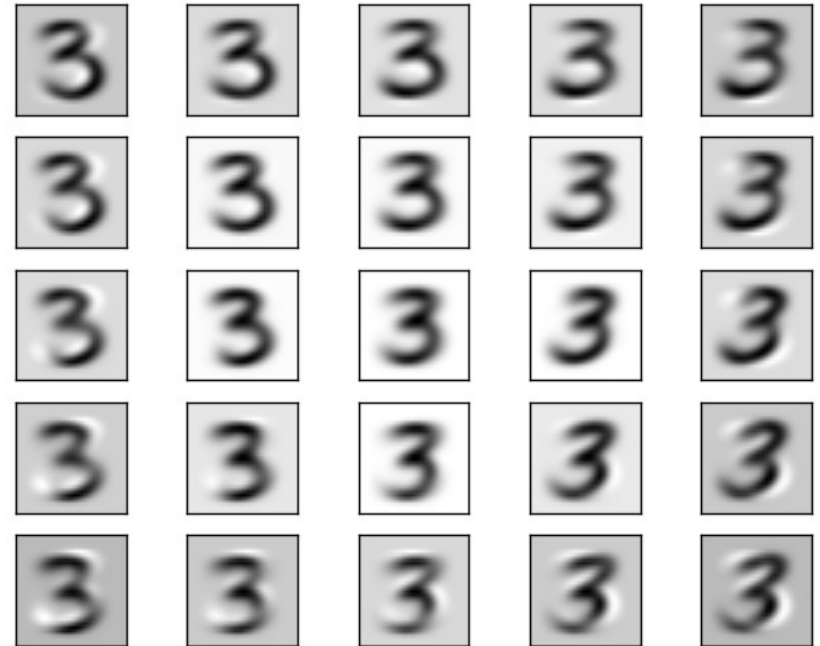
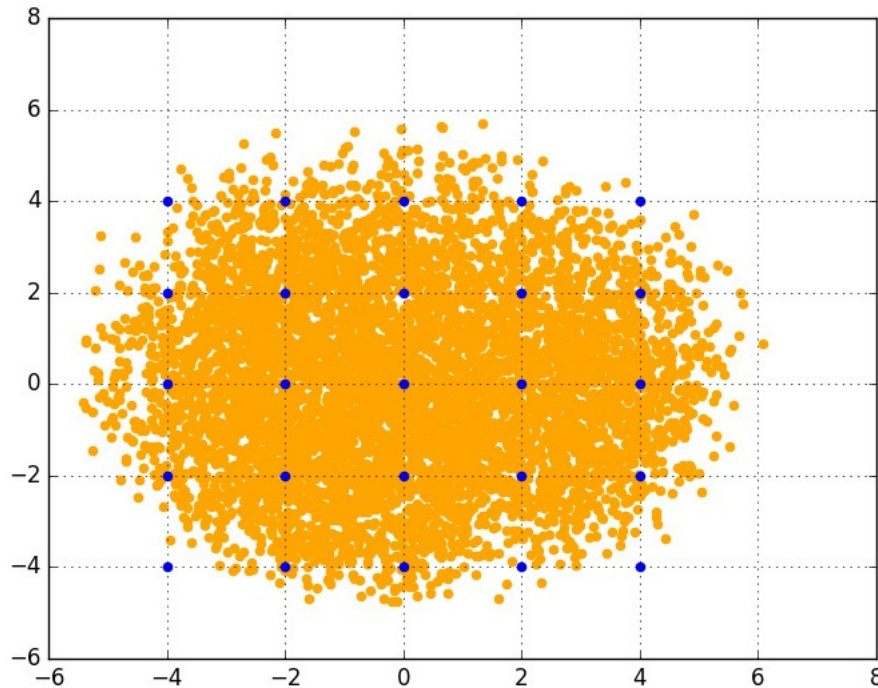
$$= \mu + \lambda_1 \mathbf{v}_1 + \lambda_2 \mathbf{v}_2$$

$$= \begin{array}{c} \boxed{\text{3}} \\ \uparrow \\ \text{mean} \end{array} + \lambda_1 \cdot \begin{array}{c} \boxed{\text{3}} \\ \uparrow \\ \text{principle components} \end{array} + \lambda_2 \cdot \begin{array}{c} \boxed{\text{3}} \\ \uparrow \\ \text{principle components} \end{array}$$

The diagram illustrates the PCA representation of a handwritten digit '3'. It shows the digit as a sum of three components: a mean image (a blurry '3' on a white background) and two principal component images (blurry '3's on a gray background). Arrows point from the labels 'mean' and 'principle components' to their respective images in the equation.

Principal Component Analysis (PCA)

Example: handwritten digits

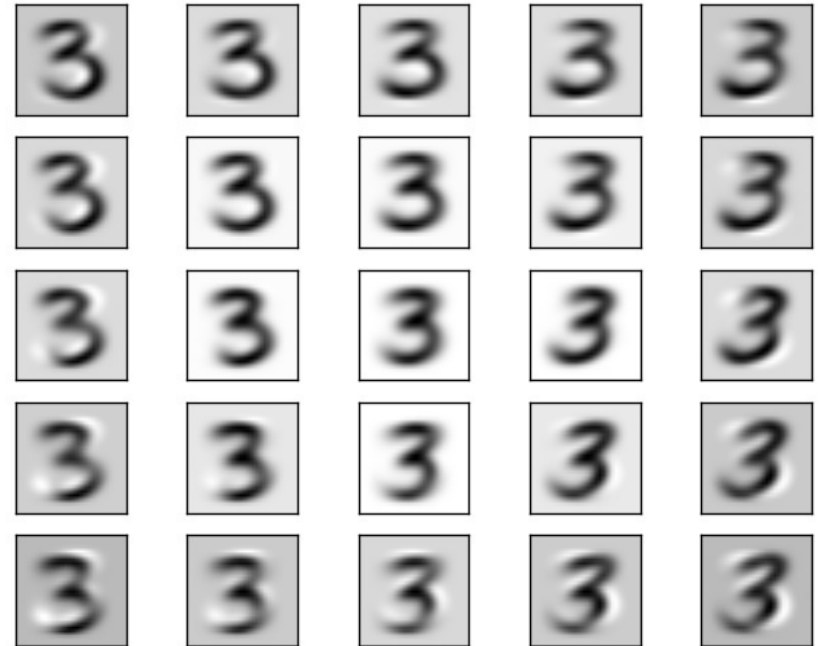
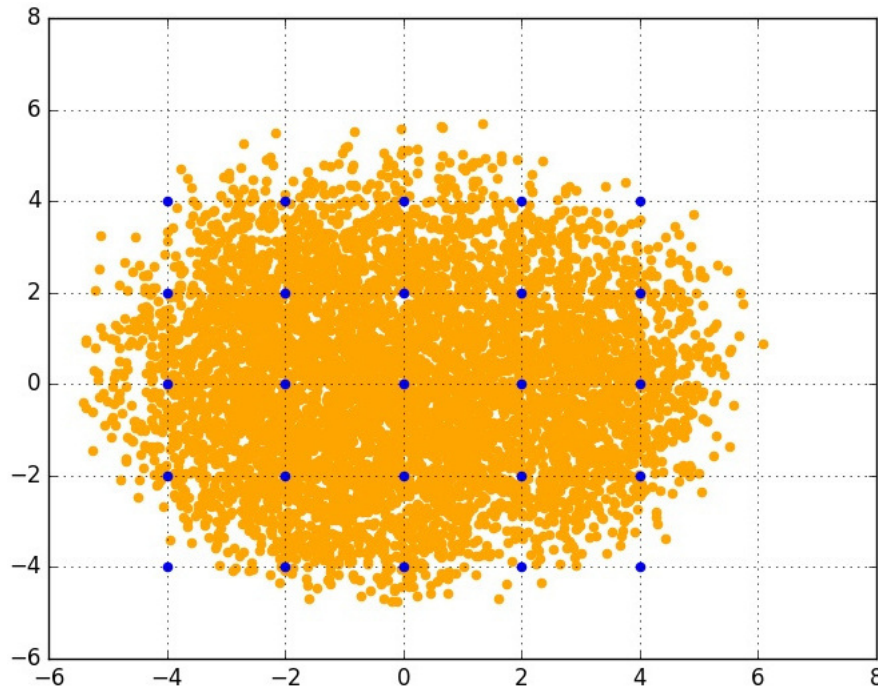


$$\begin{array}{|c|} \hline \text{3} \\ \hline \end{array} + \lambda_1 \cdot \begin{array}{|c|} \hline \text{3} \\ \hline \end{array} + \lambda_2 \cdot \begin{array}{|c|} \hline \text{3} \\ \hline \end{array}$$

Interpretation?

Principal Component Analysis (PCA)

Example: handwritten digits



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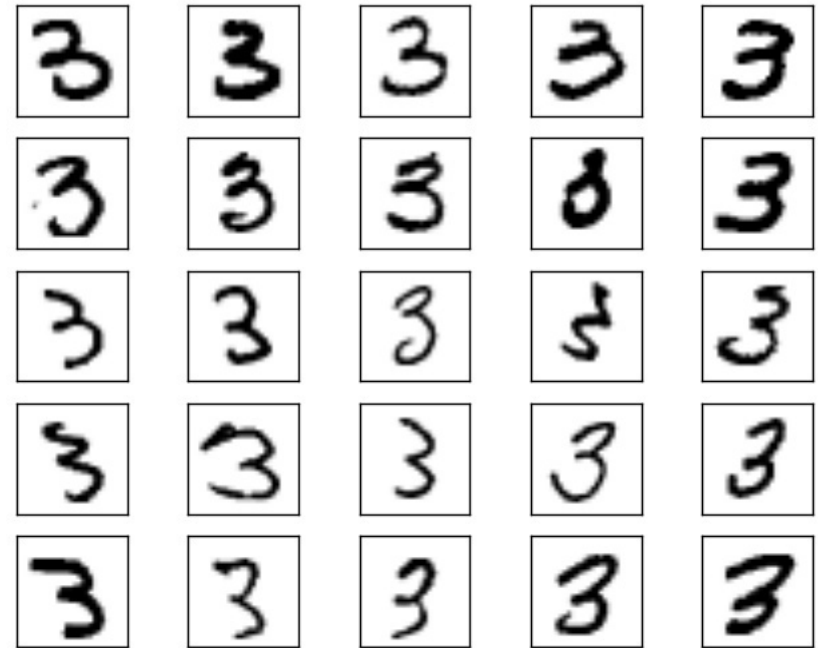
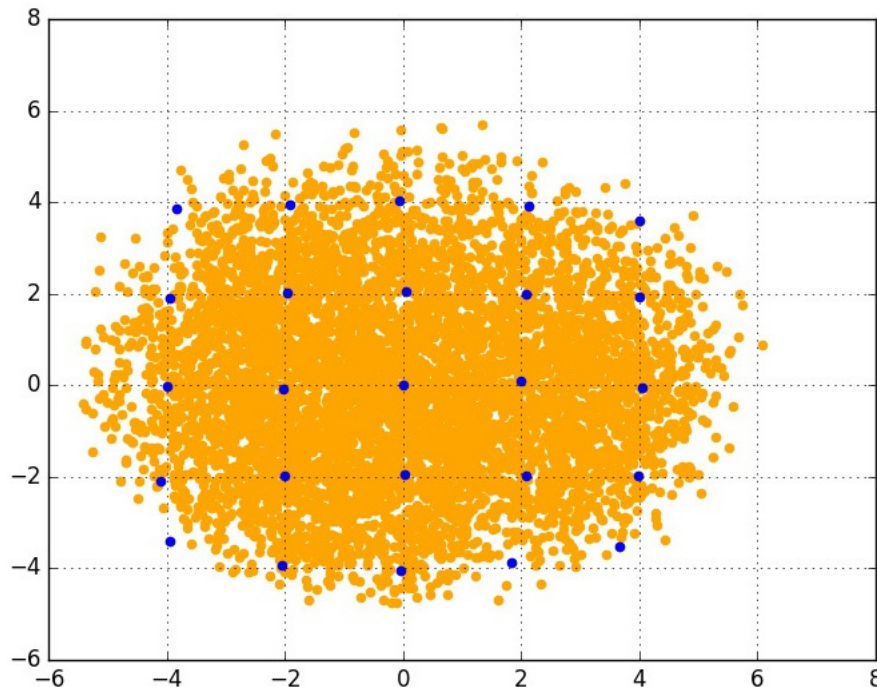
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"slanting"

"lengthening of lower tail"

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Principal Component Analysis (PCA)

We have defined PCA as an optimization problem:
Fitting a k -dimensional hyperplane to the data

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How do we compute \mathbf{V} ?

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How do we compute \mathbf{V} ?

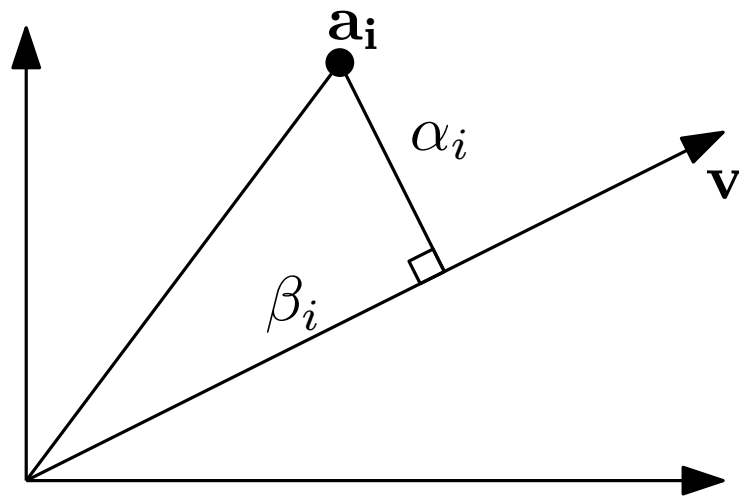
In the following, let \mathbf{A} be a $n \times d$ matrix with row vectors \mathbf{a}_i with

$$\mathbf{a}_i = (\mathbf{p}_i - \mu)^T$$

\mathbf{A} is a **centered** version of P

Computing the principal components

Simplest case: fitting a line through the origin to \mathbf{A}

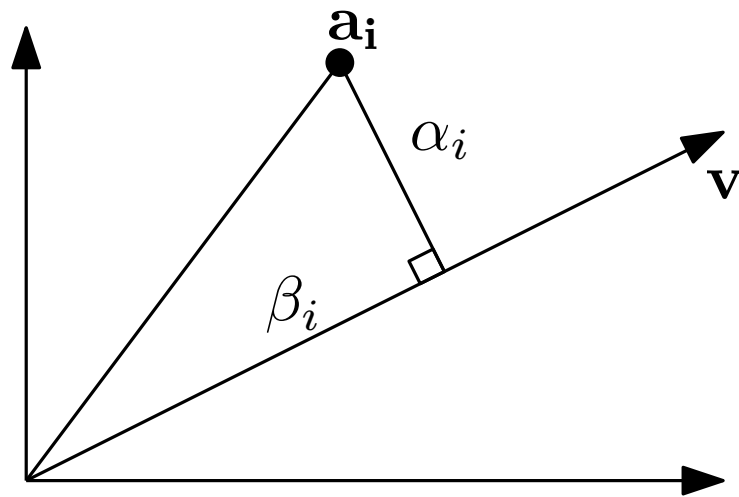


(Pythagoras)

$$\|\mathbf{a}_i\|^2 = \alpha_i^2 + \beta_i^2$$

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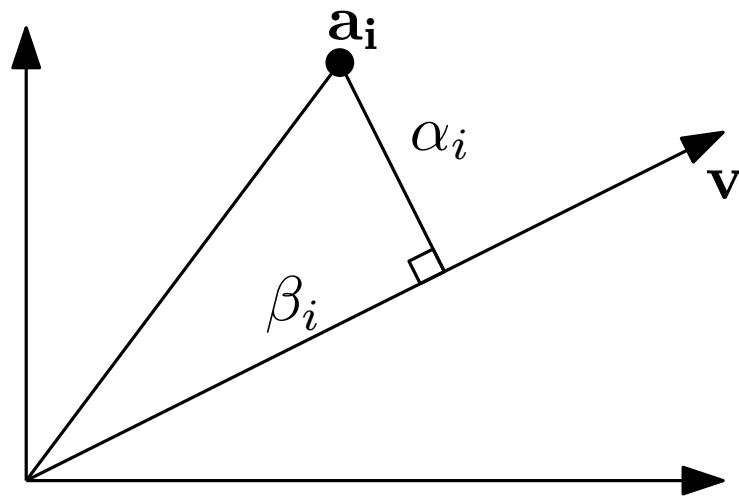
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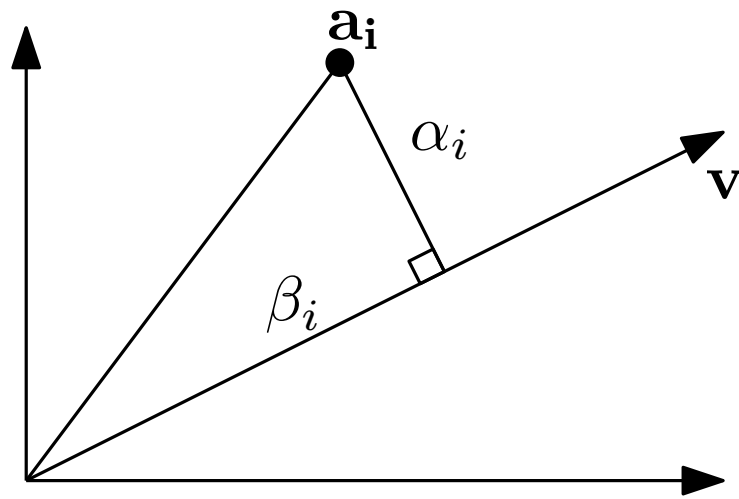
$$\Leftrightarrow \alpha_i^2 = \|\mathbf{a}_i\|^2 - \beta_i^2$$

$$\operatorname{argmin}_{\|\mathbf{v}\|=1} \sum_{1 \leq i \leq n} \alpha_i^2 = \operatorname{argmin}_{\|\mathbf{v}\|=1} \sum_{1 \leq i \leq n} \|\mathbf{a}_i\|^2 - \beta_i^2$$

"best fitting"

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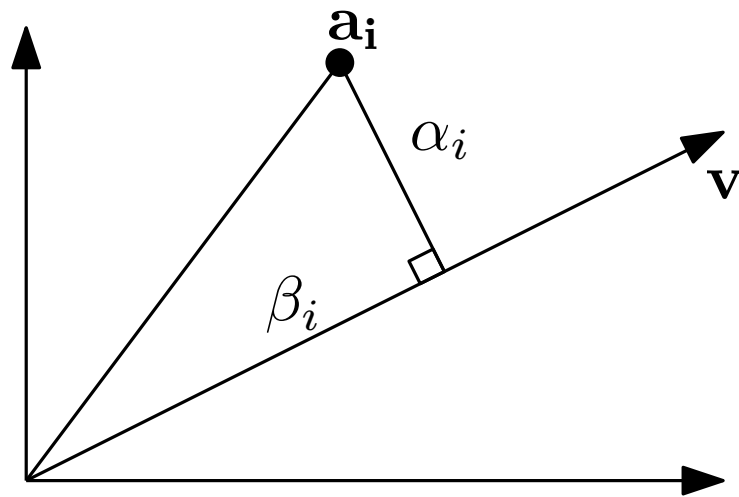
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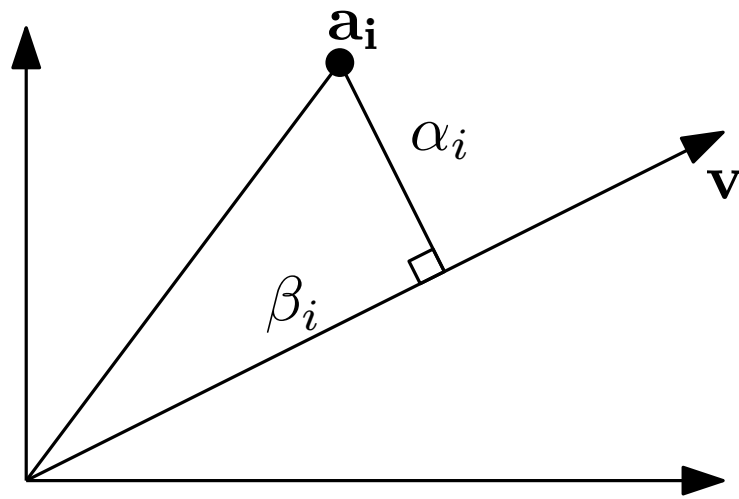
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$$= \operatorname{argmax}_{\|\mathbf{v}\|=1} \sum_{1 \leq i \leq n} (\mathbf{a}_i \mathbf{v})^2$$

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Computing the principal components

\mathbf{A} is a $n \times d$ matrix with row vectors \mathbf{a}_i

The first singular vector of A is:

$$\mathbf{v}_1 = \operatorname{argmax}_{\|\mathbf{v}\|=1} \|\mathbf{A}\mathbf{v}\|$$

The first singular value of A is:

$$\sigma_1 = \|\mathbf{A}\mathbf{v}_1\|$$

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...

The process stops when we have found singular vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r$ and singular values

$\sigma_1, \sigma_2, \dots, \sigma_r$ and

$$\max_{\substack{\|\mathbf{v}\|=1 \\ \mathbf{v} \perp \mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_r}} \|\mathbf{A}\mathbf{v}\| = 0$$

Singular Value Decomposition (SVD)

SVD is the factorization of a matrix A into three matrices

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

where

- \mathbf{U} and \mathbf{V} are orthonormal
- \mathbf{D} is diagonal with positive real entries σ_i
- σ_i are in descending order

The diagram shows the SVD factorization $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ with dimensions indicated in boxes:

- \mathbf{A} is an $n \times d$ matrix.
- \mathbf{U} is an $n \times k$ matrix.
- \mathbf{D} is a $k \times k$ matrix.
- \mathbf{V}^T is a $k \times d$ matrix.

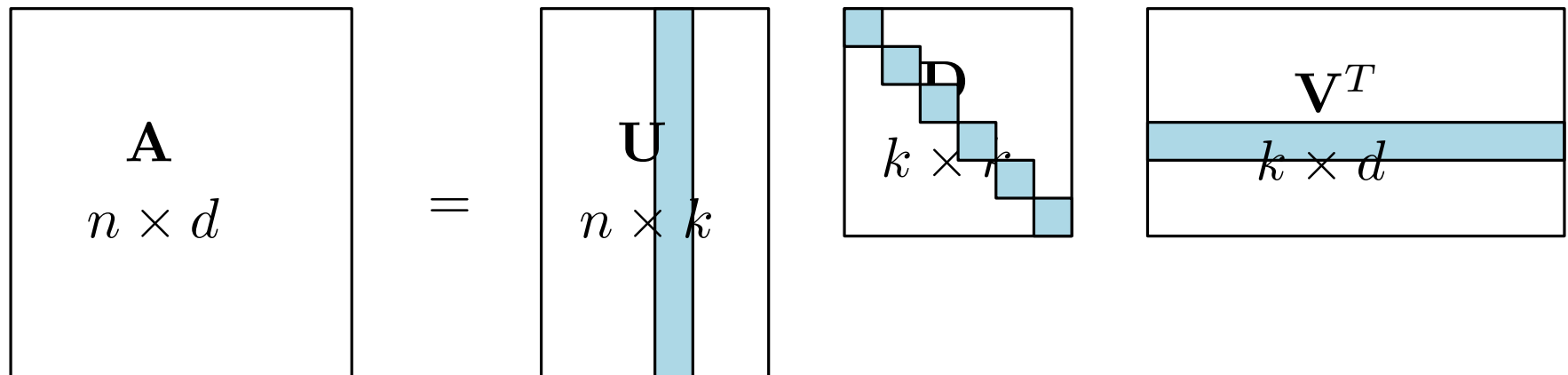
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Columns of \mathbf{V} are called **singular vectors** $\mathbf{v}_1, \mathbf{v}_2, \dots$

Diagonal entries of \mathbf{D} are called **singular values** $\sigma_1, \sigma_2, \dots$

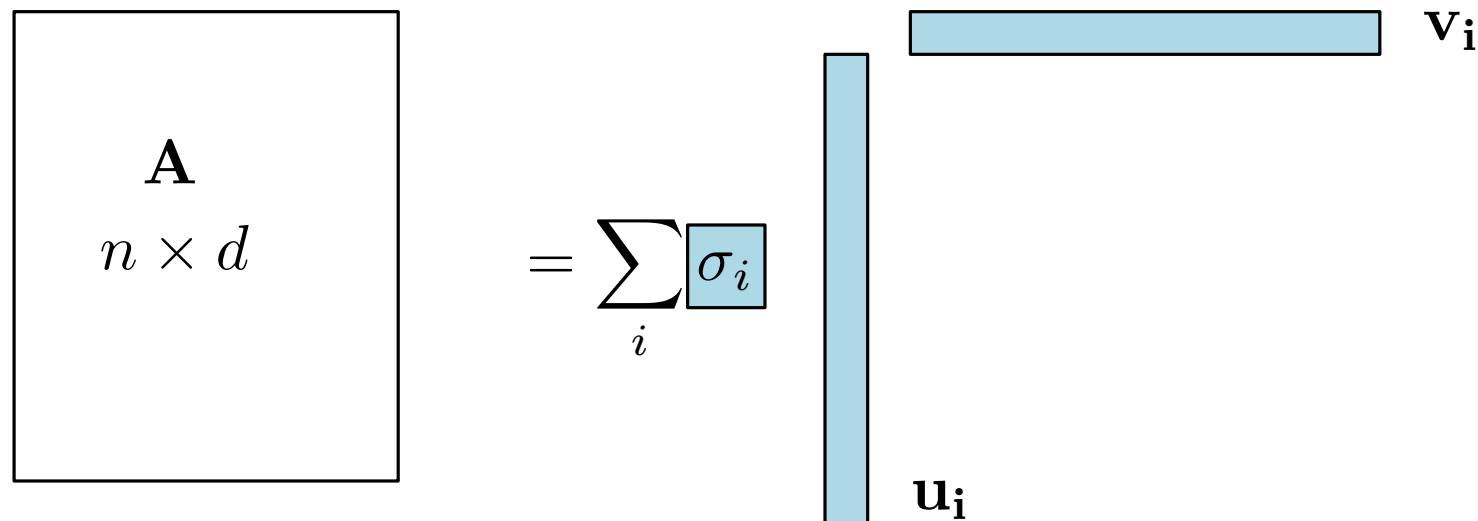
Singular Value Decomposition (SVD)

$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ can be rewritten using the sum of outer products

$$\mathbf{A} = \sum_i \sigma_i \mathbf{u}_i \mathbf{v}_i^T$$

where \mathbf{u}_i and \mathbf{v}_i are columns of \mathbf{U} and \mathbf{V}

The i^{th} term in the above sum can be viewed as giving the components of the rows of \mathbf{A} along \mathbf{v}_i



Power Method

The first principal component \mathbf{v}_1 can be computed using the **power method**:

$$\mathbf{B} = \mathbf{A}^T \mathbf{A} = \left(\sum_i \sigma_i \mathbf{u}_i \mathbf{v}_i^T \right) \left(\sum_j \sigma_j \mathbf{u}_j \mathbf{v}_j^T \right)$$

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orthogonal
for $i \neq j$

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orthogonal
for $i \neq j$

$$= \sum_i \sigma_i^2 \mathbf{v}_i \mathbf{v}_i^T$$

$$\mathbf{B}^2 = \sum_i \sum_j \sigma_i^2 \sigma_j^2 \mathbf{v}_i (\mathbf{v}_i^T \mathbf{v}_j) \mathbf{v}_j^T =$$

$$\mathbf{B}^k = \sum_i \sigma_i^{2k} \mathbf{v}_i \mathbf{v}_i^T \rightarrow \sigma_1^{2k} \mathbf{v}_1 \mathbf{v}_1^T$$

(using $\sigma_1 > \sigma_2$)

We can estimate \mathbf{v}_1 using the first column of \mathbf{B}^k normalized to unit length

Interpretation of principal components (again)

Example: handwritten digits

Assume we computed the first two principal components

We obtain an interpretable representation

$$\hat{f}(\lambda) = \mu + \mathbf{V}\lambda,$$

$$= \mu + \lambda_1 \mathbf{v}_1 + \lambda_2 \mathbf{v}_2$$

$$= \begin{array}{|c|} \hline \text{3} \\ \hline \end{array} + \lambda_1 \cdot \begin{array}{|c|} \hline \text{3} \\ \hline \end{array} + \lambda_2 \cdot \begin{array}{|c|} \hline \text{3} \\ \hline \end{array}$$

↑
mean

↑ ↑
principal components

An Alternative View

We can view \mathbf{a}_i as an observation of a multivariate distribution

\mathbf{A} contains n observations of d random variables X_1, X_2, \dots, X_d

The **covariance** of two variables X_i, X_j is defined as

$$\text{cov}(X_i, X_j) = \text{E}[(X_i - \mu_i)(X_j - \mu_j)]$$

with $\mu_i = \text{E}[X_i]$

The **sample covariance matrix** is defined as

$$\mathbf{M} = \frac{1}{n-1} \underbrace{\sum_{1 \leq i \leq n} (\mathbf{a}_i - \mu)^T (\mathbf{a}_i - \mu)}_{\mathbf{A}^T \mathbf{A}}$$

An Alternative View

A vector \mathbf{v} such that

$$B\mathbf{v} = \gamma \mathbf{v}$$

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An Alternative View

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The following holds true since $\mathbf{V}^T = \mathbf{V}^{-1}$

$$\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i \quad \text{and} \quad \mathbf{A}^T \mathbf{u}_i = \sigma_i \mathbf{v}_i$$

together this implies

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Therefore, the **singular vectors** of \mathbf{A} are the **eigenvectors** of the sample covariance matrix

Multidimensional scaling (Torgerson (1952))

Assume matrix \mathbf{A} is not available, but instead we are given all squared pairwise distances as $n \times n$ matrix Δ

$$\Delta_{ij} = \|\mathbf{a}_i - \mathbf{a}_j\|^2$$

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- \mathbf{I} denotes the $n \times n$ identity matrix
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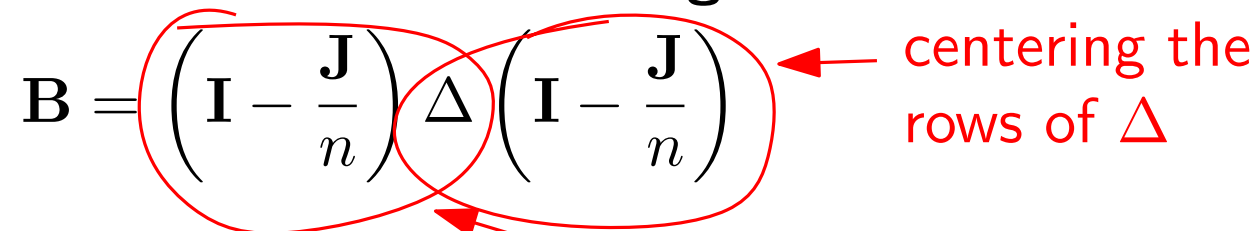
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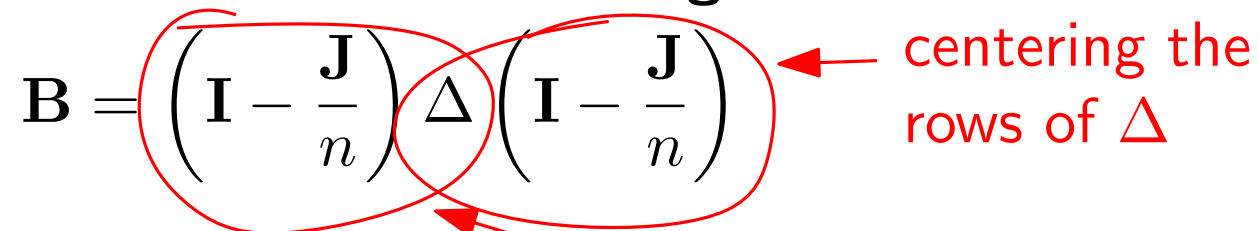
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If \mathbf{A} is mean-centered, one can show that $(-\frac{1}{2})\mathbf{B} = \mathbf{A}\mathbf{A}^T$

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Recall that from SVD we have

$$\mathbf{A}\mathbf{v}_i = \sigma_i \mathbf{u}_i \quad \text{and} \quad \mathbf{A}^T \mathbf{u}_i = \sigma_i \mathbf{v}_i$$

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The result is called an **embedding** of \mathbf{A} and the process is called classical multidimensional scaling (MDS).

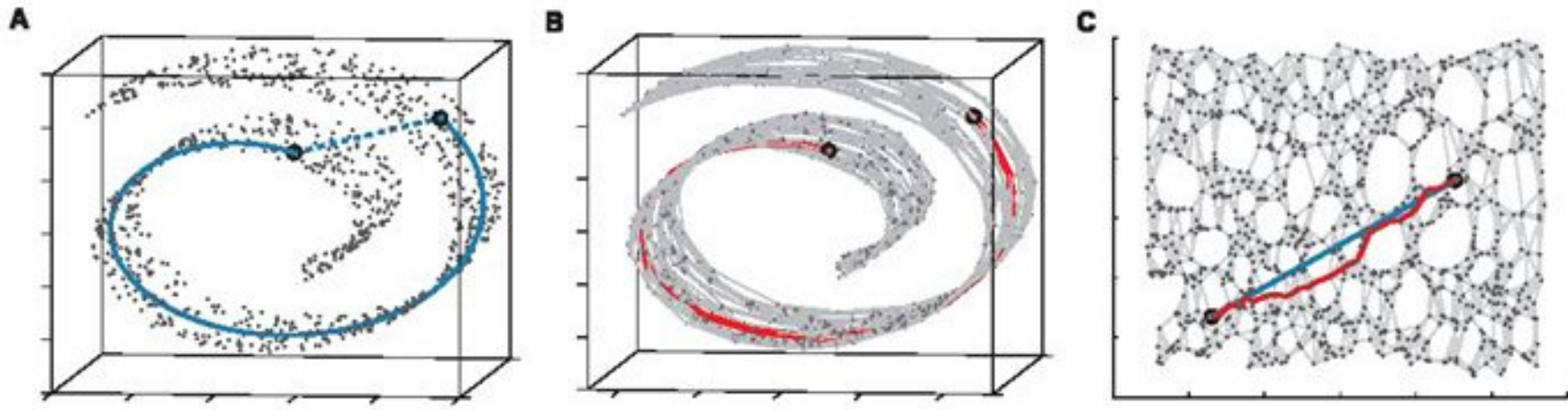
Isomap

Isomap is a non-linear embedding algorithm which assumes that the data lies on an Euclidean manifold

Isomap is due to Tenenbaum, Silva and Langford (2000)

Algorithm:

- Compute the k -nearest neighbor graph G
- Compute all pairwise shortest paths in G
- Use Multidimensional scaling on the obtained distances



Summary

- Principal Component Analysis (PCA)
- Interpretation of Principal Components
- Computing Principal Components
- Singular-Value Decomposition (SVD)
- Power Method
- Eigenvectors of the Sample Covariance Matrix
- Multidimensional scaling
- Isomap

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Foundations of Data Science
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Elements of Statistical Learning
- J. B. Tenenbaum, V. de Silva, J. C. Langford, "A Global Geometric Framework for Nonlinear Dimensionality Reduction", *Science* 290, (2000).