Metodi Numerici dell'Informatica

Singular Value Decomposition and Principal Component Analysis

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Motivation

Isometries

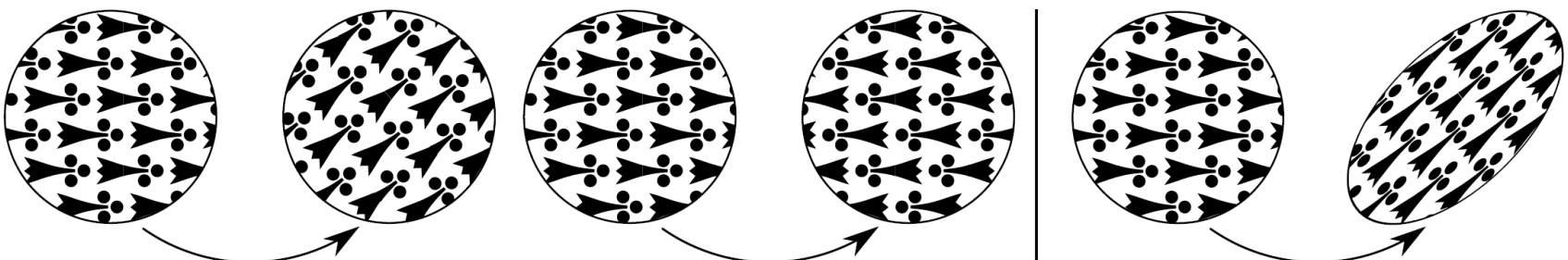
We have seen that orthogonal matrices preserve lengths:

$$\|\mathbf{Qx}\|_2^2 = \mathbf{x}^\top \mathbf{Q}^\top \mathbf{Qx} = \mathbf{x}^\top \mathbf{Ix} = \mathbf{x}^\top \mathbf{x} = \|\mathbf{x}\|_2^2$$

...and they also preserve angles (i.e. inner products):

$$\langle \mathbf{Qx}, \mathbf{Qy} \rangle = \mathbf{x}^\top \mathbf{Q}^\top \mathbf{Qy} = \mathbf{x}^\top \mathbf{Iy} = \mathbf{x}^\top \mathbf{y}$$

By these properties, the map $\mathbf{x} \mapsto \mathbf{Qx}$ is an isometry of $\mathbb{R}^n$.



(a) Isometric (b) Not isometric

General transformations

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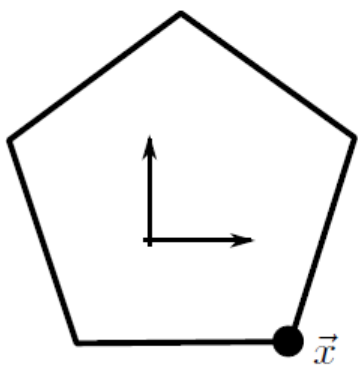

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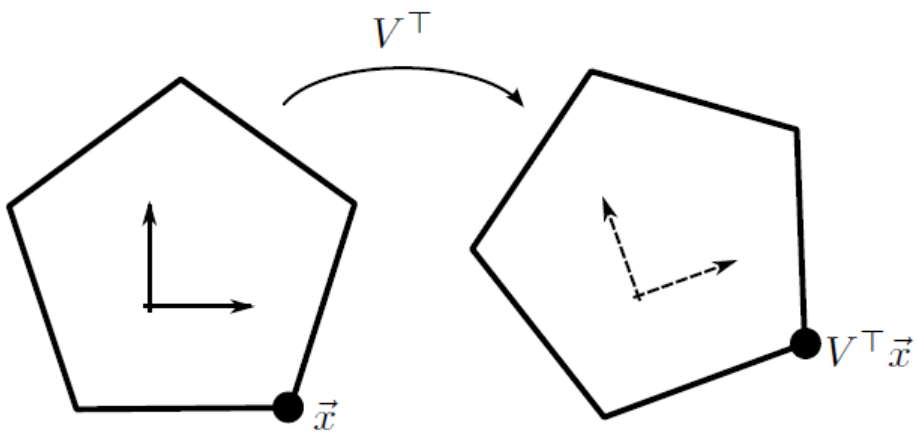

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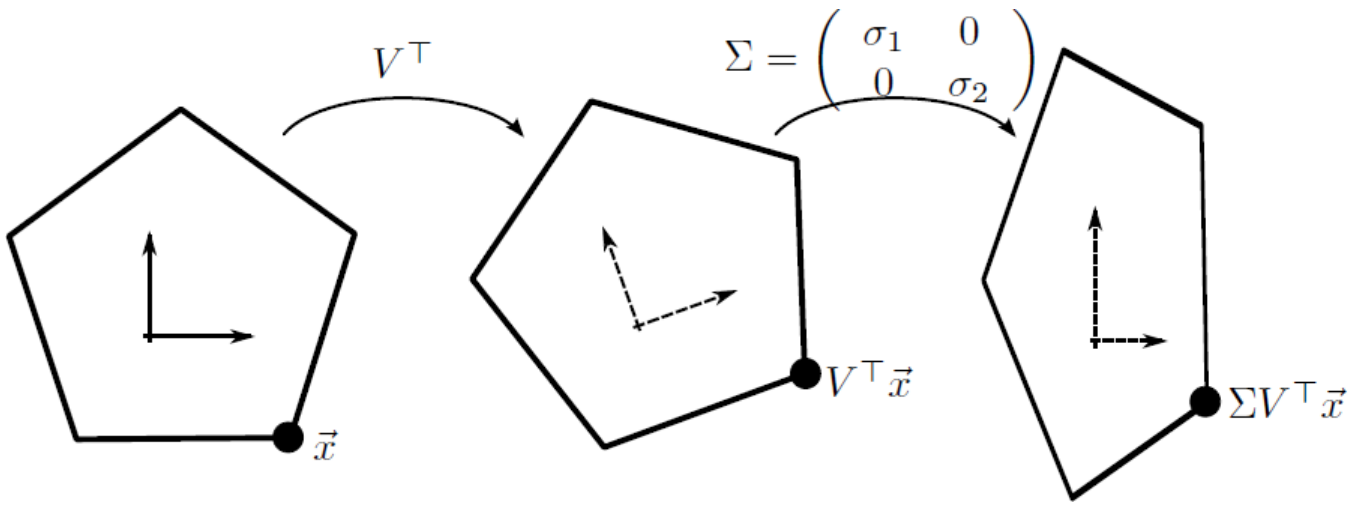

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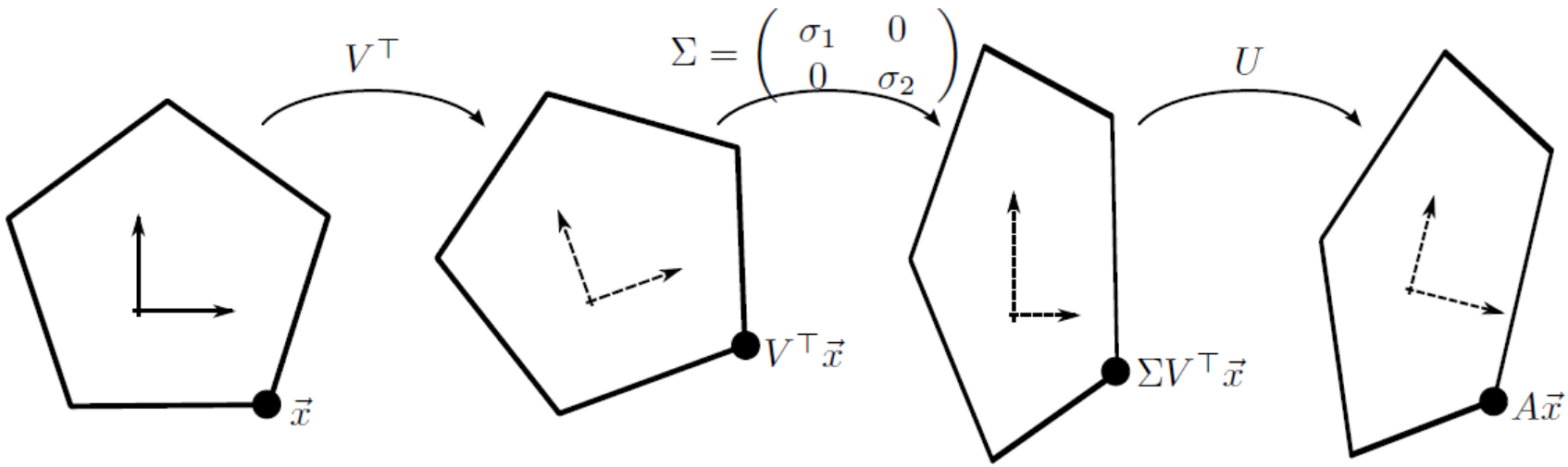

Singular Value Decomposition (SVD)

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The factorization

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$$

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which looks quite similar to the eigenvalue equation.

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Algorithms to compute the SVD are variants of those used for eigenvalues. We will not study them in detail.

Series of outer products

We can equivalently rewrite the decomposition $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top$ as

$$\mathbf{A} = \sum_{i=1}^{\ell} \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$$

where $\mathbf{u}_i$ and $\mathbf{v}_i$ are the i-th columns of $\mathbf{U}$ and $\mathbf{V}$.

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If we round small values of σ_i to zero, we are approximating $\mathbf{A}$ with fewer terms:

$$\mathbf{A} \approx \mathbf{U}\tilde{\mathbf{\Sigma}}\mathbf{V}^\top$$

where $\tilde{\mathbf{\Sigma}}$ has the small σ_i truncated to zero.

Low-rank approximations

Construct the matrix:

$$\tilde{\mathbf{A}} \equiv \mathbf{U}\tilde{\mathbf{\Sigma}}\mathbf{V}^\top$$

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The rank of a matrix is the dimension of its column space.

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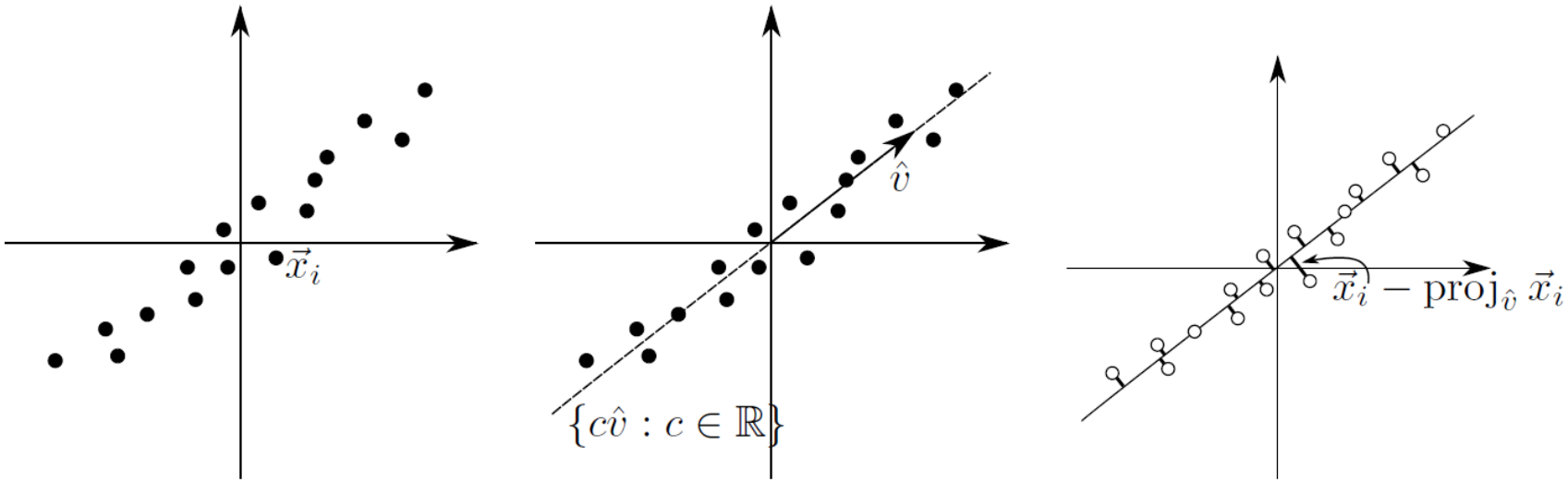
Low-rank approximations have numerous applications!

Principal Component Analysis (PCA)

Principal component

Consider the two-dimensional data in this plot:



(a) Input data (b) Principal axis (c) Projection error

Q: Find the vector $\mathbf{v}$ such that each data point $\mathbf{x}_i$ can be written as

$$\mathbf{x}_i = c_i \mathbf{v}$$

where each $\mathbf{x}_i$ has its own c_i

Another perspective

Let us be given n data points stored in matrix $\mathbf{X} \in \mathbb{R}^{d \times n}$:

$$\mathbf{X}^\top = \begin{pmatrix} — & \mathbf{x}_1^\top & — \\ & \vdots & \\ — & \mathbf{x}_n^\top & — \end{pmatrix}$$

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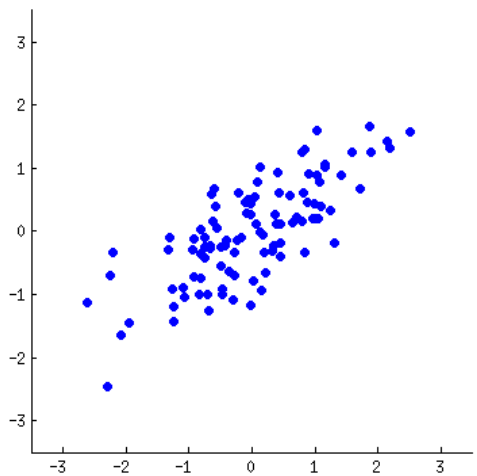

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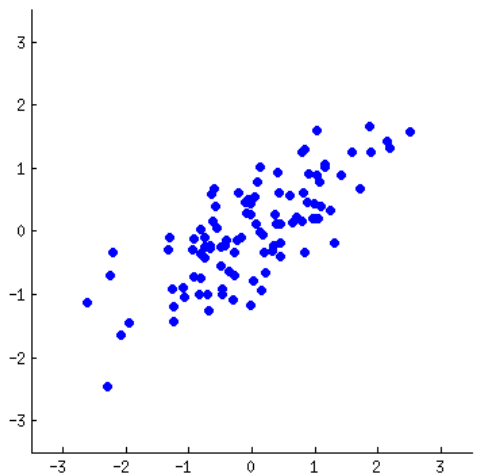
We want to replace them with a lower-dimensional approximation $\tilde{\mathbf{X}} \in \mathbb{R}^{k \times n}$, with $k \ll d$.



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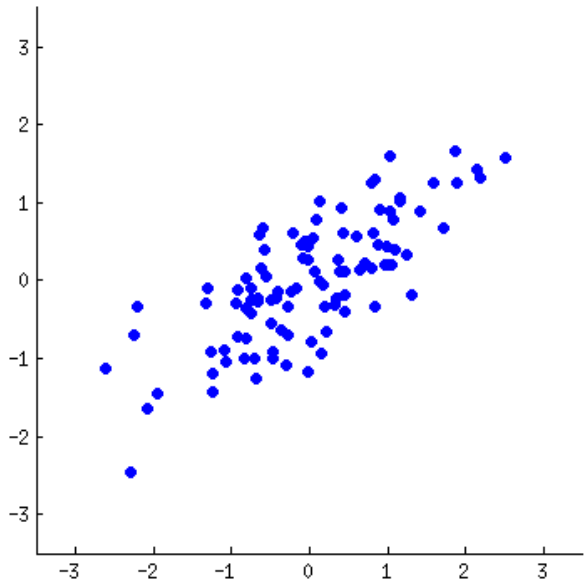
Regard our data as n points in $\mathbb{R}^d$:



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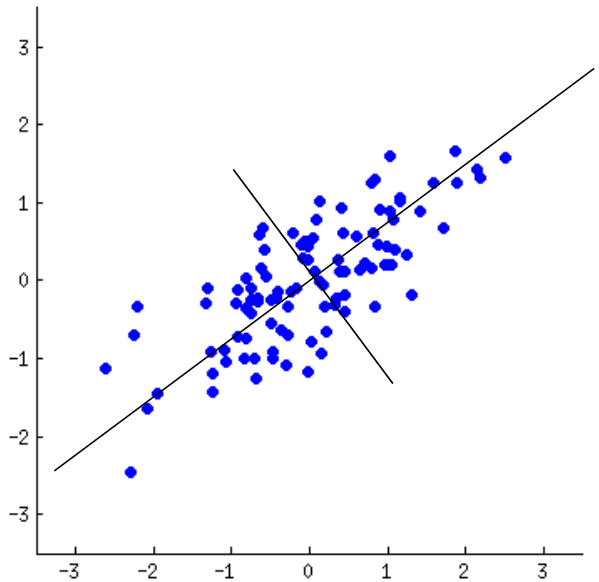

Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
  These span a k-dimensional subspace of the data.

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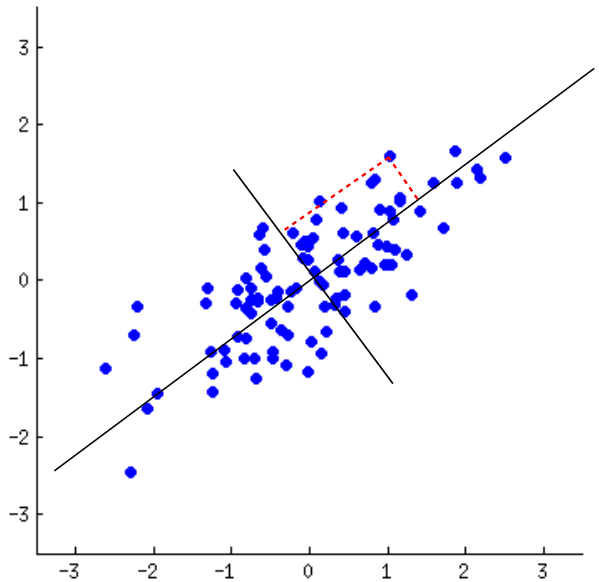

Overall idea:

- Find $k \leq d$ orthogonal directions with the most variance.
  These span a k-dimensional subspace of the data.
- Project all the data points onto these directions.
  This is lossy, but can be done with the smallest possible error.

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We seek the direction $\mathbf{w}$ that:

- Minimizes the projection/reconstruction error.
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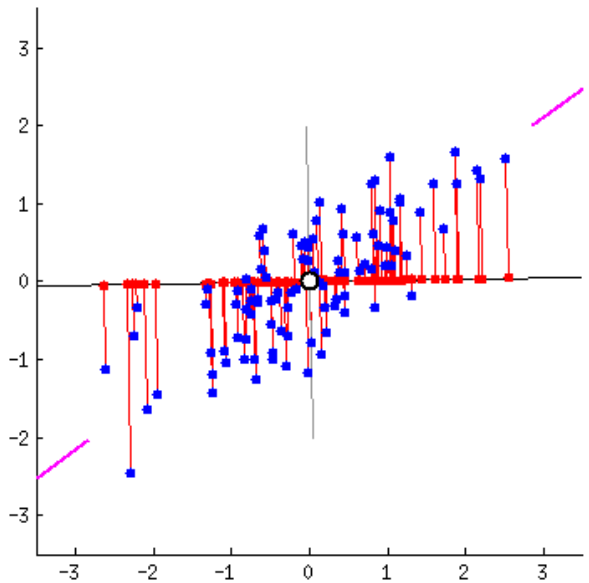

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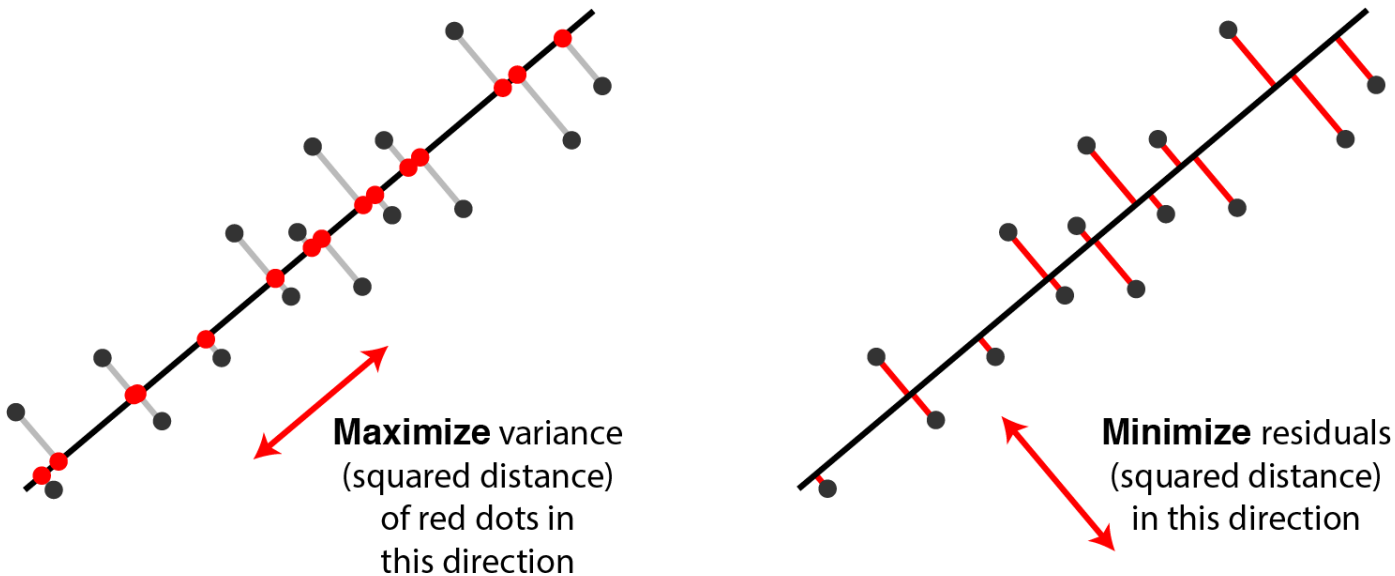

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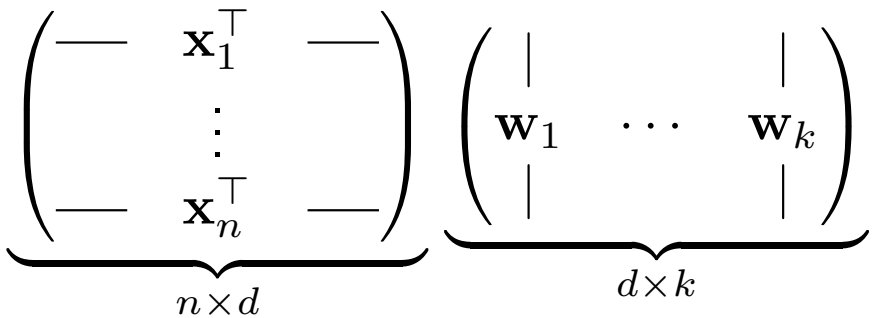

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Assuming $\mathbf{W}^\top \mathbf{W} = \mathbf{I}$, for $k = d$ we get:

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We call the columns of $\mathbf{W}$ principal components.

They are unknown and must be computed.

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where $\mathbf{C} \in \mathbb{R}^{d \times d}$ is the symmetric covariance matrix.

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The solution is $\mathbf{w} =$ principal eigenvector of $\mathbf{C}$ (Courant minmax principle), and the value $\mathbf{w}^\top \mathbf{C}\mathbf{w}$ is the corresponding eigenvalue.

Principal component analysis (PCA)

After solving the problem:

$$\mathbf{w}_1 = \arg\max_{\mathbf{w}} \mathbf{w}^\top \mathbf{C}\mathbf{w}$$
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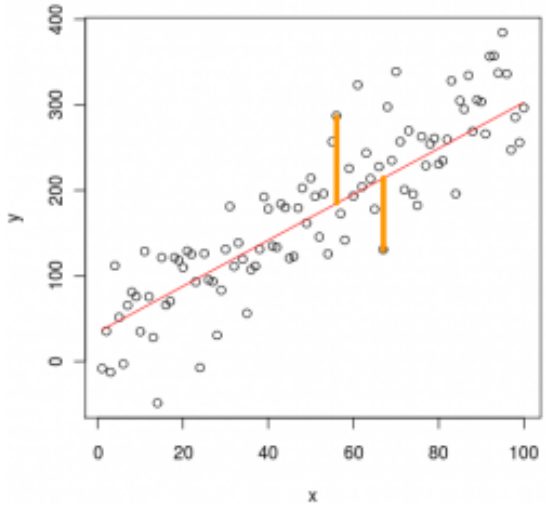
which is the second eigenvector of $\mathbf{C}$, and so on for all $\mathbf{w}_{i=2\ldots k}$.

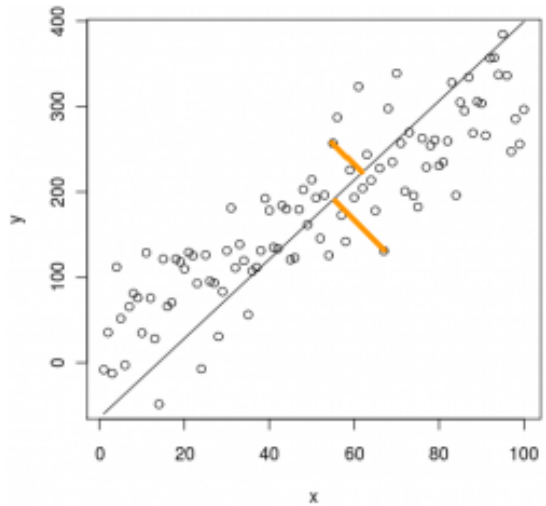
The principal components are thus the first $k \ll d$ eigenvectors of $\mathbf{C}$, sorted by decreasing eigenvalue.

PCA is not linear regression

With linear regression we measure the error along the y coordinate:



With PCA we measure the error orthogonal to the principal direction:



PCA as a generative model

Given the $\mathbf{W}$ satisfying, for the observations $\mathbf{X}$:

$$\mathbf{X}^\top \mathbf{W} = \mathbf{Z}^\top \quad \text{projection}$$
$$\mathbf{X} \approx \mathbf{W}\mathbf{Z} \quad \text{reconstruction}$$

We can generate new data just by sampling $\mathbf{z}_{\text{new}} \in \mathbb{R}^k$ and computing:

$$\mathbf{x}_{\text{new}} = \mathbf{W}\mathbf{z}_{\text{new}}$$

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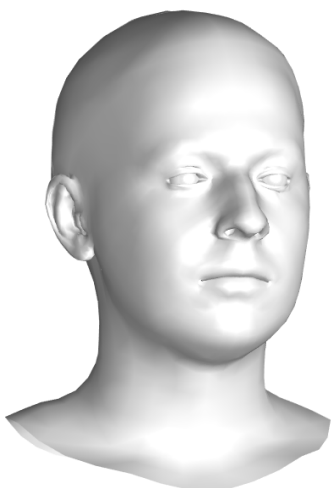
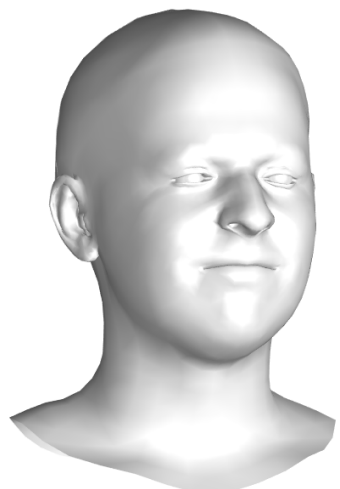
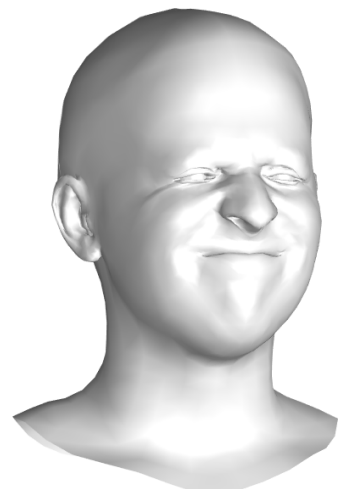
Example:



Data point $\mathbf{x}_1$



Generated
$\mathbf{x}_{\text{new}} = \frac{1}{2}\mathbf{W}(\mathbf{z}_1 + \mathbf{z}_2)$



Data point $\mathbf{x}_2$

Suggested reading

Read Sections 7.1, 7.2.2, 7.2.5 of the book:

J. Solomon, "Numerical Algorithms"