# Dimensionality Reduction with Principa Analysis



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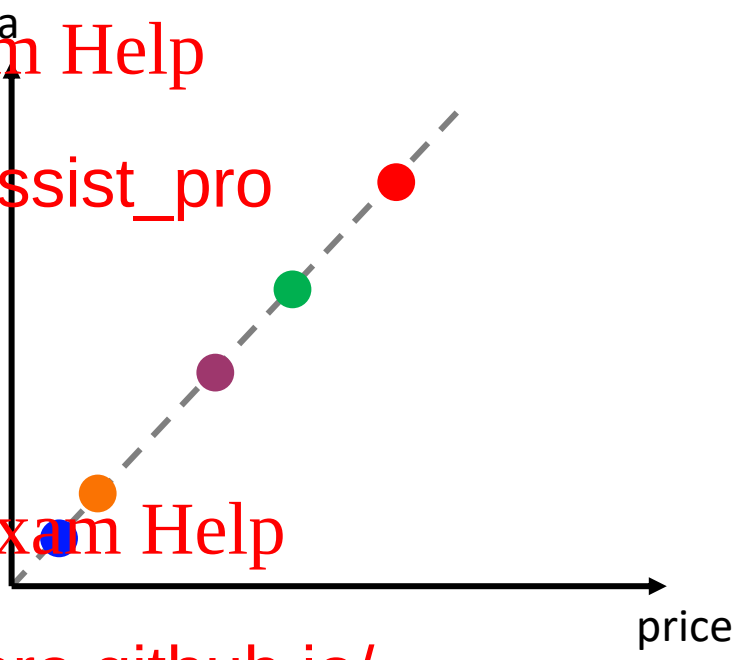
Meta Sim: Learning to Generate Synthetic Datasets. Kar et al., ICCV 2019

# Idea of PCA

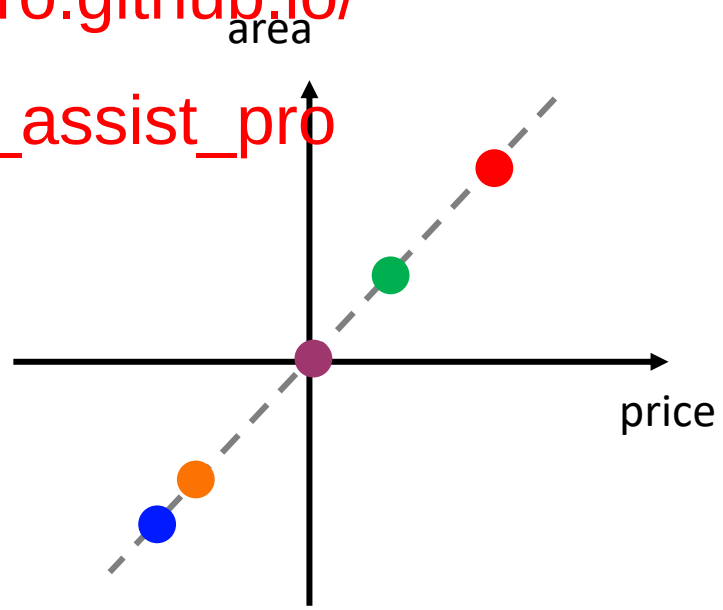


| | House price (million) | House area (100 |
|---|---|---|
| a | 10 | 10 |
| b | 2 | 2 |
| c | 7 | 7 |
| d | 1 | 1 |
| e | 5 | |



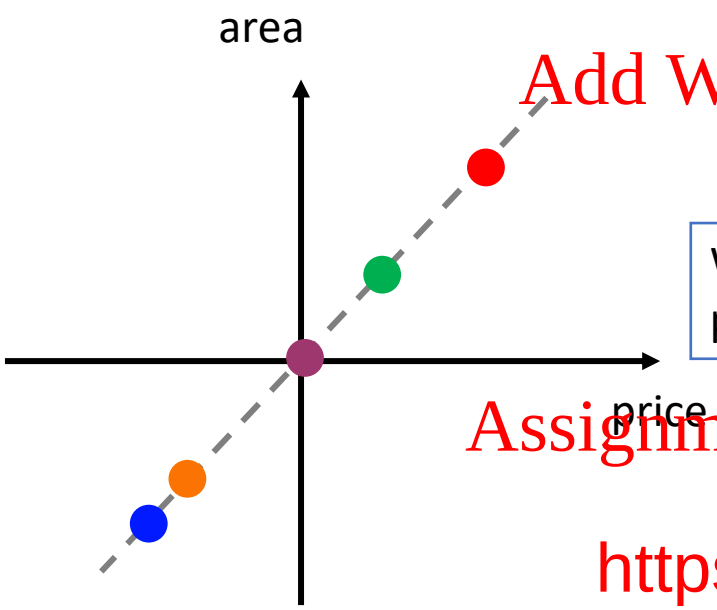

We subtract means from data points

| | House price (normalised) | House area (normalised) |
|---|---|---|
| a | 5 | 5 |
| b | -3 | -3 |
| c | 2 | 2 |
| d | -4 | -4 |
| e | 0 | 0 |

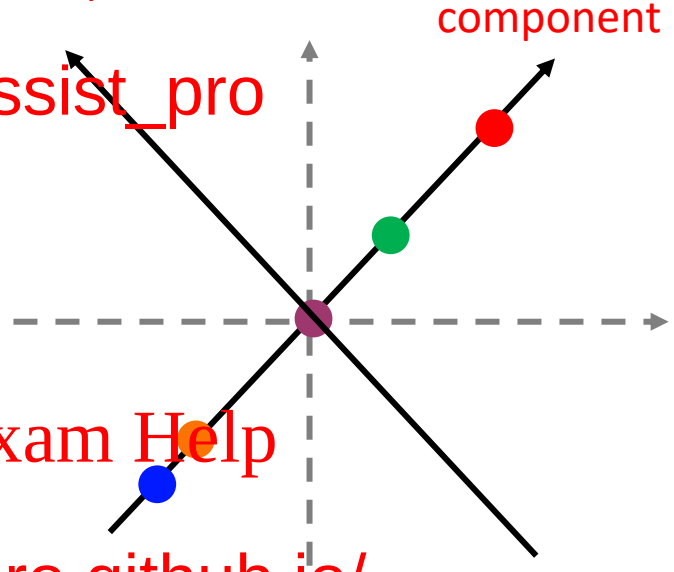


# Idea of PCA






We rotate our price and area axis






| | House price (normalised) | House area (normalised) |
|---|---|---|
| a | 5 | 5 |
| b | -3 | -3 |
| c | 2 | 2 |
| d | -4 | -4 |
| e | 0 | 0 |

| | ncipal ent | Second principal component |
|---|---|---|
| a | 7.07 | 0 |
| b | -4.24 | 0 |
| c | 2.82 | 0 |
| d | -5.66 | 0 |
| e | 0 | 0 |

# Motivation



- High-dimensional data, such as ima e analyze, interpretate, and visualize, and expensive to store.
- Good news
- high-dimensional data is often overcomplete, i.e., many dimensions are redundant and can be explained by a combination of other dimensions



- Furthermore, dimensions in high-dimensional data are often correlated so that the data possesse nal structure.





e data in (a) does not vary uch in the $x_2$-direction, so at we can express it as if it were on a line – with nearly no loss; see (b).

To describe the data in (b), only the $x_2$ -coordinate is required, and the data lies in a one-dimensional subspace of $\mathbb{R}^2$

# 10.1 Problem Setting



- In PCA, we are interested in finding $M$ of data points $\boldsymbol{x}_n$ that are as similar to the original data p ssible, but which have a significantly lower intrinsic dimensionality
- We consider an i.i.d. dataset $\boldsymbol{\mathcal{X}} = \{\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N\}, \boldsymbol{x}_n \in \mathbb{R}^D$, with mean $\boldsymbol{0}$ that possesses the data covariance matrix



$$\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^T$$



- We assume there exist ssed representation (code)

$$\boldsymbol{z}_n = \boldsymbol{B}\ \boldsymbol{x}_n$$



of $\boldsymbol{x}_n$, where we define the projection ma

$$\boldsymbol{B} := [\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M] \in \mathbb{R}^{D \times M}$$

- **Example (Coordinate Representati**



- Consider $\mathbb{R}^2$ with the canonical basis $\boldsymbol{e}_1 = [1,0]^{\mathrm{T}}$, $\boldsymbol{e}_2 = [0,1]^{\mathrm{T}}$.
- $\boldsymbol{x} \in \mathbb{R}^2$ can be represented as a linear combination of these basis vectors, e.g.,

$$\begin{bmatrix} 5 \\ 3 \end{bmatrix} = 5\boldsymbol{e}_1 + 3\boldsymbol{e}_2$$

- However, when we consider vectors of the form



$$\begin{bmatrix} 0 \\ \end{bmatrix}$$



they can always be writ $1 \quad 2$



- To represent these vectors it is sufficien ordinate/code $z$ of $\tilde{\boldsymbol{x}}$ with respect to the $\boldsymbol{e}_2$ vector.

# 10.2 PCA from Maximum Variance Perspective



- We ignore $x_2$ -coordinate of the data because it did not add too much information: the compressed data (b) is similar to the original data in (a)
- We derive PCA so as to maximize the variance in the low-dimensional representation of the data to retain as much information as possible
- Retaining most information after data compression is equivalent to capturing the largest amount of variance in the low-dimensional code (Hotelling, 1933)

# 10.2.1 Direction with Maximal Variance



- Data centering
- In the data covariance matrix, we assume centered data.

$$\boldsymbol{S} = \frac{1}{N}\sum_{n=1}^{N} \boldsymbol{x}_n \boldsymbol{x}_n^{\mathrm{T}}$$



- Let us assume that $\boldsymbol{\mu}$ sing the properties of the variance, we obtain



$$\mathbb{V}_{\boldsymbol{z}}[\boldsymbol{z}] = \mathbb{V}_{\boldsymbol{x}}[\quad(\quad)] \quad {}_{\boldsymbol{x}}[\quad] = \mathbb{V}_{\boldsymbol{x}}[\boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}]$$



- That is, the variance of the low-dimensio s not depend on the mean of the data.
- With this assumption the mean of the low-dimensional code is also $\mathbf{0}$ since

$$\mathbb{E}_{\boldsymbol{z}}[\boldsymbol{z}] = \mathbb{E}_{\boldsymbol{x}}[\boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}] = \boldsymbol{B}^{\mathrm{T}}\mathbb{E}_{\boldsymbol{x}}[\boldsymbol{x}] = \mathbf{0}$$

- To maximize the variance of the low-dimensional code, we first seek a single vector $\boldsymbol{b}_1 \in \mathbb{R}^D$ that maximizes the variance of the projected data, i.e., we aim to maximize the variance of the first coordinate $z_1$ of $\boldsymbol{z} \in \mathbb{R}^M$ so that



$$V_1 := \mathbb{V}[z_1] = \frac{1}{N}\sum_{n=1}^{N} z_{1n}^2$$

is maximized, where we defined $z_{1n}$ as the first coordinate of the low-dimensional representation $\boldsymbol{z}_n \in \mathbb{R}^M$ of $\boldsymbol{x}_n \in \mathbb{R}^D$. $z_{1n}$ is given by,



$$z_{1n} = \boldsymbol{b}_1^{\mathrm{T}}\boldsymbol{x}_n$$



i.e., it is the coordinate of $\boldsymbol{x}_n$ onto the one-dimensional subspace spanned by $\boldsymbol{b}_1$. We can substitute $z_{1n}$ into $V_1$ and obtain,



$$V_1 = \frac{1}{N}\sum_{n=1}^{N}(\boldsymbol{b}_1^{\mathrm{T}}\boldsymbol{x}_n)^2 = \frac{1}{N}\sum_{n=1}^{N}\boldsymbol{b}_1^{\mathrm{T}}\boldsymbol{x}_n\boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{b}_1$$

$$= \boldsymbol{b}_1^{\mathrm{T}}\left(\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{x}_n\boldsymbol{x}_n^{\mathrm{T}}\right)\boldsymbol{b}_1 = \boldsymbol{b}_1^{\mathrm{T}}\boldsymbol{S}\boldsymbol{b}_1$$

where $\boldsymbol{S}$ is the data covariance matrix.

- We further restrict all solutions to $\|\boldsymbol{b}_1\|^2 = 1$

- We have the following constrained optimization problem

$$\max_{\boldsymbol{b}_1} \quad \text{subject t} \quad \|\ _1\|$$



- We obtain the Lagrangian (not required in this course),

$$\mathfrak{L}(\boldsymbol{b}_1, \lambda) = \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{S} \boldsymbol{b}_1 + \lambda_1 \left(1 - \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{b}_1\right)$$

- The partial derivatives of $\mathfrak{L}$ with respect to $\boldsymbol{b}_1$ and $\lambda_1$ are



$$\frac{\partial \mathfrak{L}}{\partial \boldsymbol{b}_1} = 2\boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{S} - 2\lambda_1 \boldsymbol{b}_1^{\mathrm{T}}, \qquad \frac{\partial \mathfrak{L}}{\partial \lambda_1} = 1 - \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{b}_1$$

- Setting these partial deriv



s

$$\boldsymbol{S}\boldsymbol{b}_1 = \lambda_1$$

$$\boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{b}_1 =$$



- We see that $\boldsymbol{b}_1$ is an eigenvector of $\boldsymbol{S}$, and $\lambda_1$ is the corresponding eigenvalue. We rewrite our objective as,

$$V_1 = \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{S} \boldsymbol{b}_1 = \lambda_1 \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{b}_1 = \lambda_1$$

- i.e., the variance of the data projected onto a one-dimensional subspace equals the eigenvalue that is associated with the basis vector $\boldsymbol{b}_1$ that spans this subspace.
- To maximize the variance of the low-dimensional code, we choose the basis vector associated with the largest eigenvalue of the data covariance matrix. This eigenvector is called the first principal component.

# 10.2.2 $M$-dimensional Subspace with Maximal Variance



- Assume we have found the $m-1$ eigenvectors of $S$ that are associated with the largest $m-1$ eigenvalues.
- We want to find the $m$th principal component.
- We subtract the effect of the first $m-1$ principal components $\boldsymbol{b}_1 \cdots, \boldsymbol{b}_{m-1}$ from the data, and find principal components that compress the remaining information. We then arrive at the new data matrix,



$$\widehat{\boldsymbol{X}} \quad \text{https://eduassistpro.github.io/} \quad \boldsymbol{X}$$

where $\boldsymbol{X} = [\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N] \in \mathbb{R}^{D \times N}$ contain nts as column vectors and $\boldsymbol{B}_{m-1} := \sum_{i=1}^{m-1} \boldsymbol{b}_i \boldsymbol{b}_i^{\mathrm{T}}$ is a projection ma cts onto the subspace spanned by $\boldsymbol{b}_1, \cdots, \boldsymbol{b}_{m-1}$.



- To find the $m$th principal component, we maximize the variance

$$V_m = \mathbb{V}[z_m] = \frac{1}{N}\sum_{n=1}^{N} z_{mn}^2 = \frac{1}{N}\sum_{n=1}^{N} (\boldsymbol{b}_m^{\mathrm{T}} \widehat{\boldsymbol{x}_n})^2 = \boldsymbol{b}_m^{\mathrm{T}} \widehat{\boldsymbol{S}} \boldsymbol{b}_m$$

subject to $\|\boldsymbol{b}_m\|^2 = 1$, and we define $\widehat{\boldsymbol{S}}$ as the data covariance matrix of the transformed dataset $\widehat{\boldsymbol{X}} := \{\widehat{\boldsymbol{x}}_1, \cdots, \widehat{\boldsymbol{x}}_N\}$.

- The optimal solution $\boldsymbol{b}_m$ is the eigenvector of $\widehat{\boldsymbol{S}}$ that is associated with the largest eigenvalue of $\widehat{\boldsymbol{S}}$.



- In fact, we can derive that

$$\widehat{\boldsymbol{S}}\boldsymbol{b}_m = \boldsymbol{S}\boldsymbol{b}_m = \lambda_m \boldsymbol{b}_m \quad (1)$$

- $\boldsymbol{b}_m$ is not only an eigenvector of $\boldsymbol{S}$ but also of $\widehat{\boldsymbol{S}}$ .



- Specifically, $\lambda_m$ is the largest eigenvalue of and is the $m$th largest eigenvalue of $\boldsymbol{S}$, and both have the associated eigenvector $\boldsymbol{b}_m$.



- Moreover, $\boldsymbol{b}_1, \cdots, \boldsymbol{b}_{m-1}$ ut they are associated with eigenvalue $0$.



- Considering (1) and, $\boldsymbol{b}_m^{\mathrm{T}}\boldsymbol{b}_m = 1$, the vari ata projected onto the $m$th principal component is

$$V_m = \boldsymbol{b}_m^{\mathrm{T}}\boldsymbol{S}\boldsymbol{b}_m = \lambda_m \boldsymbol{b}_m^{\mathrm{T}}\boldsymbol{b}_m = \lambda_m$$

- This means that the variance of the data, when projected onto an $M$-dimensional subspace, equals the sum of the eigenvalues that are associated with the corresponding eigenvectors of the data covariance matrix.

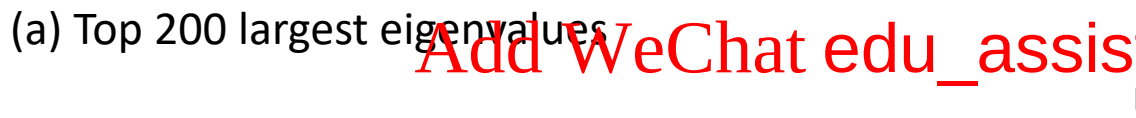
# MNIST dataset



- 60,000 examples of handwritten digit .
- Each digit is a grayscale image of size 28×28, i.e., it contains 784 pixels.
- We can interpret every image in this dataset as a vector $x \in \mathbb{R}^{784}$

# Example - Eigenvalues of MNIST digit “8”





(a) Top 200 largest eigenvalues

aptured by the
mponents.

- A $784$-dim vector is used to represent an image
- Taking all images of “8” in MNIST, we compute the eigenvalues of the data covariance matrix.
- We see that only a few of them have a value that differs significantly from $0$.
- Most of the variance, when projecting data onto the subspace spanned by the corresponding eigenvectors, is captured by only a few principal components

# Overall



- To find an $M$-dimensional subspace of $\mathbb{R}$ that retains as much information as possible,
- We choose the columns of $\boldsymbol{B} = [\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M] \in \mathbb{R}^{D \times M}$ as the $M$ eigenvectors of the data covariance matrix $\boldsymbol{S}$ that are associated with the $M$ largest eigenvalues.



- The maximum amount e with the first $M$ principal components is



$$V_M = \sum_{m=}$$



where the $\lambda_m$ are the $M$ largest eigenvalues of the data covariance matrix $\boldsymbol{S}$.

- The variance lost by data compression via PCA is

$$J_M = \sum_{j=M+1}^{D} \lambda_j = V_D - V_M$$

- Instead of these absolute quantities, we can define the relative variance captured as $\frac{V_M}{V_D}$, and the relative variance lost by compression as $1 - \frac{V_M}{V_D}$ .

# 10.3 PCA from Projection Perspective



- Previously, we derived PCA by maximizing the variance in the projected space to retain as much information as possible

$$\max_{\boldsymbol{b_1}} \boldsymbol{b}_1^{\mathrm{T}} \boldsymbol{S} \boldsymbol{b}_1$$

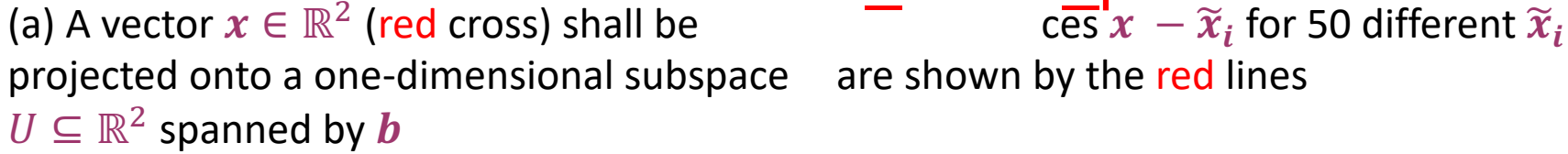
$$\text{subject to } \|\boldsymbol{b}_1\|^2 = 1$$



- Alternatively, we derive PCA as an algorithm that directly minimizes the average reconstruction

# 10.3.1 Setting and Objective





(a) A vector $\boldsymbol{x} \in \mathbb{R}^2$ (red cross) shall be projected onto a one-dimensional subspace $U \subseteq \mathbb{R}^2$ spanned by $\boldsymbol{b}$

ces $\boldsymbol{x} - \tilde{\boldsymbol{x}}_i$ for 50 different $\tilde{\boldsymbol{x}}_i$ are shown by the red lines

- We wish to project $\boldsymbol{x}$ to $\tilde{\boldsymbol{x}}$ in a lower-dimensional space, such that $\tilde{\boldsymbol{x}}$ is similar to the original data point $\boldsymbol{x}$. That is,
- We aim to minimize the (Euclidean) distance $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|$

- Given an orthonormal basis $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_D)$ of $\mathbb{R}^D$, any $\boldsymbol{x} \in \mathbb{R}^D$ can be written as a linear combination of the basis vectors of $\mathbb{R}^D$:

$$\boldsymbol{x} = \sum_{d=1}^{D} \zeta_d \, \boldsymbol{b}_d = \sum_{m=1}^{M} \zeta_m \, \boldsymbol{b}_m + \sum_{j=M+1}^{D} \zeta_j \, \boldsymbol{b}_j$$



for suitable coordinates

- We aim to find vectors  nsionally lower-dimensional subspace $U \subseteq \mathbb{R}^D$, $\dim(U) = M$, so that



$$\tilde{\boldsymbol{x}} = \sum_{m=1}^{M} z_m \, \boldsymbol{b}_m$$

is as similar to $\boldsymbol{x}$ as possible.

- We have a dataset $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, $\boldsymbol{x}_N \in \mathbb{R}^D$ centered at $\mathbf{0}$, i.e., $\mathbb{E}[\mathcal{X}] = \mathbf{0}$.
- We want to find the best linear projec c a lower dimensional subspace $U \subseteq \mathbb{R}^D$, $\dim(U) = M$. Also, ormal basis vectors $\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M$.
- We call this subspace $U$ the principal subspace.
- The projections of the data points are denoted by $\tilde{\boldsymbol{x}}_n \in \mathbb{R}^D$.







where $\boldsymbol{z}_n := [z_{1n}, \cdots, z_{Mn}] \in \mathbb{R}$ is the c tor of $\tilde{\boldsymbol{x}}_n$ with respect to the basis $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M)$.



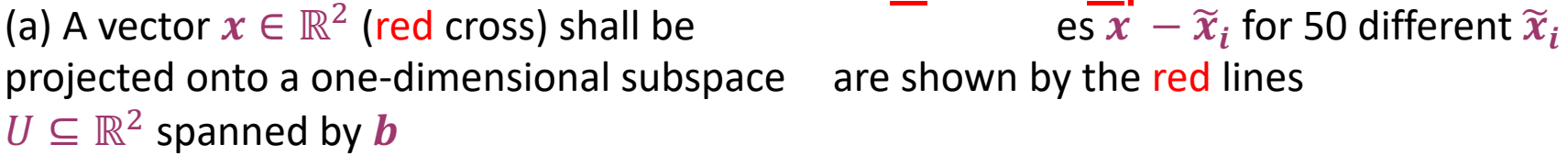
- We want to have $\tilde{\boldsymbol{x}}_n$ as similar to $\boldsymbol{x}_n$ as possible.
- We define our objective as minimizing the average squared Euclidean distance (reconstruction error)

$$J_M := \frac{1}{N}\sum_{n=1}^{N} \|\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n\|^2$$

- We need to find the orthonormal basis of the principal subspace and the coordinates $z_n \in \mathbb{R}^M$ of the projections with respect to this basis.

# 10.3.2 Finding Optimal Coordinates






- We want to find $\tilde{\boldsymbol{x}}$ in a subspace spanned by $\boldsymbol{b}$ that minimizes $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|$.
- Apparently, this will be the orthogonal projection

$$J_M := \frac{1}{N}\sum_{n=1}^{N} \|\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n\|^2$$

- Given an ONB $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M)$ of $U \subseteq \mathbb{R}^D$, to find the optimal coordinates $\boldsymbol{z}_m$ with respect to this basis, we calculate the partial derivatives

$$\frac{\partial J_M}{\partial z_{in}} = \frac{\partial J_M}{\partial \tilde{\boldsymbol{x}}_n} \frac{\partial \tilde{\boldsymbol{x}}_n}{\partial z_{in}}$$

$$\frac{\partial J_M}{\partial \tilde{\boldsymbol{x}}_n} = -\frac{2}{N}(\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n)^{\mathrm{T}} \in \mathbb{R}^{1\times D}$$

$$\tilde{\boldsymbol{x}}_n := \sum_{m=1}^{M} z_{mn}\boldsymbol{b}_m = \boldsymbol{B}\boldsymbol{z}_n \in \mathbb{R}^D$$



$$\frac{\partial}{\partial z_{in}}\left(\sum_{m=1}^{M} z_{mn}\boldsymbol{b}_m\right) = \boldsymbol{b}_i$$

for $i = 1, \cdots, M$, such that we obtain

$$\frac{\partial J_M}{\partial z_{in}} = -\frac{2}{N}(\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n)^{\mathrm{T}}\boldsymbol{b}_i = -\frac{2}{N}\left(\boldsymbol{x}_n - \sum_{m=1}^{M} z_{mn}\boldsymbol{b}_m\right)^{\mathrm{T}}\boldsymbol{b}_i$$

$$\overset{\text{ONB}}{=} -\frac{2}{N}\left(\boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{b}_i - z_{in}\boldsymbol{b}_i^{\mathrm{T}}\boldsymbol{b}_i\right) = -\frac{2}{N}(\boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{b}_i - z_{in})$$

$$\frac{\partial J_M}{\partial z_{in}} = -\frac{2}{N}$$

- Setting this partial derivative to 0 yields immediately the optimal coordinates

$$z_{in} = \boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{b}_i = \boldsymbol{b}_i^{\mathrm{T}} \boldsymbol{x}_n$$

for $i = 1, \cdots, M$, and $n = 1, \cdots, N$.



- The optimal coordinates $z_{in}$ of the projection $\tilde{\boldsymbol{x}}_n$ are the coordinates of the orthogonal projection o nto the one-dimensional subspace that is spann



- The optimal linear projection $\tilde{\boldsymbol{x}}_n$ of $\boldsymbol{x}_n$ is l projection.



- The coordinates of $\tilde{\boldsymbol{x}}_n$ with respect to th $_1$ $, \boldsymbol{b}_M)$ are the coordinates of the orthogonal projection of $\boldsymbol{x}_n$ onto the principal subspace.

(a) A vector $\boldsymbol{x} \in \mathbb{R}^2$ (re

nces $\boldsymbol{x} - \tilde{\boldsymbol{x}}_i$ for 50 different $\tilde{\boldsymbol{x}}_i$

projected onto a one-d

by the red lines

$U \subseteq \mathbb{R}^2$ spanned by $\boldsymbol{b}$

(c) Distances $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|$ for some $\tilde{\boldsymbol{x}} = z_1\boldsymbol{b} \in U = \text{span}[\boldsymbol{b}]$

(d) The vector $\tilde{\boldsymbol{x}}$ that minimizes $\|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|$ is the orthogonal projection of $\boldsymbol{x}$ onto $U$.

- We briefly recap orthogonal projections 3.8 (Analytic geometry).



- If $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_D)$ is an orthonormal basis o

$$\tilde{\boldsymbol{x}} = \frac{\boldsymbol{b}_j^{\mathrm{T}} \boldsymbol{x}}{\|\boldsymbol{b}_j\|^2} \boldsymbol{b}_j = \boldsymbol{b}_j \boldsymbol{b}_j^{\mathrm{T}} \boldsymbol{x} \in \mathbb{R}^D$$

is the orthogonal projection of $\boldsymbol{x}$ onto the subspace spanned by the $j$th basis vector, and $z_j = \boldsymbol{b}_j^{\mathrm{T}} \boldsymbol{x}$ is the coordinate of this projection with respect to the basis vector $\boldsymbol{b}_j$ that spans that subspace since $z_j \boldsymbol{b}_j = \tilde{\boldsymbol{x}}$.





- More generally, if we aim to project onto a al subspace of $\mathbb{R}^D$, we obtain the orthogonal projection of onto t onal subspace with orthonormal basis vectors $\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M$ as



$$\tilde{\boldsymbol{x}} = \boldsymbol{B} \underbrace{\left(\boldsymbol{B}^{\mathrm{T}} \boldsymbol{B}\right)^{-1}}_{=\boldsymbol{I}} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{x} = \boldsymbol{B} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{x}$$

where we defined $\boldsymbol{B} := [\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M] \in \mathbb{R}^{D \times M}$ . The coordinates of this projection with respect to the ordered basis $(\boldsymbol{b}_1, \cdots, \boldsymbol{b}_M)$ are $\boldsymbol{z} := \boldsymbol{B}^{\mathrm{T}} \boldsymbol{x}$

- Although $\tilde{\boldsymbol{x}} \in \mathbb{R}^D$, we only need $M$ coordinates to represent $\tilde{\boldsymbol{x}}$. The other $D - M$ coordinates with respect to the basis vectors $(\boldsymbol{b}_{M+1}, \cdots, \boldsymbol{b}_D)$ are always 0

# 10.3.3 Finding the Basis of the Principal Subspace

- So far we have shown that for a given ONB optimal coordinates of $\tilde{\boldsymbol{x}}$ by an orthogonal projection onto the principal sub llowing, we will determine what the best basis is.
- Recall the optimal coordinates of $\tilde{\boldsymbol{x}}$ given ONB is

$$z_{in} = \boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{b}_i = \boldsymbol{b}_i^{\mathrm{T}} \boldsymbol{x}_n$$

- We have



$$\tilde{\boldsymbol{x}}_n = \sum_{m=1}^{M} z_{mn} \boldsymbol{b}_m = \sum_{m=1}^{M} (\boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{b}_m) \boldsymbol{b}_m$$



- We now exploit the symme s

$$\tilde{\boldsymbol{x}}_n = \sum_{m=1}^{M} (\boldsymbol{b}_m^{\mathrm{T}} \boldsymbol{x}_n) \boldsymbol{b}_m = \sum_{m=1}^{M} \boldsymbol{b}_m (\boldsymbol{b}_m^{\mathrm{T}} \boldsymbol{x}_n) = \left( \sum_{m=1}^{M} \boldsymbol{b}_m \boldsymbol{b}_m^{\mathrm{T}} \right) \boldsymbol{x}_n$$



- Since we can generally write the original data point $\boldsymbol{x}_n$ as a linear combination of all basis vectors, it holds that

$$\boldsymbol{x}_n = \sum_{d=1}^{D} z_{dn} \boldsymbol{b}_d = \sum_{d=1}^{D} (\boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{b}_d) \boldsymbol{b}_d = \left( \sum_{d=1}^{D} \boldsymbol{b}_d \boldsymbol{b}_d^{\mathrm{T}} \right) \boldsymbol{x}_n$$

$$= \left( \sum_{m=1}^{M} \boldsymbol{b}_m \boldsymbol{b}_m^{\mathrm{T}} \right) \boldsymbol{x}_n + \left( \sum_{j=M+1}^{D} \boldsymbol{b}_j \boldsymbol{b}_j^{\mathrm{T}} \right) \boldsymbol{x}_n$$

where we split the sum with $D$ terms into a sum over $M$ and a sum over $D - M$ terms.

- With these results, the displacement $\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n$, i.e., the difference vector between the original data point and its projection is



$$\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n = \left( \sum_{j=M+1}^{D} \boldsymbol{b}_j \boldsymbol{b}_j^{\mathrm{T}} \right) \boldsymbol{x}_n = \sum_{j=M+1}^{D} \left( \boldsymbol{x}_n^{\mathrm{T}} \boldsymbol{b}_j \right) \boldsymbol{b}_j$$

- The displacement vector $\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n$ is exactly the projection of the data point onto the orthogonal complement of the principal subspace.

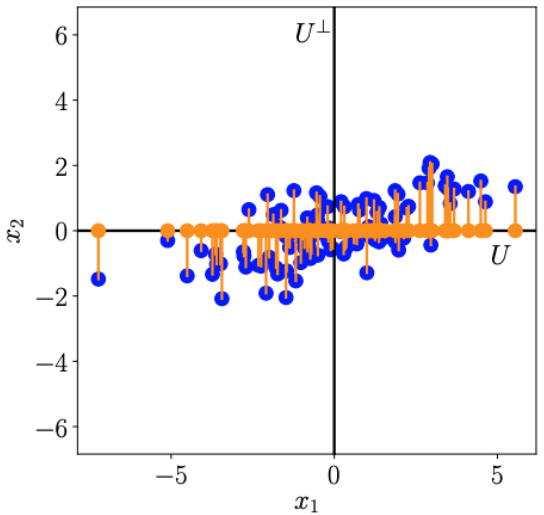


- $\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n$ lies in the sub e principal subspace.



- We identify the matrix $\sum_{j=M+1}^{D} \boldsymbol{b}_j \boldsymbol{b}_j^{\mathrm{T}}$ above as the projection matrix that performs this projection.






Orthogonal projection and displacement vectors. When projecting data points $\boldsymbol{x}_n$ (blue) onto subspace $U_1$, we obtain $\tilde{\boldsymbol{x}}_n$ (orange). The displacement vector $\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n$ lies completely in the orthogonal complement $U_2$ of $U_1$.

- Now we reformulate the loss function.



$$J_M = \frac{1}{N}\sum_{n=1}^{N} \|\boldsymbol{x}_n - \tilde{\boldsymbol{x}}_n\|^2 \qquad \frac{1}{N}\sum_{n=1}^{N}\left\|\sum_{j=M+1}^{D}(\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{x}_n)\boldsymbol{b}_j\right\|^2$$

- We explicitly compute the squared norm and exploit the fact that the $\boldsymbol{b}_j$ form an ONB:



$$J_M = \frac{1}{N}\sum_{n}\sum_{j=M+1}^{D}(\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{x}_n)^2 = \frac{1}{N}\sum_{n=1}^{N}\sum_{j=M+1}^{D}\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{x}_n\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{x}_n$$



$$n=1\ j=M+1$$



where we exploited the symmetry of the do e last step to write $\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{x}_n = \boldsymbol{x}_n^{\mathrm{T}}\boldsymbol{b}_j$. We now swap the sums and obtain

$$J_M = \sum_{j=M+1}^{D}\boldsymbol{b}_j^{\mathrm{T}}\left(\frac{1}{N}\sum_{n=1}^{N}\boldsymbol{x}_n\boldsymbol{x}_n^{\mathrm{T}}\right)\boldsymbol{b}_j = \sum_{j=M+1}^{D}\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{S}\boldsymbol{b}_j$$

$$= \sum_{j=M+1}^{D}\mathrm{tr}(\boldsymbol{b}_j^{\mathrm{T}}\boldsymbol{S}\boldsymbol{b}_j) = \sum_{j=M+1}^{D}\mathrm{tr}(\boldsymbol{S}\boldsymbol{b}_j\boldsymbol{b}_j^{\mathrm{T}}) = \mathrm{tr}\left(\left(\sum_{j=M+1}^{D}\boldsymbol{b}_j\boldsymbol{b}_j^{\mathrm{T}}\right)\boldsymbol{S}\right)$$

where we exploited the property that the trace operator $\mathrm{tr}(\cdot)$ is linear and invariant to cyclic permutations of its arguments

$$J_M = \sum_{j=M+1}^{D} \boldsymbol{b}_j^{\mathrm{T}} \boldsymbol{S} \boldsymbol{b}_j = \left( \sum_{j=M+1} {}_j\boldsymbol{b}_j^{\mathrm{T}} \right) \boldsymbol{S}$$

projection matrix

- The loss is formulated as the covariance matrix of the data, projected onto the orthogonal complement of the principal subspace.
- Minimizing the average r is therefore equivalent to minimizing the varianc onto the subspace we ignore, i.e., the orthogo ipal subspace.
- Equivalently, we maximize the variance ion that we retain in the principal subspace, which links the proje ediately to the maximum-variance formulation of PCA in Section 10.2.
- In Section 10.2, the average squared reconstruction error, when projecting onto the $M$-dimensional principal subspace, is

$$J_M = \sum_{j=M+1}^{D} \lambda_j$$

- where $\lambda_j$ are the eigenvalues of the data covariance matrix.

$$J_M = \sum_{j=M+1} \lambda_j$$

- To minimize it, we need to select the smallest $D - M$ eigenvalues. Their corresponding eigenvectors are the basis of the orthogonal complement of the principal subspace.
- Consequently, this me ctpal subspace comprises the eigenvectors $\boldsymbol{b}_1, \ldots, \ _M$ that are asso e largest $M$ eigenvalues of the data covariance matrix.

# 10.5 PCA in High Dimensions



- In order to do PCA, we need to compute the data covariance matrix $\boldsymbol{S}$
- In $D$ dimensions, $\boldsymbol{S}$ is a $D \times D$ matrix.
- Computing the eigenvalues and eigenvectors of this matrix is computationally expensive as it scales cubically in $D$.



- Therefore, PCA will be sions



- For example, if $\boldsymbol{x}_n$ are i e would need to compute the eigendecomposition of a $10{,}000 \times 10{,}$



- We provide a solution to this problem for t we have substantially fewer data points than dimensions, i.e., $N \ll D$
- Assume we have a centered dataset $\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N,\ \boldsymbol{x}_n \in \mathbb{R}^D$. Then the data covariance matrix is given as

$$\boldsymbol{S} = \frac{1}{N}\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}} \in \mathbb{R}^{D \times D}$$

where $\boldsymbol{X} = [\boldsymbol{x}_1, \cdots, \boldsymbol{x}_N]$ is a $D \times N$ matrix whose columns are the data points.

- We now assume that $N \ll D$, i.e., the number of data points is smaller than the dimensionality of the data.



- With $N \ll D$ data points, the rank of the covariance matrix $S$ is at most $N$, so it has at least $D - N$ eigenvalues that are $0$.
- Intuitively, this means that there are some redundancies. In the following, we will exploit this and turn the $D \times D$ covariance matrix into an $N \times N$ covariance matrix whose eigenvalues are all positive.



- In PCA, we ended up



$$\boldsymbol{S}\boldsymbol{b}_m = \lambda_m \boldsymbol{b}_m$$

where $\boldsymbol{b}_m$ is a basis vector of the principal subspace. Let us rewrite this equation a bit: With $\boldsymbol{S} = \frac{1}{N}\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}} \in \mathbb{R}^{D \times D}$, we



$$\boldsymbol{S}\boldsymbol{b}_m = \frac{1}{N}\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{b}_m = \lambda_m \boldsymbol{b}_m$$

- We now multiply $\boldsymbol{X}^{\mathrm{T}} \in \mathbb{R}^{N \times D}$ from the left-hand side, which yields

$$\frac{1}{N}\underbrace{\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}}_{N \times N}\underbrace{\boldsymbol{X}^{\mathrm{T}}\boldsymbol{b}_m}_{=:\boldsymbol{c}_m} = \lambda_m \boldsymbol{X}^{\mathrm{T}}\boldsymbol{b}_m \Leftrightarrow \frac{1}{N}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}\boldsymbol{c}_m = \lambda_m \boldsymbol{c}_m$$

- We get a new eigenvector/eigenvalue equation: $\lambda_m$ remains eigenvalue, which confirms our results from exercise 4.11 that the nonzero eigenvalues of $\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}$ equal the nonzero eigenvalues of $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$.
- We obtain the eigenvector of the matrix $\frac{1}{N}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X} \in \mathbb{R}^{N\times N}$ associated with $\lambda_m$ as $\boldsymbol{c}_m := \boldsymbol{X}^{\mathrm{T}}\boldsymbol{b}_m$ .



- This also implies that $\frac{1}{N}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ has the same (nonzero) eigenvalues as the data covariance matrix $\boldsymbol{S}$.



- But $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ now an $N\times N$ m the eigenvalues and eigenvectors much more efficiently than fo $\times D$ data covariance matrix.



- Now that we have the eigenvectors of $\frac{1}{N}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$, we are going to recover the original eigenvectors, which we still need for PCA. Currently, we know the eigenvectors of $\frac{1}{N}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$. If we left-multiply our eigenvalue/ eigenvector equation with $\boldsymbol{X}$, we get

$$\underbrace{\frac{1}{N}\boldsymbol{X}\boldsymbol{X}^{\mathrm{T}}}_{\boldsymbol{S}}\boldsymbol{X}\boldsymbol{c}_m = \lambda_m \boldsymbol{X}\boldsymbol{c}_m$$

and we recover the data covariance matrix again. This now also means that we recover $\boldsymbol{X}\boldsymbol{c}_m$ as an eigenvector of $\boldsymbol{S}$.

# 10.6 Key Steps of PCA in Practice



eigendecomposition

- **Step 1. Mean subtraction**



- We center the data by computing the mean $\mu$ of the dataset and subtracting it from every single data point. This ensures that the dataset has mean $0$.

- **Step 2. Standardization** Divide the data points by the standard deviation σd of the dataset for every dimension $d = 1, \ldots, D$. Now the data has variance 1 along each axis.

- **Step 3. Eigendecomposition of the matrix**



- Compute the data covariance matrix values and corresponding eigenvectors. The longer vector (larger eigenvalue) spans the principal subspace $U$

- 4. **Projection** We can project any d $\mathbb{R}^D$ onto the principal subspace: To get this right, we need e $\boldsymbol{x}_*$ using the mean $\mu_d$ and standard deviation $\sigma_d$ of the training data in the $d$th dimension, respectively, so that



$$x_*^{(d)} \leftarrow \frac{x_*^{(d)} - \mu_d}{\sigma_d}, \qquad d = 1, \cdots, D$$



where $x_*^{(d)}$ is the $d$th c

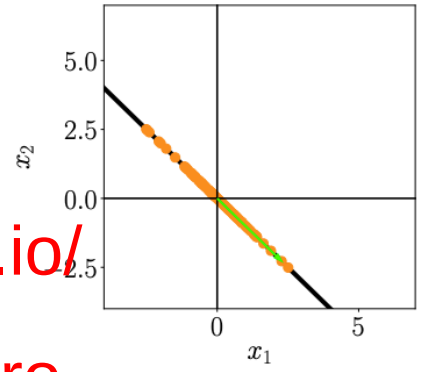
- We obtain the projectio



$$\tilde{\boldsymbol{x}}_* = \boldsymbol{B}\boldsymbol{B}$$



with coordinates




(e) Step 4: Project data onto the principal subspace.

$$\boldsymbol{z}_* = \boldsymbol{B}^{\mathrm{T}}\boldsymbol{x}_*$$

with respect to the basis of the principal subspace. Here, $\boldsymbol{B}$ is the matrix that contains the eigenvectors that are associated with the largest eigenvalues of the data covariance matrix as columns.

- Note that PCA returns the coordinates $\boldsymbol{z}_*$, not the projections of $\boldsymbol{x}_*$.

- Having standardized our dataset, $\tilde{x}_*$ yields the projections in the context of the standardized datas



- To obtain our projection in the original data space (i.e., before standardization), we need to undo the standardization: multiply by the standard deviation before adding the mean.
- We obtain



$\tilde{x}_*^{(d)}$ $^{(d)}$ $\ldots, D$

- Figure 10.10(f) illustrat al data space.