Principal Component Analysis

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Outline

- Overview
- Principle Component Analysis: Main Idea
- The PCA Algorithm
- PCA and SVD
- Summary

Motivating Example: Data Visualization

53 blood and urine samples (features) from 65 people

- Matrix format (65x53)

Instances

	H-WBC	H-RBC	H-Hgb	H-Hct	H-MCV	H-MCH	H-MCHC
A1	8.0000	4.8200	14.1000	41.0000	85.0000	29.0000	34.0000
A2	7.3000	5.0200	14.7000	43.0000	86.0000	29.0000	34.0000
A3	4.3000	4.4800	14.1000	41.0000	91.0000	32.0000	35.0000
A4	7.5000	4.4700	14.9000	45.0000	101.0000	33.0000	33.0000
A5	7.3000	5.5200	15.4000	46.0000	84.0000	28.0000	33.0000
A6	6.9000	4.8600	16.0000	47.0000	97.0000	33.0000	34.0000
A7	7.8000	4.6800	14.7000	43.0000	92.0000	31.0000	34.0000
A8	8.6000	4.8200	15.8000	42.0000	88.0000	33.0000	37.0000
A9	5.1000	4.7100	14.0000	43.0000	92.0000	30.0000	32.0000

Features

Difficult to see the correlations of different features

Motivating Example: Data Visualization

Is there a representation better than the coordinate axes?

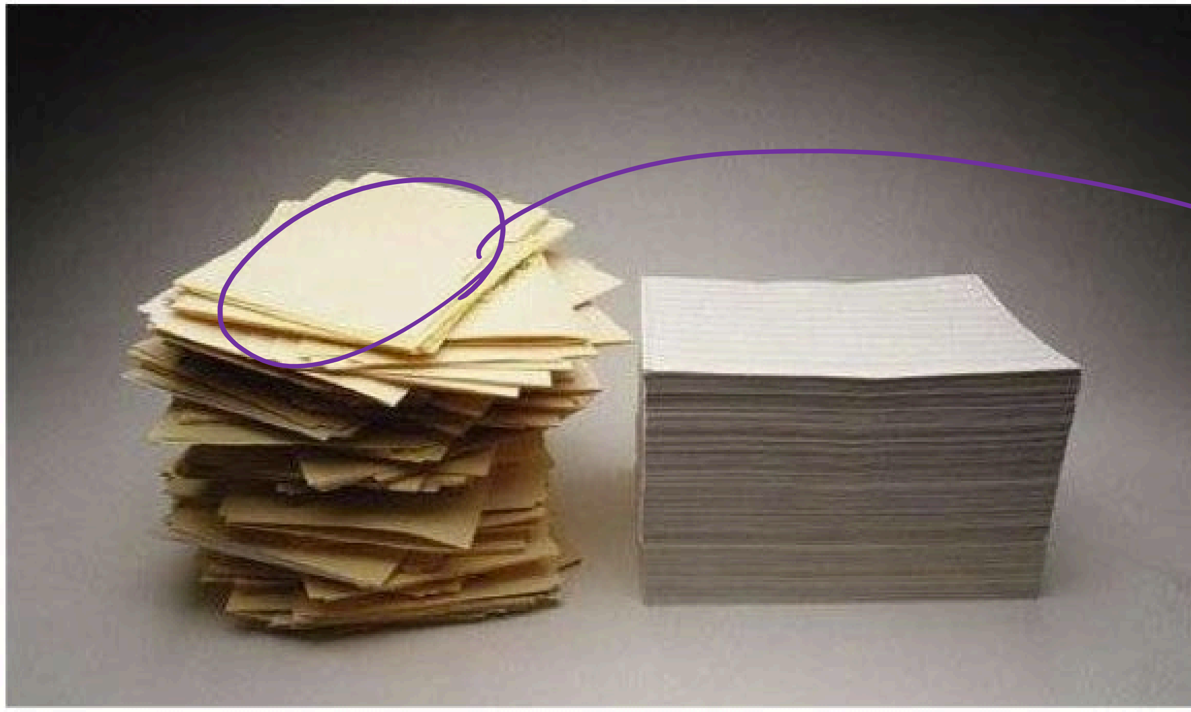
Is it really necessary to show all the 53 dimensions?

- … what if there are strong correlations between the features?

How could we find
the *smallest* subspace of the 53-D space that
keeps the *most information* about the original data?

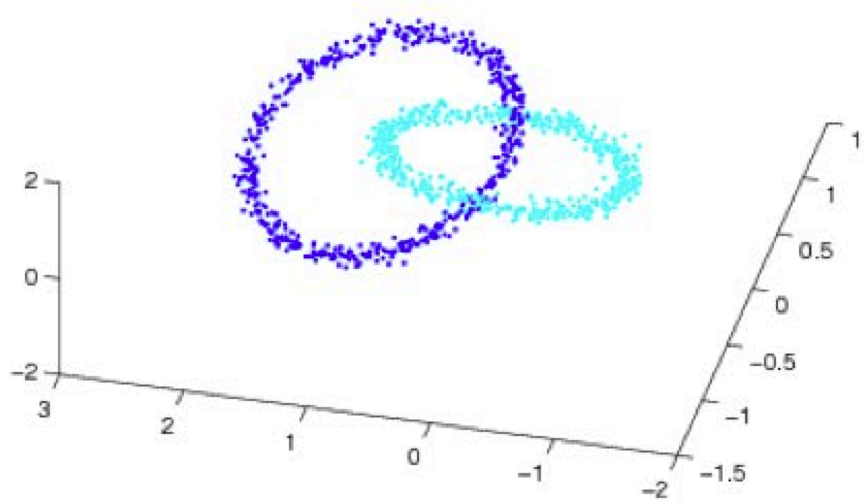
A Solution: **Dimension Reduction**

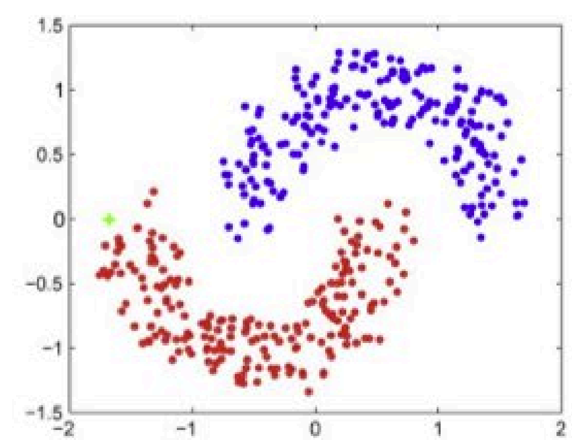
Another Example: Dimension Reduction for Text



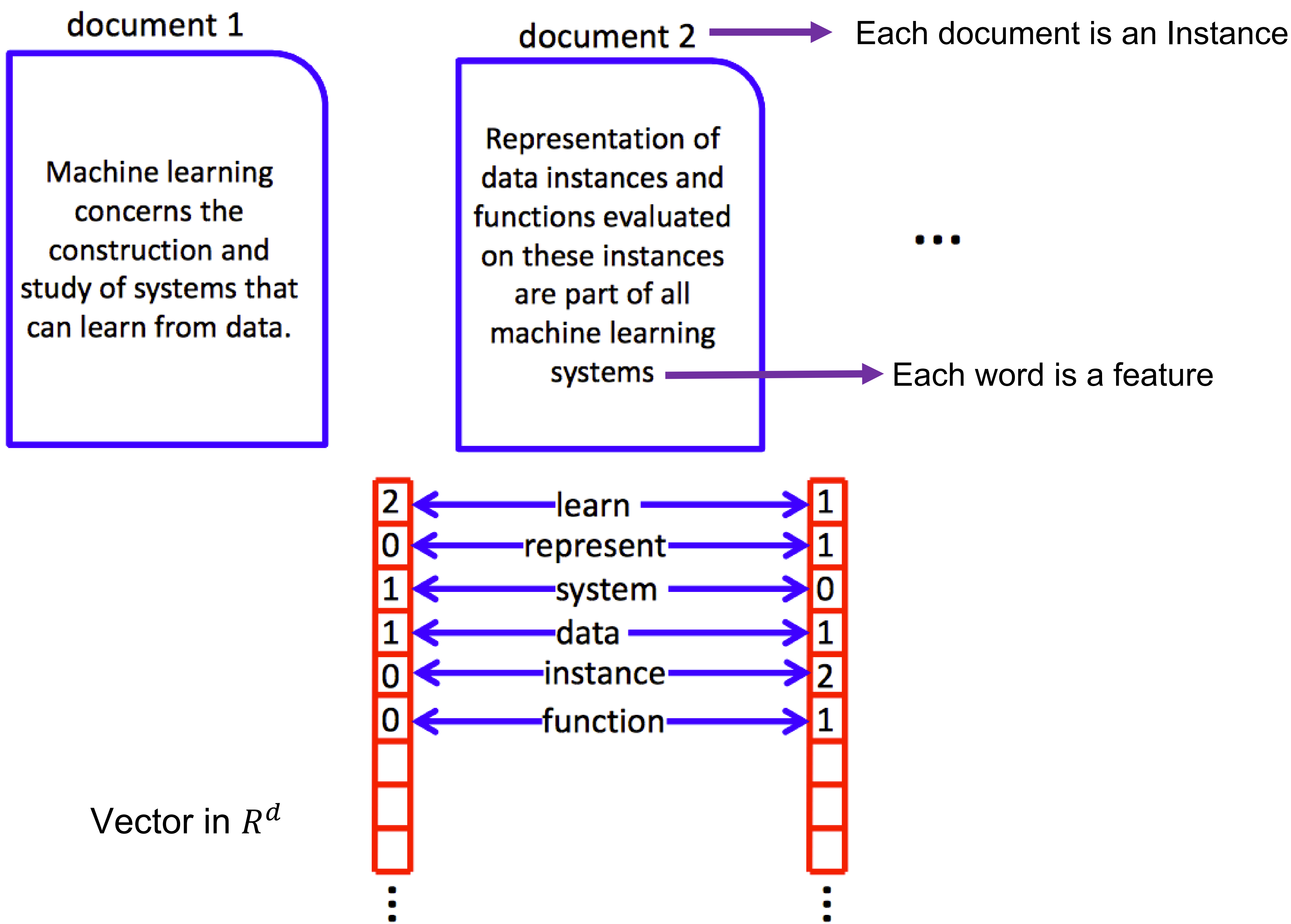
What are the relations between data points?

$X_{n \times d} =$





Bag-of-Words Representations



Term-Document Data Matrix – Bag-of-words

	database	SQL	index	regression	likelihood	linear
d1	24	21	9	0	0	3
d2	32	10	5	0	3	0
d3	12	16	5	0	0	0
d4	6	7	2	0	0	0
d5	43	31	20	0	3	0
d6	2	0	0	18	7	16
d7	0	0	1	32	12	0
d8	3	0	0	22	4	2
d9	1	0	0	34	27	25
d10	6	0	0	17	4	23

▪ ▪ ▪ Many more features

Solution:
Dimension Reduction

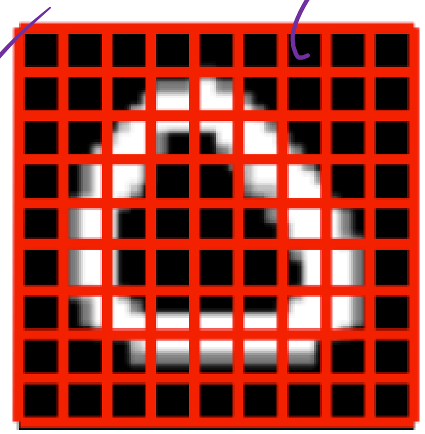
What is Dimension Reduction?

- The process of reducing the number of random variables under consideration
  - One can combine, transform or select variables
  - One can use linear or nonlinear operations

$X =$ $n \times d$

Original data point

Reduced representation



9×9

$$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

vector in R^d

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} \qquad f(x): R^d \mapsto R^k \qquad z = \begin{pmatrix} z_1 \\ z_2 \\ \vdots \\ z_k \end{pmatrix}$$

$$k \ll d$$

Applications of Dimension Reduction

- The dimension-reduced data can be used for
  - Visualizing, exploring and understanding the data
  - Aggregating weak signals in the data
  - Cleaning the data
  - Speeding up subsequent learning task
  - Building simpler model later

- Key questions of a dimensionality reduction algorithm
  - What is the criterion for carrying out the reduction process?
  - What are the algorithm steps?

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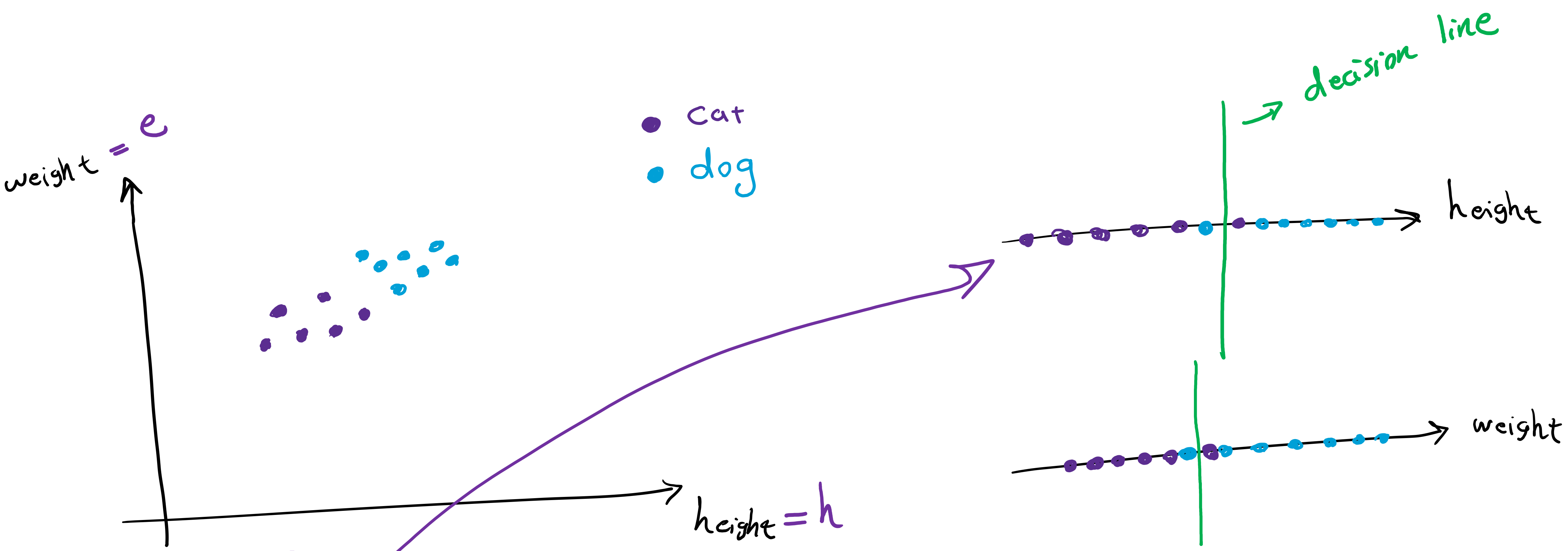
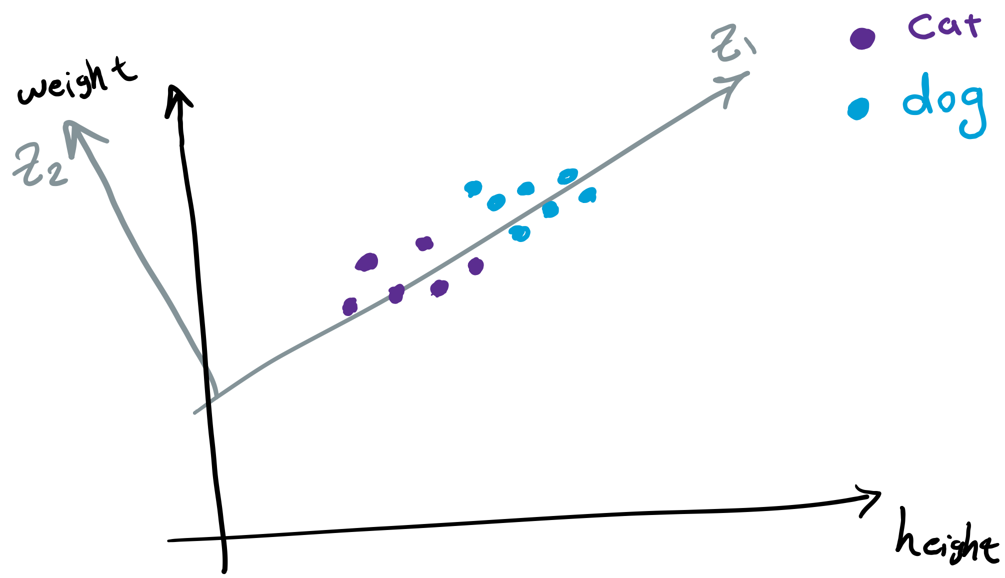
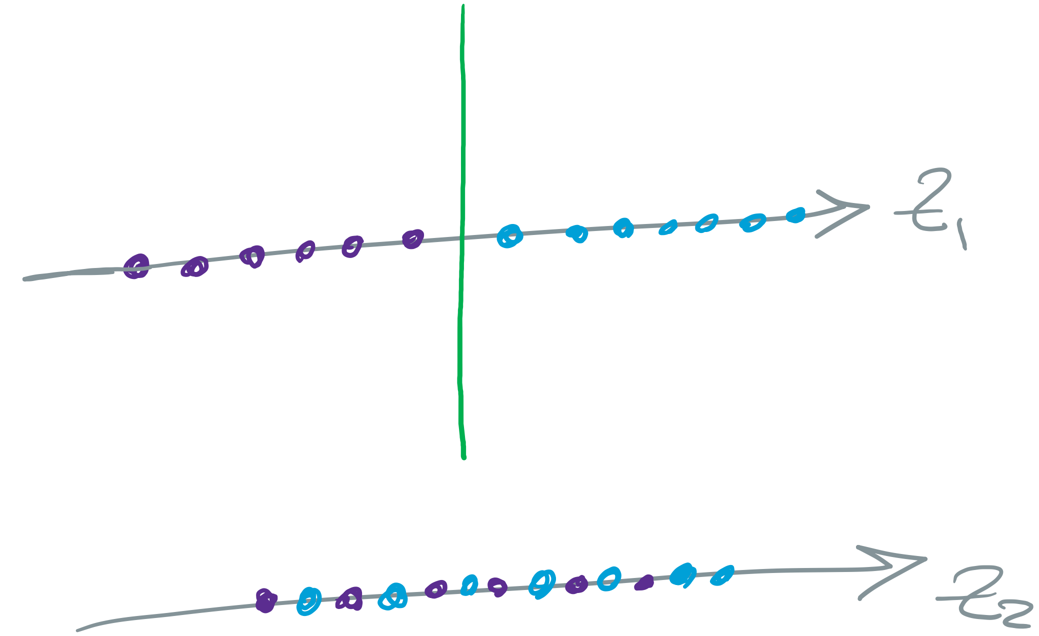


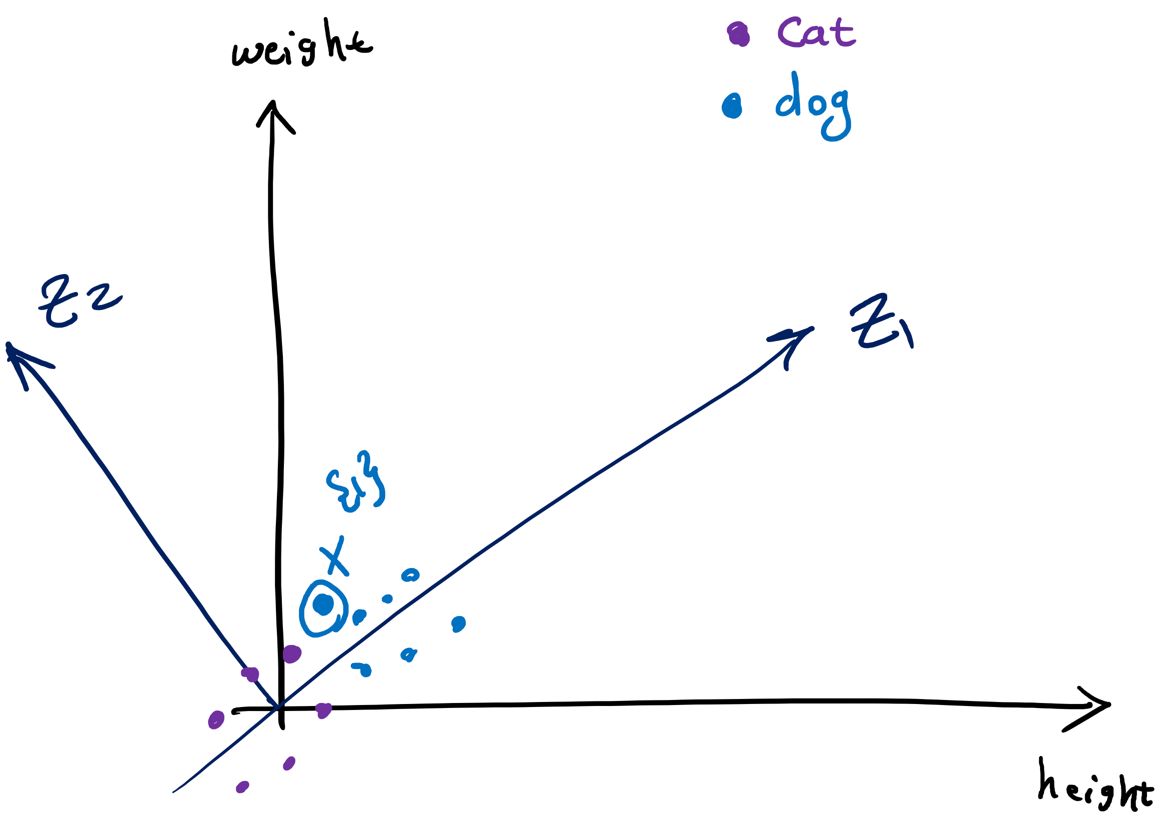
$$X = \begin{array}{c} \begin{array}{cc} h & e \end{array} \\ \begin{bmatrix} \vdots & \vdots \\ \vdots & \vdots \end{bmatrix}_{n \times 2 = d} \end{array}$$



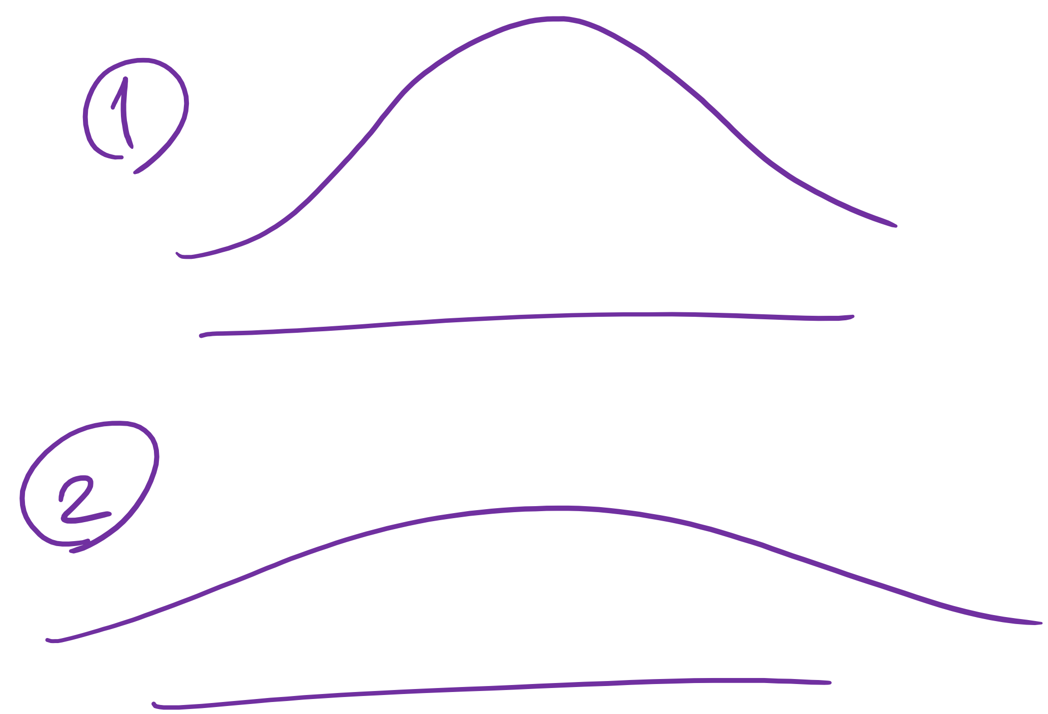
weight
z2
z1
cat
dog
height



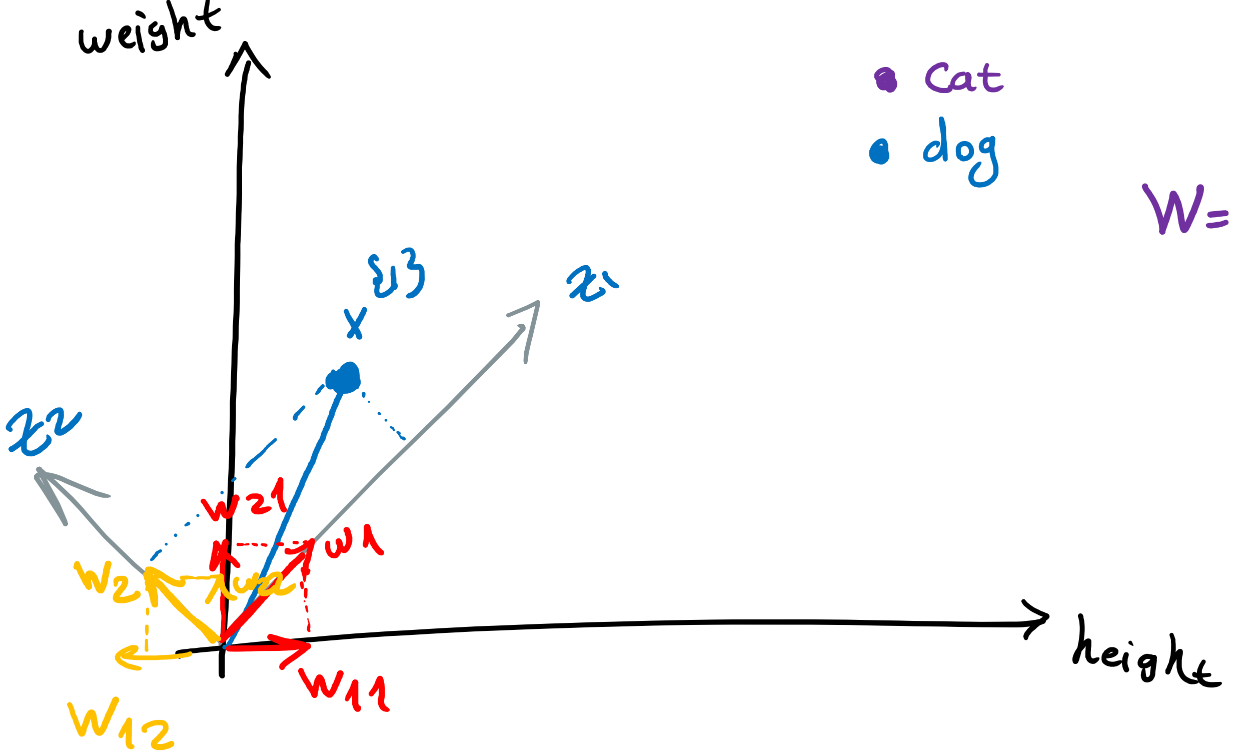
z1
z2



weight
cat
dog
z2
z1
x
height

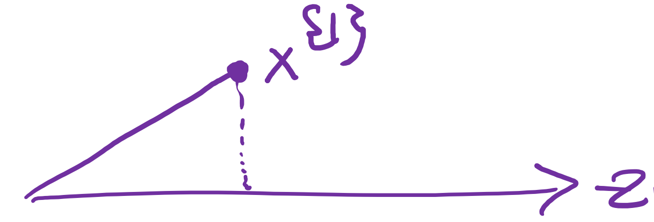


1
2



$$W = \begin{array}{cc} w_1 & w_2 \\ \hline \begin{bmatrix} w_{11} & w_{12} \\ w_{21} & w_{22} \end{bmatrix} \end{array}$$

$\|w_1\| = 1$



$\|w_1\| = 1$

$$x^{\{i\}} \cdot \frac{z_1}{\|z_1\|} = x^{\{i\}} \cdot w_1$$

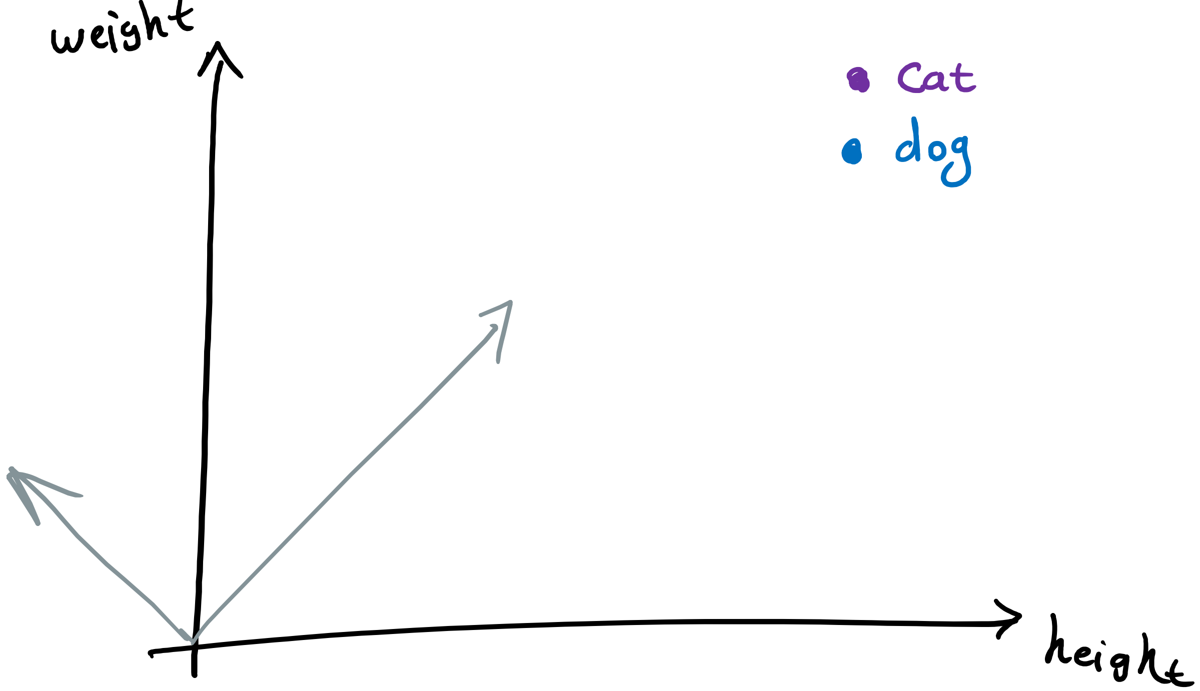
$$\|W\| = 1$$

$$x^{\{i\}} = [h^{\{i\}}, e^{\{i\}}] \qquad z^{\{i\}} = [z_1^{\{i\}}, z_2^{\{i\}}]$$

$$z_1^{\{i\}} = x^{\{i\}} \cdot w_1 = [h^{\{i\}}, e^{\{i\}}] \begin{bmatrix} w_{11} \\ w_{21} \end{bmatrix} = w_{11} h^{\{i\}} + w_{21} e^{\{i\}}$$

$$z_2^{\{i\}} = x^{\{i\}} \cdot w_2 = [h^{\{i\}}, e^{\{i\}}] \begin{bmatrix} w_{12} \\ w_{22} \end{bmatrix} = w_{12} h^{\{i\}} + w_{22} e^{\{i\}}$$

$$x^{\{i\}} = [h^{\{i\}}, e^{\{i\}}] \Rightarrow z^{\{i\}} = [w_{11} h^{\{i\}} + w_{21} e^{\{i\}}, \; w_{12} h^{\{i\}} + w_{22} e^{\{i\}}]$$

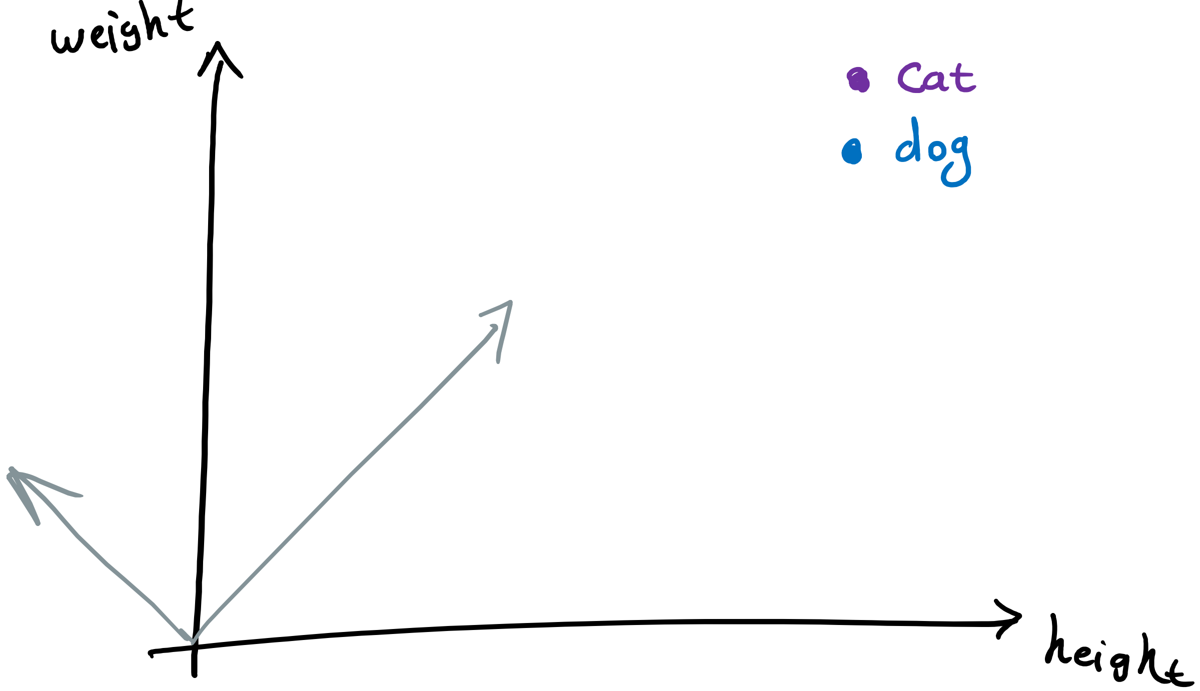


$$W = \begin{array}{cc} w_1 & w_d \\ \left[\begin{array}{c} w_{11} \\ w_{21} \\ \vdots \\ w_{d1} \end{array}\right. & \left.\begin{array}{c} \vdots \\ \vdots \\ \vdots \\ w_{dd} \end{array}\right]_{d \times d} \end{array}$$

$$Var(X) = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2$$

Maximize $\boxed{Var(Z) = \frac{1}{N} \sum_{i=1}^{N} (x_i \cdot w - \mu \cdot w)^2}$ objective function

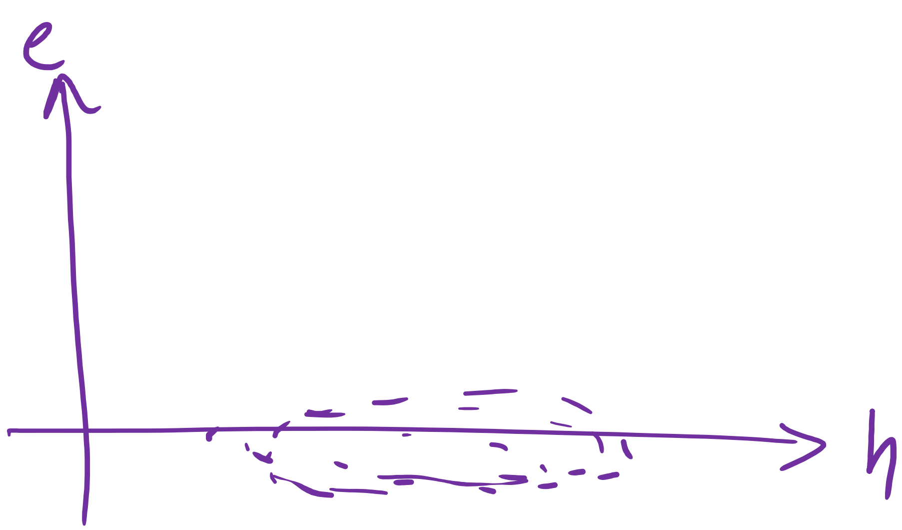
$\boxed{s.t. \ \|w\| = 1}$ → constraint function

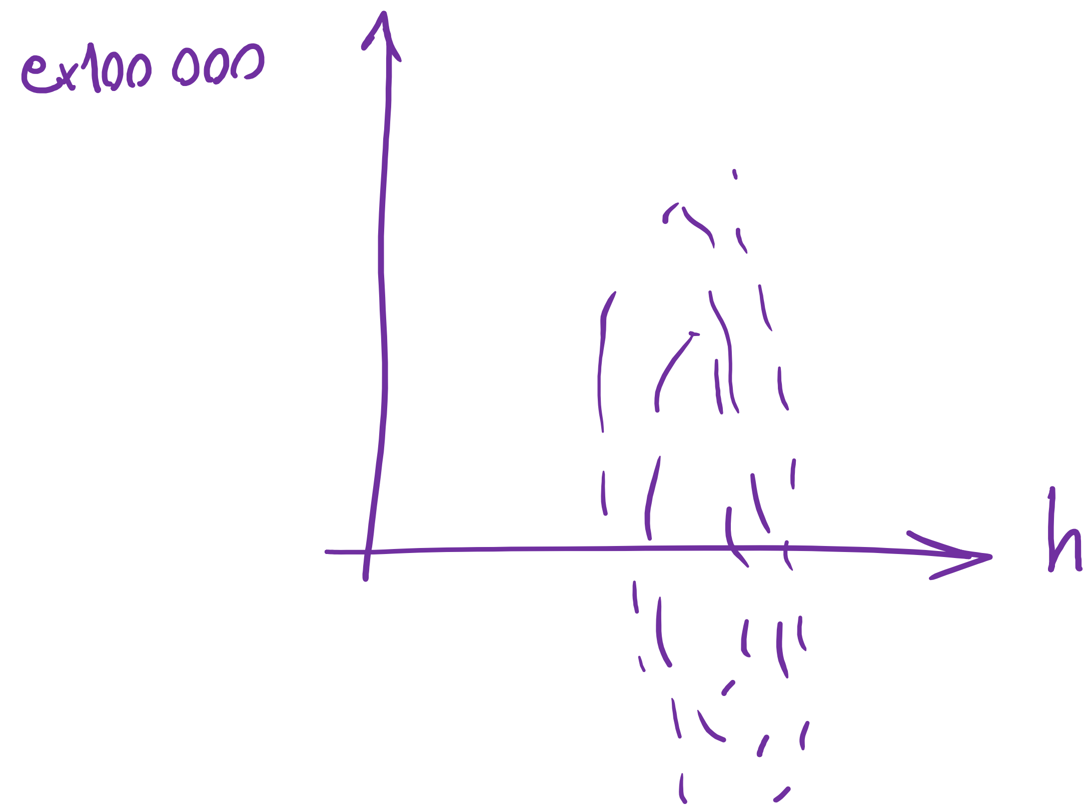


$$\bar{X}^* = \begin{array}{c} \\ \\ \end{array}\begin{array}{cc} \bar{h}^* & \bar{e}^* \end{array}$$

$$\bar{X}^* = \begin{bmatrix} \frac{x^{\{1\}} - \mu_h}{\sigma_h} & \frac{x^{\{1\}} - \mu_e}{\sigma_e} \\ \vdots & \vdots \end{bmatrix}$$

"Standardization"





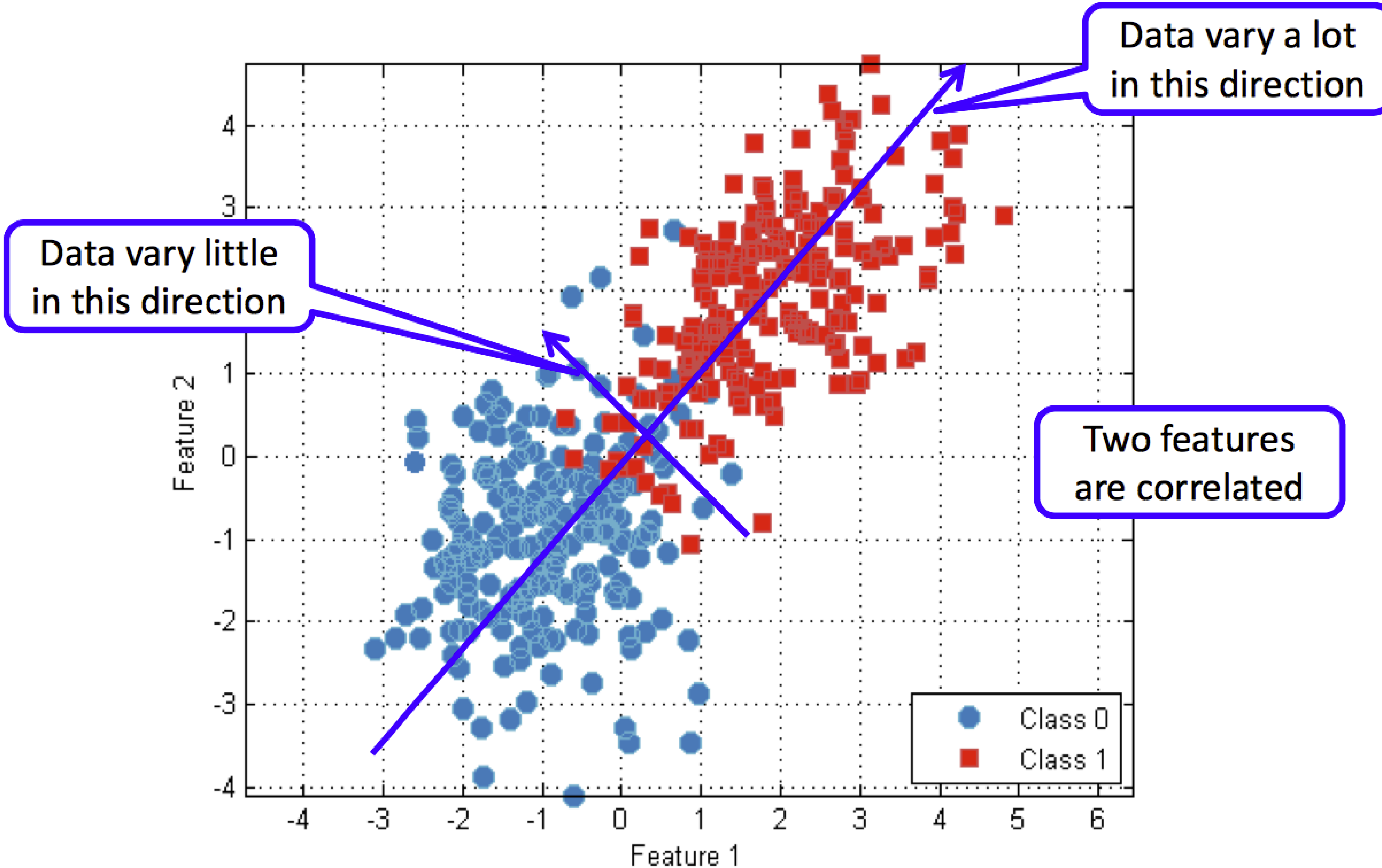
PCA: Dimension Reduction by Capturing **Variation**

- There are many criteria (geometric based, information theory based, etc.)

- One criterion: want to capture variation in data
  - variations are “signals” or information in the data
  - need to normalize each variables first

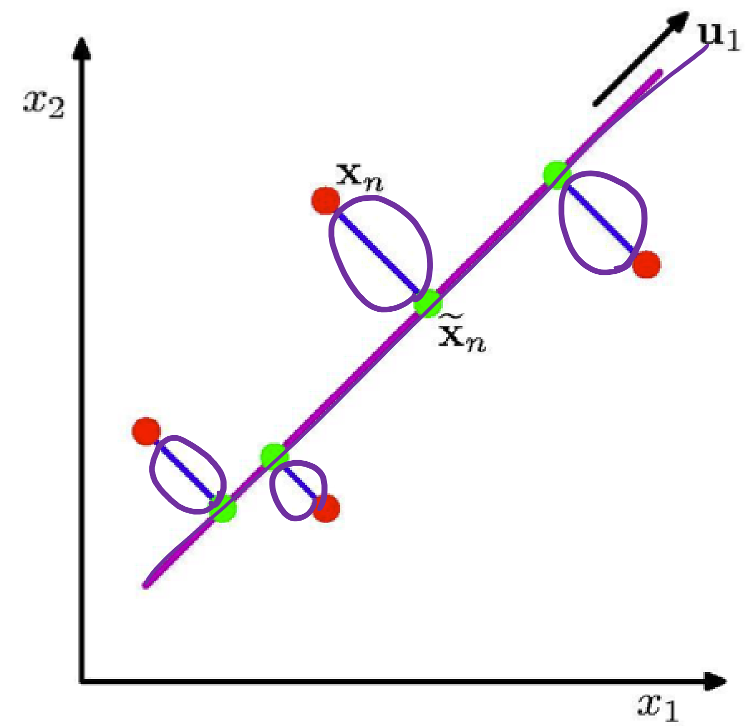
- In the process, also discover variables or dimensions highly correlated
  - represent highly related phenomena
  - combine them to form a stronger signal
  - lead to simpler presentation

Capturing Variation in Data



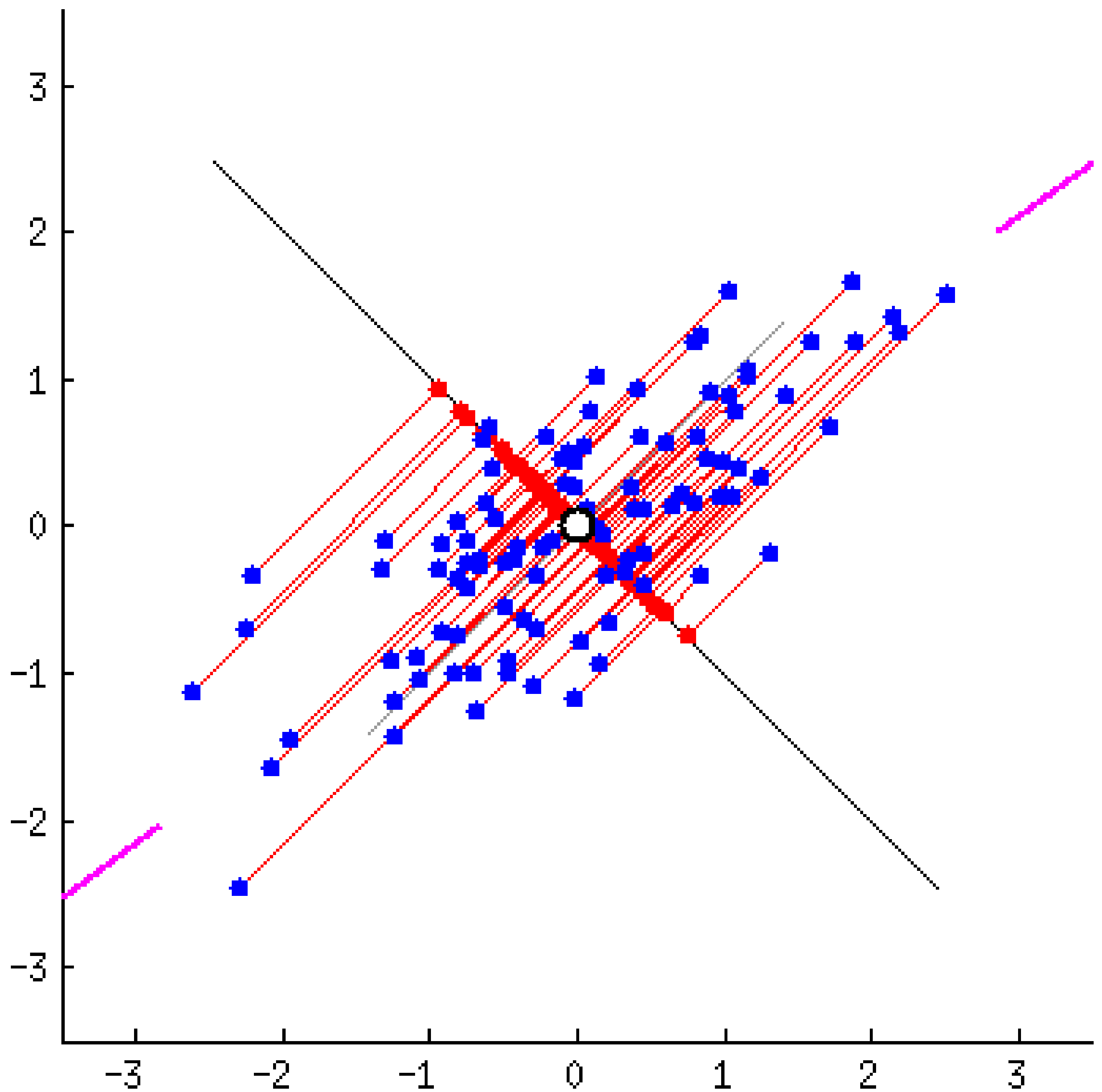
Two Equivalent Perspectives of PCA

PCA:



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

- ❑ maximizes variance of projected data (purple line)
- ❑ minimizes mean squared distance between
    - data point and
    - projections (sum of blue lines)


3
2
1
0
−1
−2
−3
−3
−2
−1
0
1
2
3

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What is variance equation?

$$Var(x) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

Formulating the Problem

- Given n data points, $\{x_1, x_2, \dots, x_n\} \in R^d$ with their mean $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$
- Find a direction $w \in R^d$ where

$$\|w\| = \sqrt{\sum_{j \in d} \omega_j^2} = 1$$

We constrain the norm of w to be equal to one to avoid having very large variance in each new dimension.

- Given n data points, $\{x_1, x_2, \dots, x_n\} \in R^d$ with their mean μ

$$\|w\| = \sqrt{\sum_{j \in d} \omega_j^2} = 1 \qquad \mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

- Such that the variance (or variation) of the data along direction w is maximized

$$Var(z) = \max_{\|w\|=1} \underbrace{\frac{1}{n}\sum_{i=1}^{n}(x_i w - \mu w)^2}_{\text{variance in new feature space}}$$

An Optimization Problem

- Manipulate the objective with linear algebra

$$\frac{1}{n}\sum_{i=1}^{n}(x_i w - \mu w)^2 = \frac{1}{n}\sum_{i=1}^{n}((x_i - \mu)w)^2 =$$

$$= \frac{1}{n}\sum_{i=1}^{n}(\underbrace{(x_i - \mu)}_{A}\underbrace{w)}_{B}{}^T((x_i - \mu)w) = \frac{1}{n}\sum_{i=1}^{n} w^T(x_i - \mu)^T (x_i - \mu)w$$

$$(AB)^T = B^T A^T$$

$$\frac{\bar{X}^T \bar{X}}{N} = \text{cov}$$

$$w^T\boxed{(\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^T (x_i - \mu))}w = w^T C w$$

Covariance matrix

Let's optimize it

Maximize

$$Var(z) = \frac{1}{N}\sum_{i=1}^{N}(x_i w - \mu_w) = w^T C w$$

$$\text{s.t.} \quad \|w\| = 1 \;;\; w^T\cdot w = 1 \Rightarrow g(w) = w^T\cdot w - 1 = 0$$

$f(x)$

s.t. $g(x) = 0$

$$L(x, \delta) = f(x) - \delta g(x)$$

$X_{n\times d}$

$$C = \left[\quad\right]_{d\times d} = \frac{\bar{X}^T \bar{X}}{N}$$

$$L(w, \delta) = w^T C w - \delta(w^T\cdot w - 1)$$

$$\frac{\partial L(w,\delta)}{\partial w} = 2Cw - 2\delta w = 0 \Rightarrow \boxed{\begin{array}{c} Ax = \delta x \\ Cw = \delta w \end{array}}$$

$$\begin{array}{cc} & \begin{array}{cccc} x_1 & x_2 & \cdots & x_d \end{array} \\ \begin{array}{c} x_1 \\ x_2 \\ \vdots \\ x_d \end{array} & \left[\begin{array}{cccc} & & & \\ & & & \\ & & & \\ & & & \end{array}\right]_{d\times d} \end{array}
\begin{array}{c} \begin{array}{ccc} w_1 & \cdots & w_d \end{array} \\ \left[\begin{array}{ccc} & & \\ & & \\ & & \end{array}\right]_{d\times d} \end{array}
= \left[\begin{array}{ccc} \delta_1 & & \\ & \ddots & \\ & & \delta_d \end{array}\right]_{d\times d}
\begin{array}{c} \begin{array}{ccc} w_1 & \cdots & w_d \end{array} \\ \left[\begin{array}{ccc} & & \\ & & \\ & & \end{array}\right]_{d\times d} \end{array}$$

$$C \quad W = \Lambda \quad W$$

$$Var(z) = \frac{1}{N}\sum_{i=1}^{N}(x_i w - \mu w)^2 = w^T C w$$

$$\underbrace{Cw} = \lambda w = w \lambda$$

$$w^T \cdot w = 1$$

$$Var(z) = w^T \underline{Cw} = w^T w \lambda = \lambda$$

$$Var(z) = \lambda$$

$$\frac{\lambda_1 + \lambda_2 + \dots}{\lambda_1 + \lambda_2 + \dots + \lambda_d} \geq 0.98 \quad \rightsquigarrow \quad z = \begin{array}{cc} z_1 & z_2 \\ \left[\begin{array}{cc} x^{(1)}\cdot w_1 & x^{(1)}\cdot w_2 \\ x^{(2)}\cdot w_1 & \vdots \\ \vdots & \\ x^{(n)}\cdot w_1 & x^{(n)}\cdot w_2 \end{array}\right]_{n\times 2} \end{array}$$

Equivalence to The Eigenvalue Problem

Objective function: $\max\limits_{||w||=1} w^T C w$

- Form lagrangian function of the optimization problem

$$L(w, \lambda) = w^T C w + \lambda(1 - w^T w)$$

If w is a maximum of the original optimization problem, then there exist a λ, where (w, λ) is a stationary point of $\mathrm{L}(\mathrm{w}, \lambda)$

Therefore:

$$\frac{\partial \mathrm{L}(\mathrm{w}, \lambda)}{\partial w} = 0 = 2Cw - 2\lambda w \Rightarrow \qquad Cw = \lambda w$$

Eigen-Value Problem

- Eigen-value problem

d: dimension

  - Given a symmetric matrix $C \in R^{d \times d}$

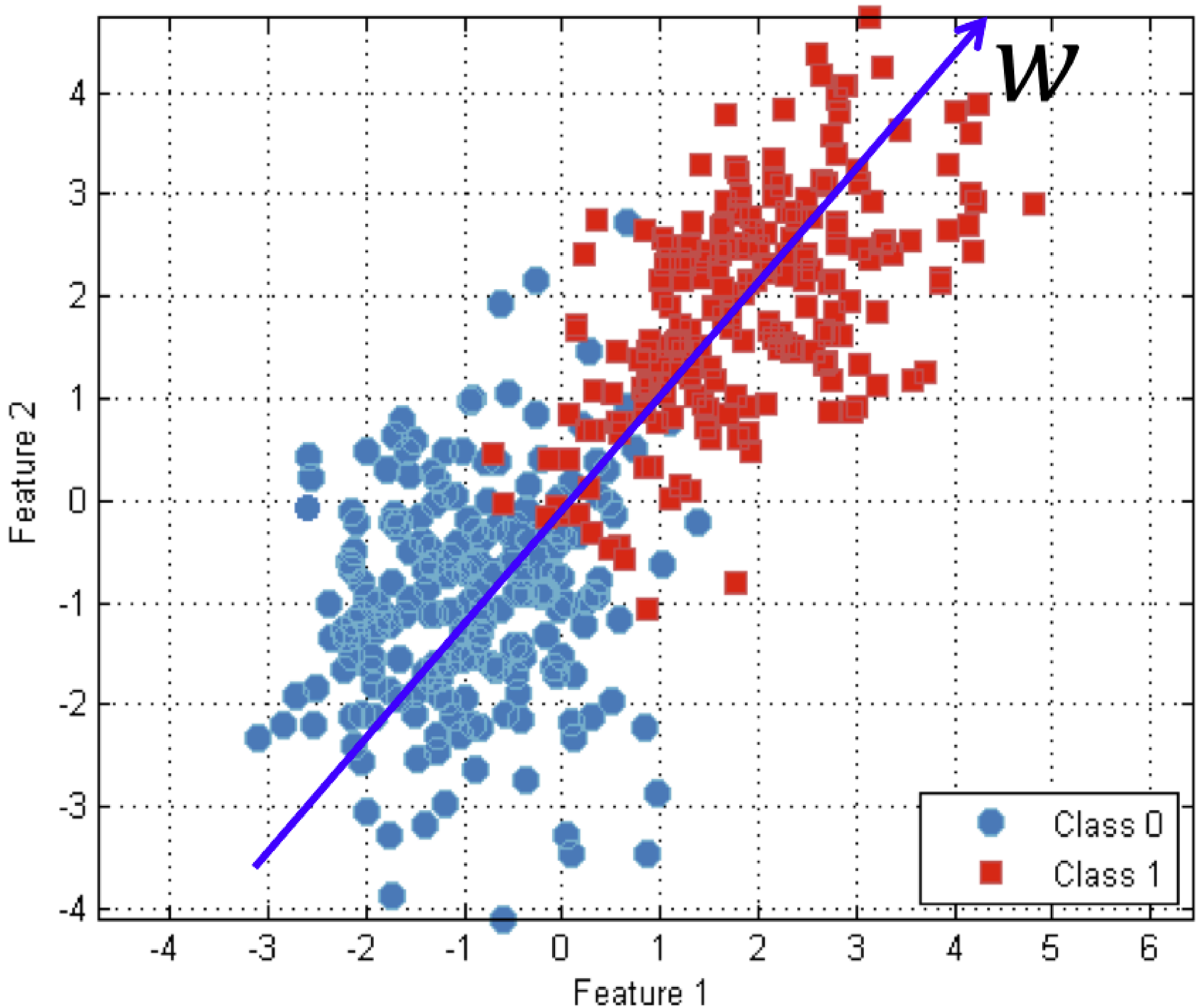
C is also a positive semidefinite matrix

  - Find a vector $w \in R^d$ and $\|w\| = 1$
  - Such that

$$Cw = \lambda w$$

- There will be multiple solution of $w_1, w_2, \dots, w_d$ for its corresponding $\lambda_1, \lambda_2, \dots, \lambda_d$
  - They are ortho-normal: $w_i^T w_i = 1 \qquad w_i^T w_j = 0$

Principal Direction of the Data



Variance in the Principal Direction

- Principal direction w satisfies

$$Cw = \lambda w = w\lambda$$

- Variance in principal direction is

$$w^T C w$$

$$= w^T w \lambda$$

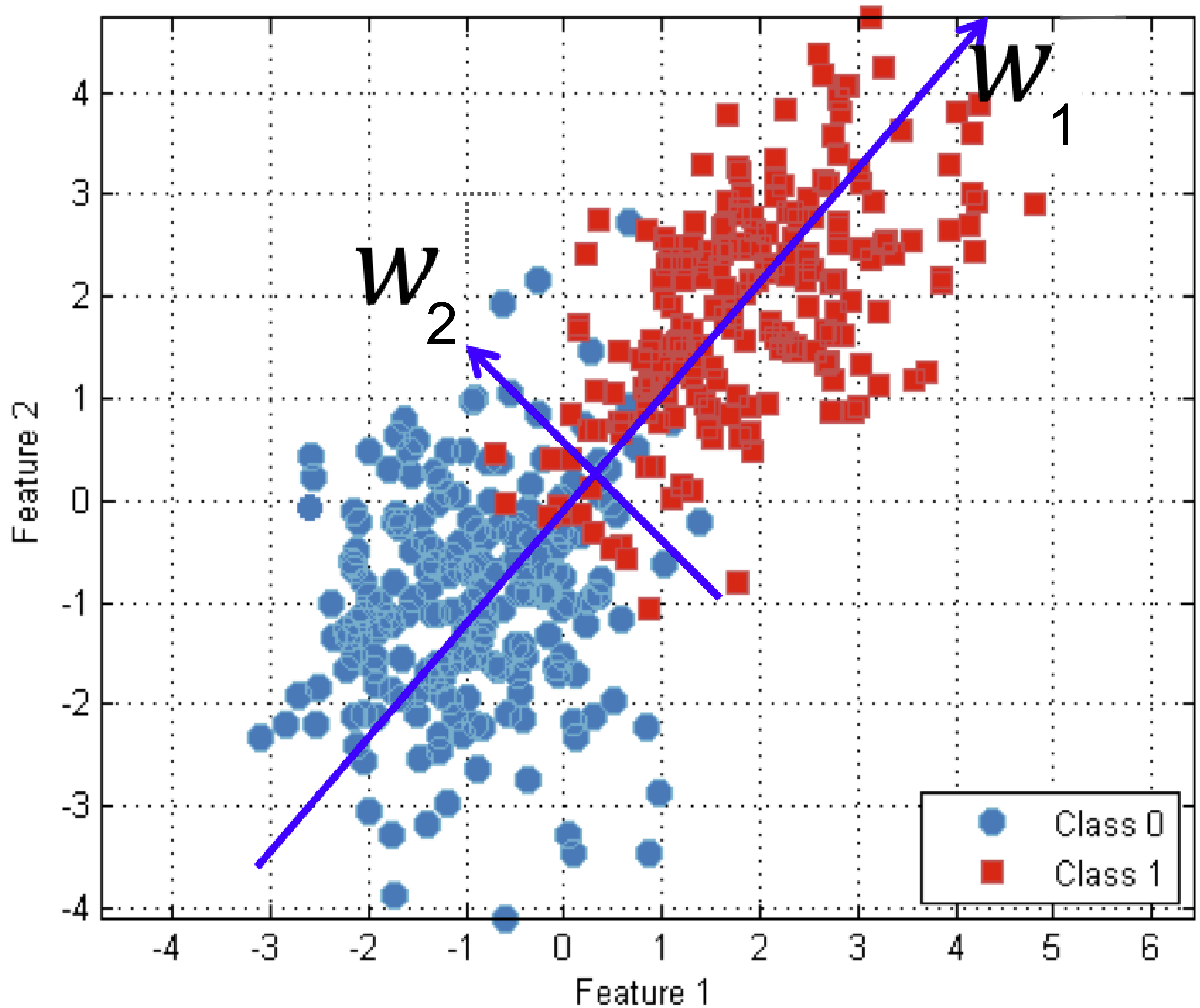
$$= \lambda$$

eigen-value

Multiple Principal Directions

- Directions $w_1, w_2, \ldots$ which has
  - the largest variances
  - but are orthogonal to each other
- Take the eigenvectors $w_1, w_2, \ldots$ of C corresponding to
  - the largest eigenvalue λ_1,
  - the second largest eigenvalue λ_2
  - …

Extra Principal Directions



Relations Between Principal Components

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**

The PCA Algorithm

- Given n data points, $\{x_1, x_2, \ldots, x_n\} \in R^d$ with mean

- Step 1: Estimate the mean and covariance matrix from data

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i \quad and \quad C = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^T (x_i - \mu)$$

Principal directions

- Step 2: Take the eigenvectors w_1, w_2 , ... of C corresponding to the largest eigenvalue λ_1, the second largest eigenvalue λ_2 ...

- Step 3: Compute reduced representation

$$z_i = \left(\frac{(x_i - \mu_1)}{\sigma_1} w_1 \quad \frac{(x_i - \mu_2)}{\sigma_2} w_2 \quad \ldots \right)$$

$$z \Rightarrow \mathrm{n} \times k$$

$$k \ll d$$

Normalizing by standard deviation

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Singular Value Decomposition

$\bar{X}_{n\times d}$

n: instances
d: dimensions
X is a centered matrix

$$U_{n\times n} \rightarrow unitary\ matrix \rightarrow\ U \times U^T = I$$

$$\bar{X} = U\Sigma V^T \qquad \Sigma_{n\times d} \rightarrow diagonal\ matrix$$

$$\mathrm{V}_{d\times d} \rightarrow unitary\ matrix \rightarrow V \times V^T = I$$

Principle direction

$$X = \underbrace{\begin{bmatrix} u_{1\times 1} & \cdots & \cdots & \cdots & u_{1\times n} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ u_{1\times 1} & \cdots & \cdots & \cdots & u_{n\times n} \end{bmatrix}}_{U} \times \underbrace{\begin{bmatrix} \sum_{1\times 1} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \sum_{d\times d} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\Sigma} \times \underbrace{\begin{bmatrix} v_{1\times 1} & \cdots & \cdots & \cdots & v_{1\times d} \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \ddots & \vdots \\ v_{d\times 1} & \cdots & \cdots & \cdots & v_{d\times d} \end{bmatrix}}_{V^T}$$

$$d < n$$

According to PCA ➔ $Cw = \lambda w = w\lambda$

$$\text{Covariance } C_{d\times d} = \frac{1}{n}\sum_{i=1}^{n}\left(x^i - \mu\right)^T \overbrace{\left(x^i - \mu\right)}^{\textbf{Centering X}} = \frac{\bar{X}^T\bar{X}}{n}$$

$$\left.\begin{array}{l} \bar{X} = U\Sigma V^T \\ \\ C = \dfrac{\bar{X}^T\bar{X}}{n} \end{array}\right\} C = \frac{V\Sigma^T U^T U\Sigma V^T}{n} = \frac{V\Sigma^2 V^T}{n}$$

$$C = \frac{V\Sigma^2 V^T}{n} = V\frac{\Sigma^2}{n}V^T$$

$\bar{X} = U\Sigma V^T$

$$CV = V\frac{\Sigma^2}{n}V^TV = V\frac{\Sigma^2}{n}$$

$S = \frac{\Sigma^2}{n}$ $V = w$

According to Eigen-decomposition definition ➔ $CV = V\Lambda$

$$\boxed{\begin{aligned} CV &= V\frac{\Sigma^2}{n} \\ Cw &= wS \end{aligned}}$$

V is the eigen vectors of covariance (Principal directions)

$\lambda_i = \frac{\sigma_i^2}{n}$ ➔ The eigenvalues of covariance matrix

Let's project the data (X) on principal directions:

$$\bar{X}V = U\Sigma V^TV = U\Sigma$$

$\bar{X}\boldsymbol{V}$ is linear combination of the original data (x-space) features

Projection of one instance (x) on the first principal direction using k dimensions

$$\mathrm{p}_1 = [u_{1\times 1}\Sigma_{1\times 1}, u_{1\times 2}\Sigma_{2\times 2}, \dots, u_{1\times k}\Sigma_{k\times k}]$$
$$\mathrm{p}_2 = [u_{2\times 1}\Sigma_{1\times 1}, u_{2\times 2}\Sigma_{2\times 2}, \dots, u_{2\times k}\Sigma_{k\times k}]$$

$U \Rightarrow n \times k$
$\Sigma \Rightarrow k \times k$
Upper left corner

Eigen values $\lambda = \frac{\Sigma^2}{n}$

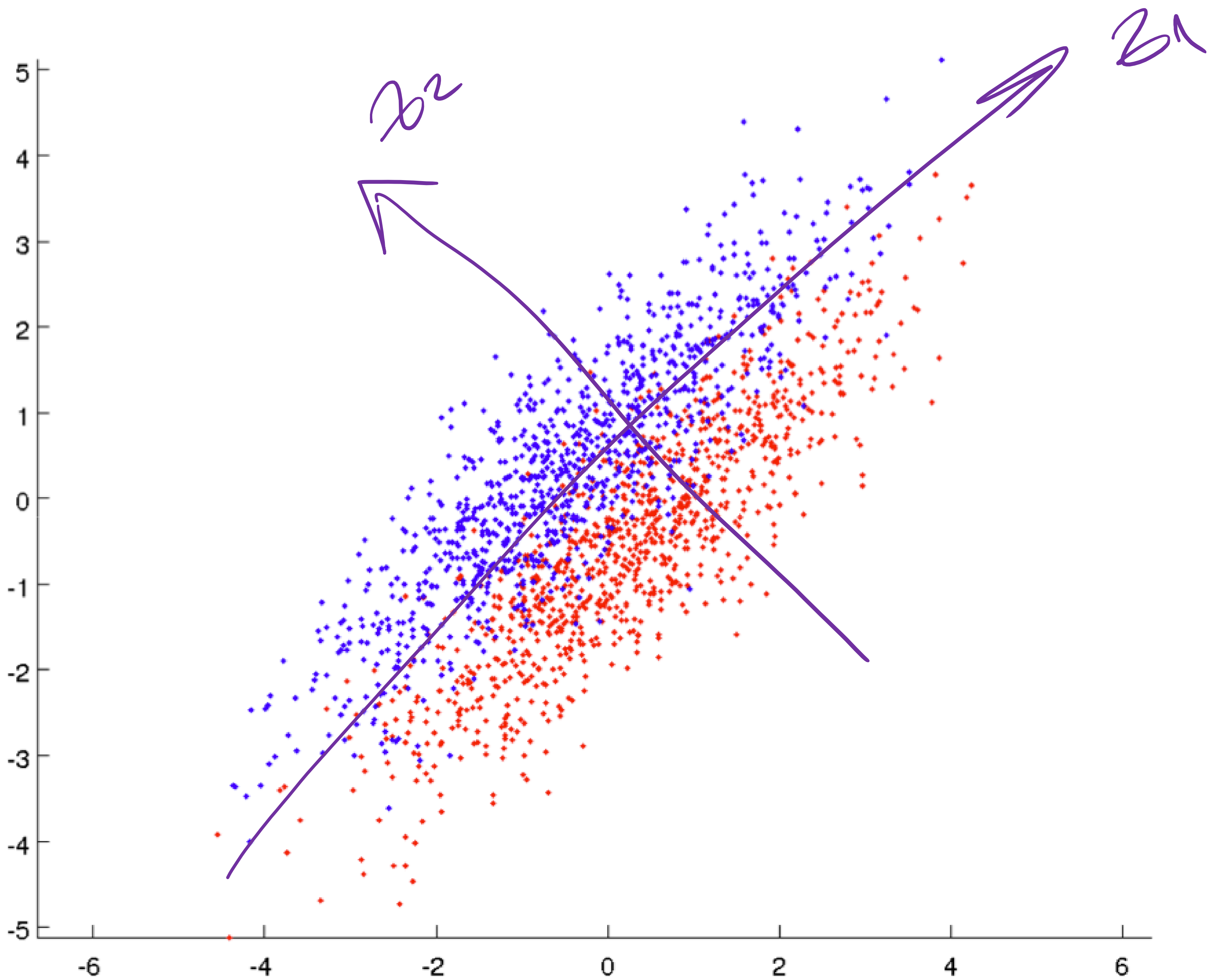
Eigenvectors (principal directions) V

$$\bar{X} = U\Sigma V^T$$

Principal components (Scores) or projections on principal directions

In fact, using the SVD to perform PCA makes much better sense numerically than forming the covariance matrix to begin with, since the formation of $X^T X$ can cause loss of precision.

Are Principal Components Good for Classification?



Why PCA potentially works in classification?

the dimension with the largest variance corresponds to the dimension with the largest entropy and thus encodes the most information (Information Theory). The smallest eigenvectors will often simply represent noise components, whereas the largest eigenvectors often correspond to the principal components that define the data.

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- PCA
  - Finds orthonormal basis for data
  - Sorts dimensions in order of “importance”
  - Discard low significance dimensions
- Uses
  - Get concise low-dimensional representations
  - Remove noise
- Not magic
  - Doesn’t know class labels
  - Can only capture linear variations

Image compression using PCA