

Data Preparation: Reduction and Transformation

Mining Massive Datasets

Prof. Carlos Castillo

Topic 05

Main Sources

- Data Mining, The Textbook (2015) by Charu Aggarwal (Chapter 2) + [slides by Lijun Zhang](#)
- Introduction to Data Mining 2nd edition (2019) by Tan et al. (Chapter 2)
- Data Mining Concepts and Techniques, 3rd edition (2011) by Han et al. (Chapter 3)

Data reduction and transformation

- Sampling
 \cong “Less rows”
- Dimensionality Reduction or Feature Selection
 \cong “Less columns”

Why reduce/transform data?

- The Advantages
 - Reduce space complexity
 - Reduce time complexity
 - Reduce noise
 - Reveal hidden structures
 - E.g., manifold learning
- The Disadvantages
 - Information loss

Sampling for static data

- **Uniform** random sampling
 - with/without replacement
- **Biased** sampling
 - e.g., emphasize recent items
- **Stratified** sampling
 - Partition data in strata, sample in each stratum

Sampling example

- There are 10000 people which contain 100 millionaires
- Uniform random sample of 100 people
 - In expectation, one millionaire will be sampled
 - There is $\approx 37\%$ chance no millionaires are sampled, why?
- Stratified Sampling
 - Unbiased Sampling 1 from 100 millionaires
 - Unbiased Sampling 99 from remaining

Sampling from data streams

- The setting
 - Data arrive sequentially
 - We want sample of them uniformly
 - There is a reservoir that can hold k data points
- The algorithm: reservoir sampling
 - The first k data points are kept
 - Insert the n -th data point with probability k/n
 - Drop one of the existing data points uniformly at random
 - [More on this in the sequence mining lecture ...](#)

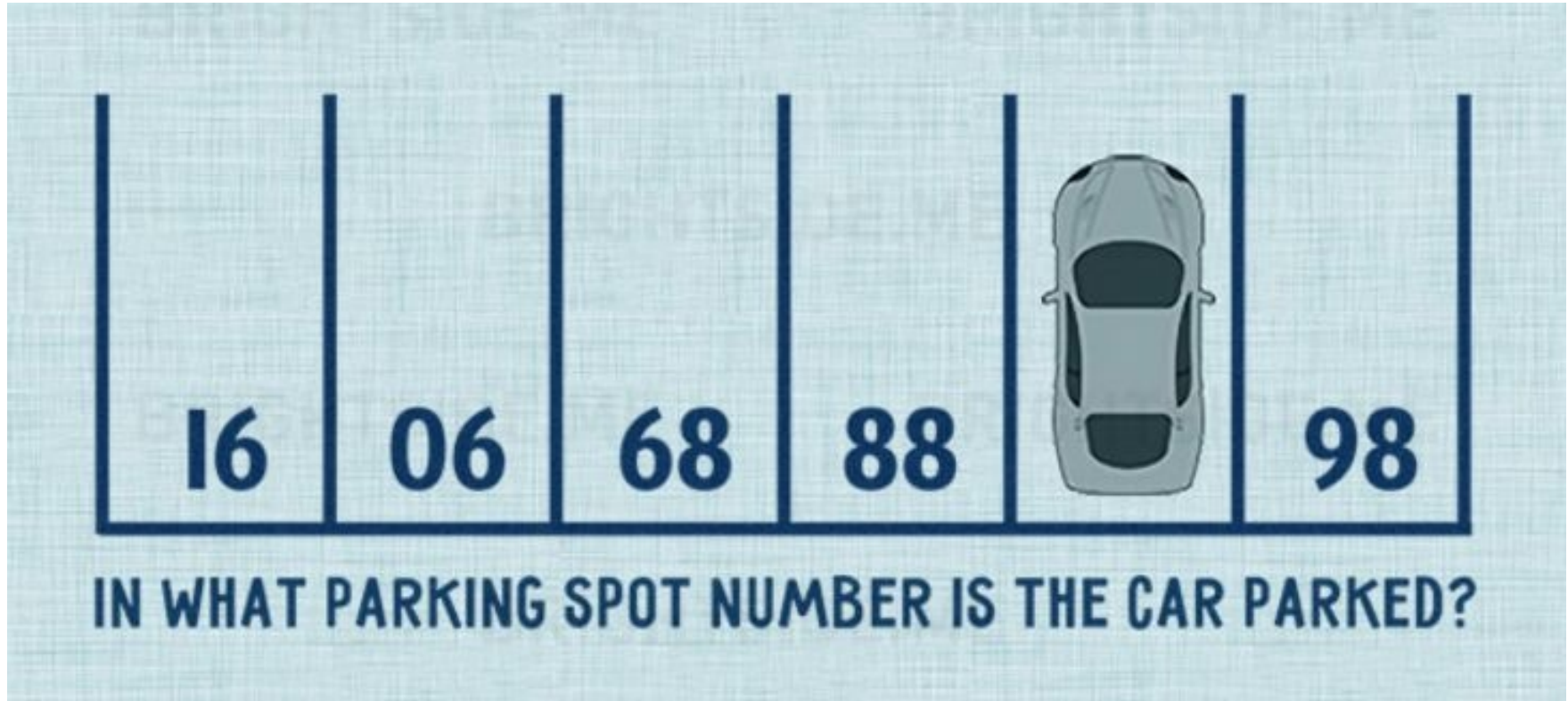
Reducing data dimensionality

Note: PCA/SVD covered well in other courses, won't be part of our exam

Feature selection

- **Unsupervised** Feature Selection
 - Using the performance of unsupervised learning (e.g, clustering) to guide the selection
- **Supervised** Feature Selection
 - Using the performance of supervised learning (e.g., classification) to guide the selection

An axis rotation may help :-)



Source: [Centauro Blog \(2017\)](#)

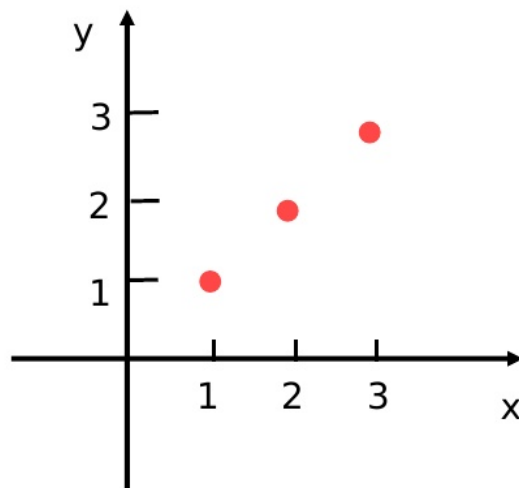
Dimensionality reduction with axis rotation (perfect case)

- Motivation: three points in a line in two-dimensional space

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 3 \\ 3 \end{bmatrix}$$



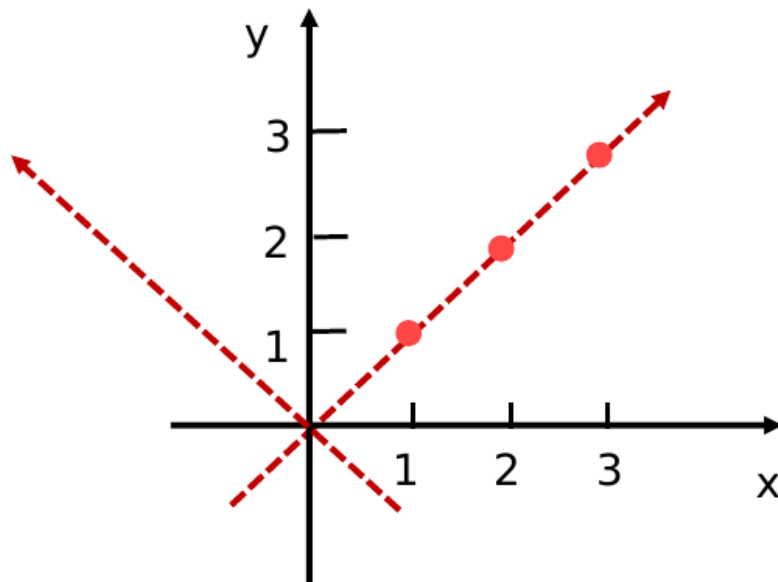
Dimensionality reduction with axis rotation (perfect case, cont.)

- Coordinates after axes rotation

$$\mathbf{x}_1 = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2\sqrt{2} \\ 0 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 3\sqrt{2} \\ 0 \end{bmatrix}$$



Dimensionality reduction with axis rotation (perfect case, cont.)

- Coordinates after axes rotation

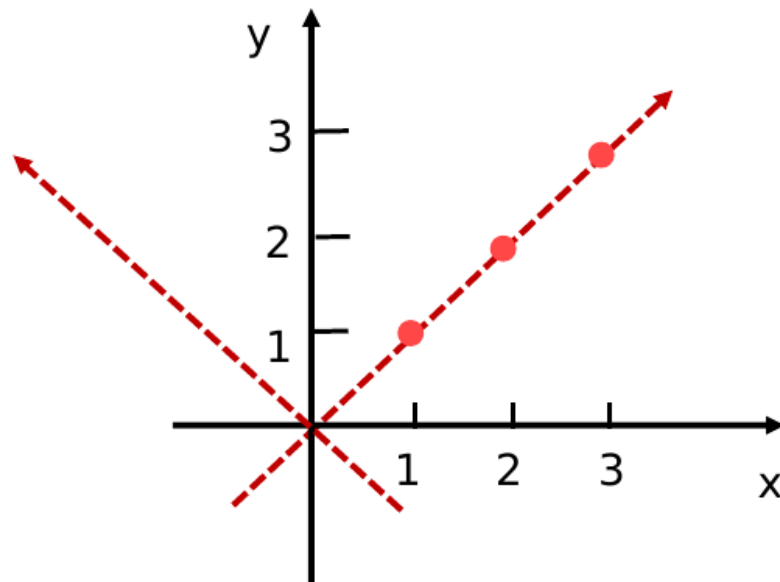
Drop second coordinate, **no** information is lost.

2D data reduced to 1D data

$$\mathbf{x}_1 = \begin{bmatrix} \sqrt{2} \\ \text{---} \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2\sqrt{2} \\ \text{---} \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 3\sqrt{2} \\ \text{---} \end{bmatrix}$$



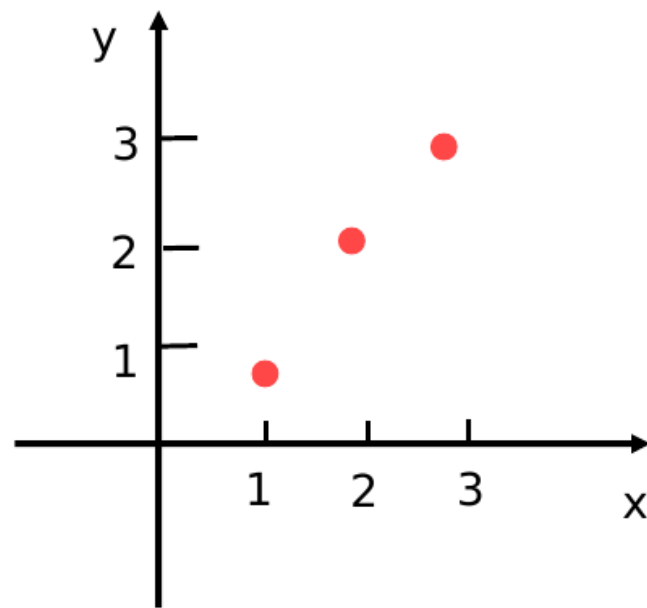
Dimensionality reduction with axis rotation (noisy case)

- Suppose points don't lie exactly on a line

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 0.9 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2.1 \\ 2 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 2.9 \\ 3.1 \end{bmatrix}$$



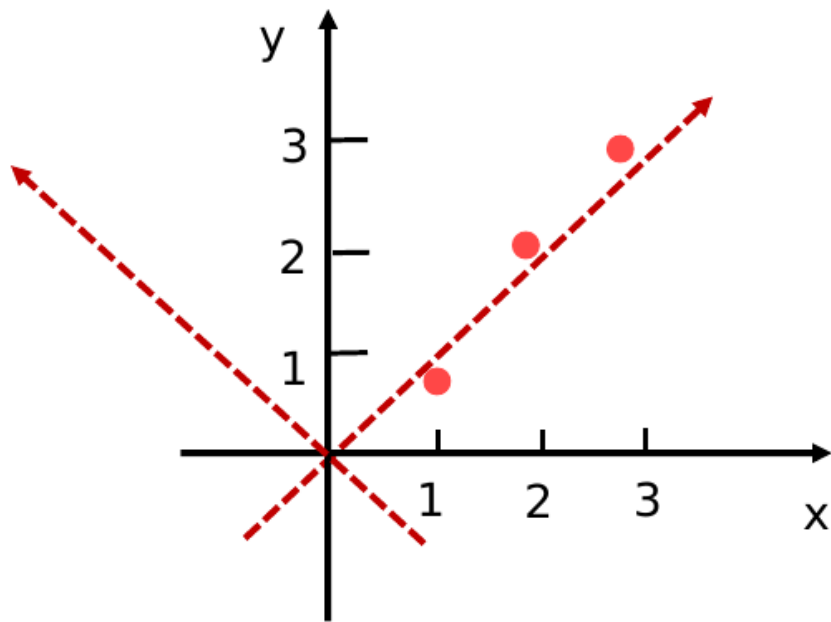
Dimensionality reduction with axis rotation (noisy case, cont.)

- Suppose points don't lie exactly on a line

$$\mathbf{x}_1 = \begin{bmatrix} 1.34 \\ 0.07 \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2.89 \\ 0.07 \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 4.24 \\ -0.14 \end{bmatrix}$$



Dimensionality reduction with axis rotation (noisy case, cont.)

- Suppose points don't lie exactly on a line

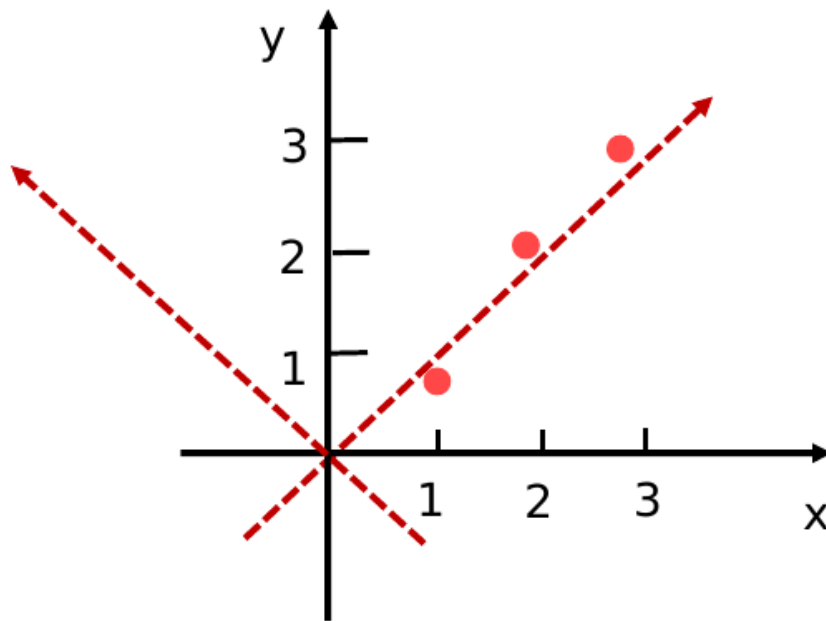
Drop second
coordinate,
some
information is
lost.

2D data
reduced to 1D
data

$$\mathbf{x}_1 = \begin{bmatrix} 1.34 \\ \text{0.07} \end{bmatrix}$$

$$\mathbf{x}_2 = \begin{bmatrix} 2.89 \\ \text{0.07} \end{bmatrix}$$

$$\mathbf{x}_3 = \begin{bmatrix} 4.24 \\ \text{-0.14} \end{bmatrix}$$



How does this work in reality?

- Change of axes **removes correlations** and **reduces dimensionality**
- Techniques
 - Principal Component Analysis (PCA)
 - Singular-Value Decomposition (SVD)

(Seen elsewhere: **not in the exams** on this subject, the next slides are just here for completeness)

Axis rotation - formulation

- Points are usually described with respect to the standard basis

$$\mathbf{x} = \begin{bmatrix} x^1 \\ x^2 \\ \vdots \\ x^d \end{bmatrix} \in \mathbb{R}^d \longleftrightarrow \mathbf{x} = x^1 \mathbf{e}_1 + x^2 \mathbf{e}_2 + \cdots + x^d \mathbf{e}_d$$

Axis rotation – formulation (cont.)

We will determine **new coordinates** under basis W :


$W = [\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_d]$ is a orthonormal matrix

$$\begin{aligned}\mathbf{x} &= WW^T \mathbf{x} = \left(\sum_{i=1}^d \mathbf{w}_i \mathbf{w}_i^T \right) \mathbf{x} = \sum_{i=1}^d \mathbf{w}_i (\mathbf{w}_i^T \mathbf{x}) \\ &= (\mathbf{w}_1^T \mathbf{x}) \mathbf{w}_1 + (\mathbf{w}_2^T \mathbf{x}) \mathbf{w}_2 + \dots + (\mathbf{w}_d^T \mathbf{x}) \mathbf{w}_d\end{aligned}$$

Thus, the new coordinates are

$$\mathbf{y} = \begin{bmatrix} \mathbf{w}_1^T \mathbf{x} \\ \mathbf{w}_2^T \mathbf{x} \\ \vdots \\ \mathbf{w}_d^T \mathbf{x} \end{bmatrix} \in \mathbb{R}^d$$

Vector \mathbf{x} has n dimensions, but
vector \mathbf{y} has $d \leq n$ dimensions

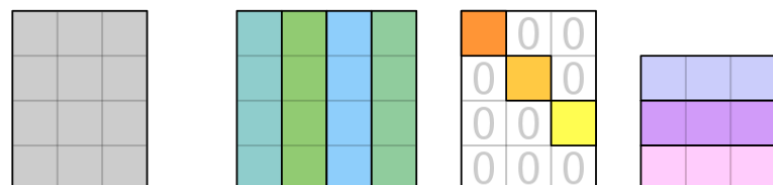


PCA formulation: optimization

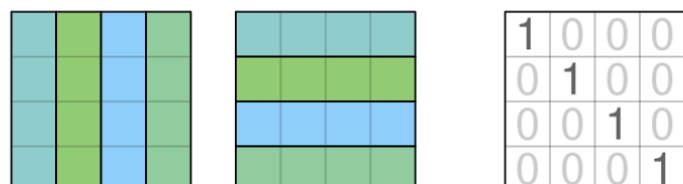
- Find new basis $\{ \mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k \}$, with $k \leq d$ such that the variance of this set is maximized:

$$\left\{ \mathbf{y}_1 = \begin{bmatrix} \mathbf{w}_1^\top \mathbf{x}_1 \\ \mathbf{w}_2^\top \mathbf{x}_1 \\ \vdots \\ \mathbf{w}_k^\top \mathbf{x}_1 \end{bmatrix}, \mathbf{y}_2 = \begin{bmatrix} \mathbf{w}_1^\top \mathbf{x}_2 \\ \mathbf{w}_2^\top \mathbf{x}_2 \\ \vdots \\ \mathbf{w}_k^\top \mathbf{x}_2 \end{bmatrix}, \dots, \mathbf{y}_n = \begin{bmatrix} \mathbf{w}_1^\top \mathbf{x}_n \\ \mathbf{w}_2^\top \mathbf{x}_n \\ \vdots \\ \mathbf{w}_k^\top \mathbf{x}_n \end{bmatrix} \right\}$$

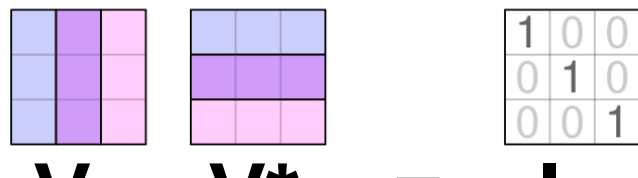
SVD formulation



$$\begin{matrix} \text{4} \times \text{4} \\ \mathbf{X} = & \begin{matrix} \text{4} \times \text{4} \\ \mathbf{U} \end{matrix} & \begin{matrix} \text{4} \times \text{4} \\ \mathbf{\Sigma} \end{matrix} & \begin{matrix} \text{4} \times \text{4} \\ \mathbf{V}^* \end{matrix} \end{matrix}$$



$$\begin{matrix} \text{4} \times \text{4} \\ \mathbf{U} \end{matrix} \quad \begin{matrix} \text{4} \times \text{4} \\ \mathbf{U}^* \end{matrix} = \begin{matrix} \text{4} \times \text{4} \\ \mathbf{I}_d \end{matrix}$$



$$\begin{matrix} \text{4} \times \text{4} \\ \mathbf{V} \end{matrix} \quad \begin{matrix} \text{4} \times \text{4} \\ \mathbf{V}^* \end{matrix} = \begin{matrix} \text{4} \times \text{4} \\ \mathbf{I}_n \end{matrix}$$

- \mathbf{U} and \mathbf{V} are rotation matrices; $\mathbf{\Sigma}$ is a scaling matrix
- The rotated data is obtained by multiplying $\mathbf{U}^T \mathbf{X}$

Algorithms for PCA and SVD

- PCA $\left\{ \begin{array}{l} 1. \text{ Calculate the mean vector } \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \\ 2. \text{ Calculate the covariance matrix } C = \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{x}_i - \bar{\mathbf{x}})^\top \\ 3. \text{ Calculate the } k\text{-largest eigenvectors of } C \end{array} \right.$
- SVD $\left\{ \begin{array}{l} 1. \text{ Calculate the mean vector } \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \\ 2. \text{ Calculate the } k \text{ largest left singular vectors of } \bar{X} = [\mathbf{x}_1 - \bar{\mathbf{x}}, \dots, \mathbf{x}_n - \bar{\mathbf{x}}] \end{array} \right.$

Summary

Things to remember

- Data sampling methods
- Why would we want to reduce dimensionality?
- What are the main techniques for doing so

Exercises for TT03-TT05

- Exercises 3.7 of Data Mining Concepts and Techniques, 3rd edition (2011) by Han et al.
- Exercises 2.6 of Introduction to Data Mining, Second Edition (2019) by Tan et al.
 - Mostly the first exercises, say 1-6