Data Preparation: Reduction and Transformation

Mining Massive Datasets

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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

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≃ "Less rows"
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Dimensionality Reduction or Feature Selection

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≃ "Less columns"
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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 ...

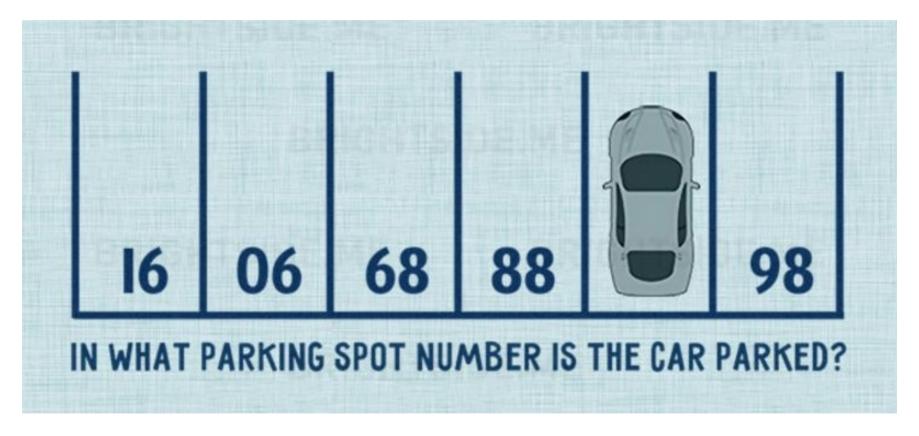
Reducing data dimensionality

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 twodimensional space

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

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

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

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

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

Coordinates after axes rotation

$$\mathbf{x}_{1} = \begin{bmatrix} \sqrt{2} \\ 0 \end{bmatrix} \qquad \qquad \mathbf{y}$$

$$\mathbf{x}_{2} = \begin{bmatrix} 2\sqrt{2} \\ 0 \end{bmatrix} \qquad \qquad \mathbf{z}$$

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

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

Coordinates after axes rotation

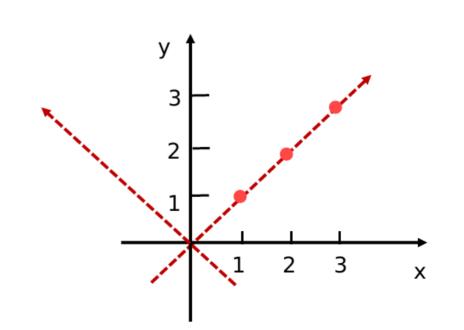
Drop second coordinate, **no** information is lost.

2D data reduced to 1D data

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

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

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



Dimensionality reduction with axis rotation (noisy case)

• Suppose points don't lie exactly on a line

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

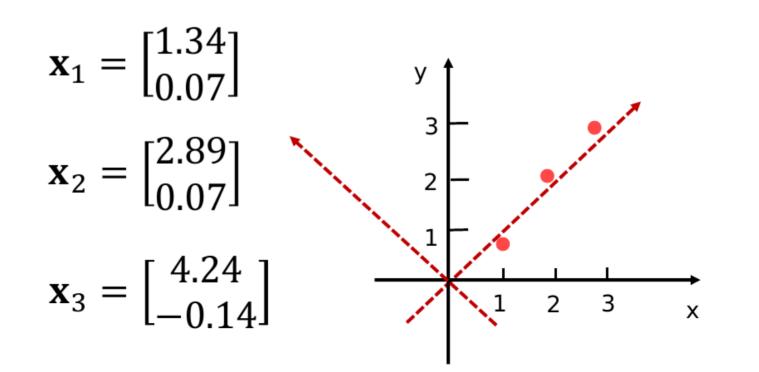
$$\mathbf{x}_{2} = \begin{bmatrix} 2.1 \\ 2 \end{bmatrix}$$

$$\mathbf{x}_{3} = \begin{bmatrix} 2.9 \\ 3.1 \end{bmatrix}$$

$$\mathbf{x}_{3} = \begin{bmatrix} 2.9 \\ 3.1 \end{bmatrix}$$

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

• Suppose points don't lie exactly on a line



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

Suppose points don't lie exactly on a line

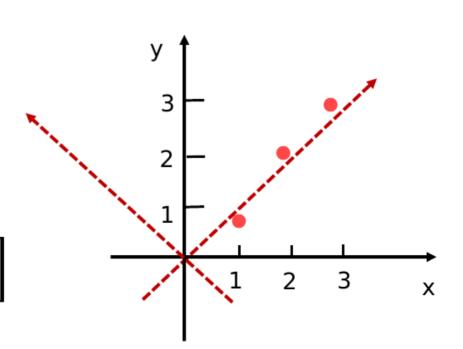
Drop second coordinate, some information is lost.

2D data reduced to 1D data

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

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

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



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

$$\mathbf{x} = \begin{bmatrix} x^{1} \\ x^{2} \\ \vdots \\ x^{d} \end{bmatrix} \in \mathbb{R}^{d} \iff \mathbf{x} = x^{1} \mathbf{e}_{1} + x^{2} \mathbf{e}_{2} + \dots + x^{d} \mathbf{e}_{d}$$

Axis rotation – formulation (cont.)

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

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

$$\mathbf{x} = WW^{\mathsf{T}}\mathbf{x} = \left(\sum_{i=1}^{d} \mathbf{w}_{i} \mathbf{w}_{i}^{\mathsf{T}}\right) \mathbf{x} = \sum_{i=1}^{d} \mathbf{w}_{i} (\mathbf{w}_{i}^{\mathsf{T}} \mathbf{x})$$
$$= (\mathbf{w}_{1}^{\mathsf{T}} \mathbf{x}) \mathbf{w}_{1} + (\mathbf{w}_{2}^{\mathsf{T}} \mathbf{x}) \mathbf{w}_{2} + \dots + (\mathbf{w}_{d}^{\mathsf{T}} \mathbf{x}) \mathbf{w}_{d}$$

Thus, the new coordinates are

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

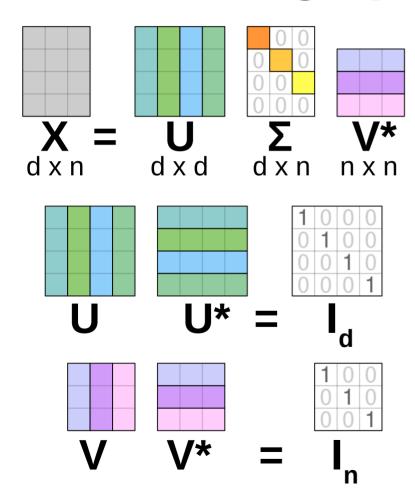
Vector x has n dimensions, but vector y has $d \le n$ dimensions

PCA formulation: optimization

• Find new basis $\{w_1, w_2, ..., w_k\}$, with $k \le d$ such that the variance of this set is maximized:

$$\left\{\mathbf{y}_{1} = \begin{bmatrix} \mathbf{w}_{1}^{\mathsf{T}} \mathbf{x}_{1} \\ \mathbf{w}_{2}^{\mathsf{T}} \mathbf{x}_{1} \\ \vdots \\ \mathbf{w}_{k}^{\mathsf{T}} \mathbf{x}_{1} \end{bmatrix}, \mathbf{y}_{2} = \begin{bmatrix} \mathbf{w}_{1}^{\mathsf{T}} \mathbf{x}_{2} \\ \mathbf{w}_{2}^{\mathsf{T}} \mathbf{x}_{2} \\ \vdots \\ \mathbf{w}_{k}^{\mathsf{T}} \mathbf{x}_{2} \end{bmatrix}, \cdots, \mathbf{y}_{n} = \begin{bmatrix} \mathbf{w}_{1}^{\mathsf{T}} \mathbf{x}_{n} \\ \mathbf{w}_{2}^{\mathsf{T}} \mathbf{x}_{n} \\ \vdots \\ \mathbf{w}_{k}^{\mathsf{T}} \mathbf{x}_{n} \end{bmatrix} \right\}$$

SVD formulation



- U and V are rotation matrices; Σ is a scaling matrix
- The rotated data is obtained by multiplying U^TX

Algorithms for PCA and SVD

- PCA $\begin{cases} \textbf{1.} & \text{Calculate the mean vector } \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \\ \textbf{2.} & \text{Calculate the covariance matrix } \mathcal{C} = \\ & \frac{1}{n} \sum_{i=1}^n (\mathbf{x}_i \bar{\mathbf{x}}) (\mathbf{x}_i \bar{\mathbf{x}})^{\mathsf{T}} \\ \textbf{3.} & \text{Calculate the k-largest eigenvectors of \mathcal{C}} \end{cases}$

- SVD $\begin{cases} \textbf{1.} & \text{Calculate the mean vector } \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_i \\ \textbf{2.} & \text{Calculate the } k \text{ largest left singular vectors of } \bar{X} = [\mathbf{x}_1 \bar{\mathbf{x}}, ..., \mathbf{x}_n \bar{\mathbf{x}}] \end{cases}$

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