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KYOTO UNIVERSITY

Statistical Learning Theory
- Introduction -

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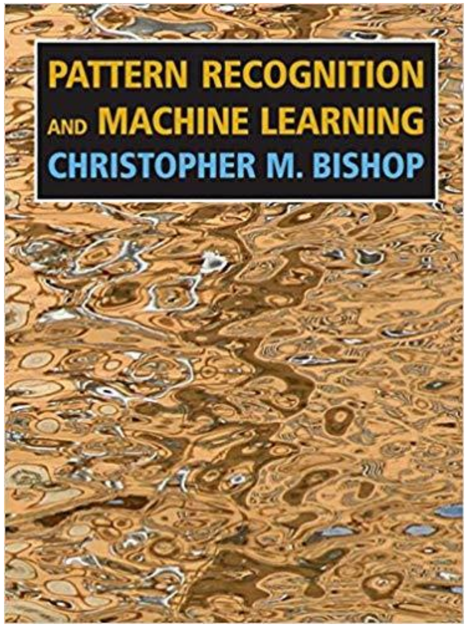
AND TECHNOLOGY

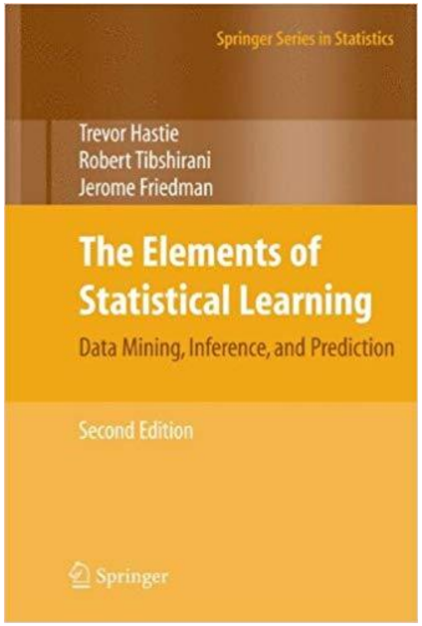
Statistical learning theory:
Foundations of recent data analysis technologies

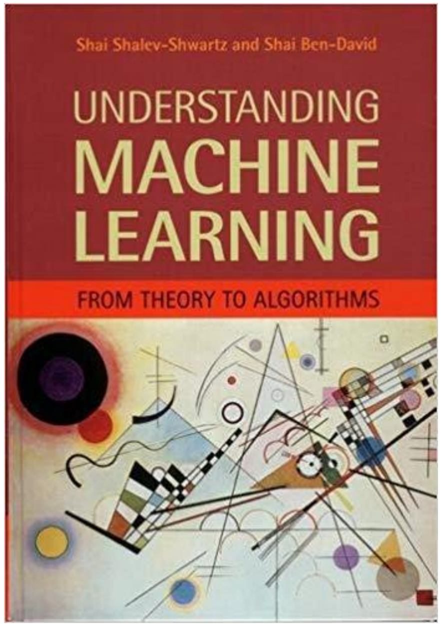
- This lecture will cover:
  - Basic ideas, problems, solutions, and applications of statistical machine learning
    - Supervised & unsupervised learning
    - Models & algorithms: linear regression, SVM, neural nets, …
  - Statistical learning theory
    - Theoretical foundation of statistical machine learning
  - Hands-on practice
- Advanced topics: TBD

Textbooks?:
Most of the topics can be found in...

- Pattern recognition and machine learning / Bishop
- The elements of statistical learning / Hastie & Tibshirani
- Understanding machine learning / Shalev-Shwartz & Ben-David




Springer Series in Statistics
Trevor Hastie
Robert Tibshirani
Jerome Friedman
The Elements of Statistical Learning
Data Mining, Inference, and Prediction
Second Edition
Springer


Shai Shalev-Shwartz and Shai Ben-David
UNDERSTANDING MACHINE LEARNING
FROM THEORY TO ALGORITHMS

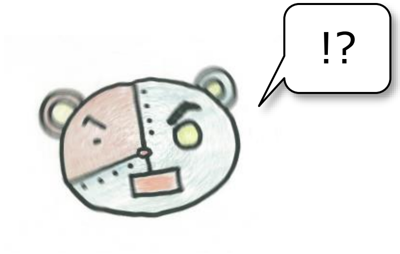
Evaluations:
Final Exam is All You Need

- Evaluation is based on the final exam
- The examination is a standard written exam and does not allow the use of reference materials.

Introduction:
Basic ideas of machine learning and applications

1. What is machine learning?
2. Machine learning applications
3. Some machine learning topics
    1. Recommender systems
    2. Anomaly detection

What is machine learning?



“The third A.I. boom”: Machine learning is a core technology

- You can see many successes of “Artificial Intelligence”:
  - Q.A. machine beating quiz champions and Go program surpassing top players
  - Protein folding, that was thought to be unsolvable, was solved
  - Are large language models (LLMs) the realization of general-purpose artificial intelligence?
- Current A.I. boom owes machine learning
  - Especially, deep learning

What is machine learning? ：
A branch of artificial intelligence

- Originally started as a branch of artificial intelligence
  - has its more-than-50-years history
  - Computer programs that “learns” from experience
  - Based on logical inference
- Pioneers who invented the computer also already dreamed of realizing artificial intelligence

What is machine learning?：
A data analytics technology

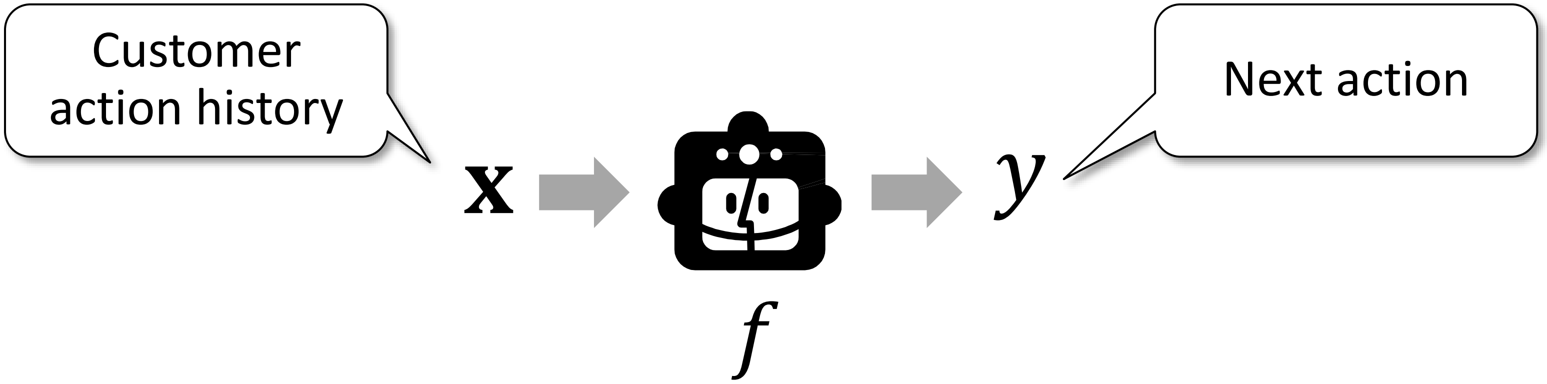
- Rise of “statistical” machine learning
  - Successes in bioinformatics, natural language processing, and other business areas
- Recently rather considered as a data analysis technology
  - Buzzwords: “big data” and “data scientist”
    - Data scientist is “the sexiest job in the 21st century” (?)
- Led the success of deep learning
  - The 3rd AI boom

What can machine learning do?: Prediction, discovery, … and generation

1. Prediction
   - “What will happen in future data?”
   - Given past data, predict about future data
2. Discovery
   - “What is happening in data in hand?”
   - Given past data, find insights in them
3. Data generation
   - “Generate new data satisfying certain properties”
   - Given past data, generate similar data

Prediction machine:
A function from a vector to a scalar

- We model the intelligent machine as a mathematical function
- Relationship of input and output $f: \mathbf{x} \to y$
  - Input $\mathbf{x} = (x_1, x_2, \ldots, x_D)^\top \in \mathbb{R}^D$ is a D-dimensional vector
  - Output y is one dimensional
    - Regression: real-valued output $y \in \mathbb{R}$
    - Classification: discrete output $y \in \{C_1, C_2, \ldots, C_M\}$



Customer action history

$\mathbf{x}$

f

y

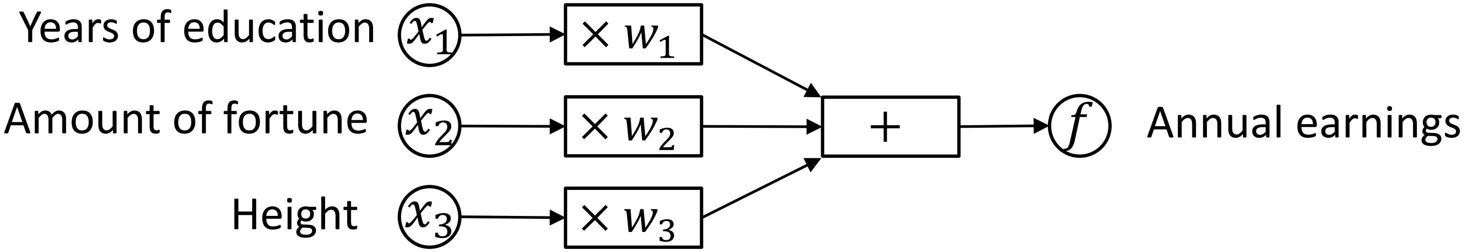
Next action

A model for regression: Linear regression model

- Model f takes an input $\mathbf{x} = (x_1, x_2, \dots, x_D)^\top$ and outputs a real value

$$\boxed{f(\mathbf{x}) = w_1 x_1 + w_2 x_2 + \cdots + w_D x_D}$$

  – Model parameter $\mathbf{w} = (w_1, w_2, \dots, w_D)^\top \in \mathbb{R}^D$

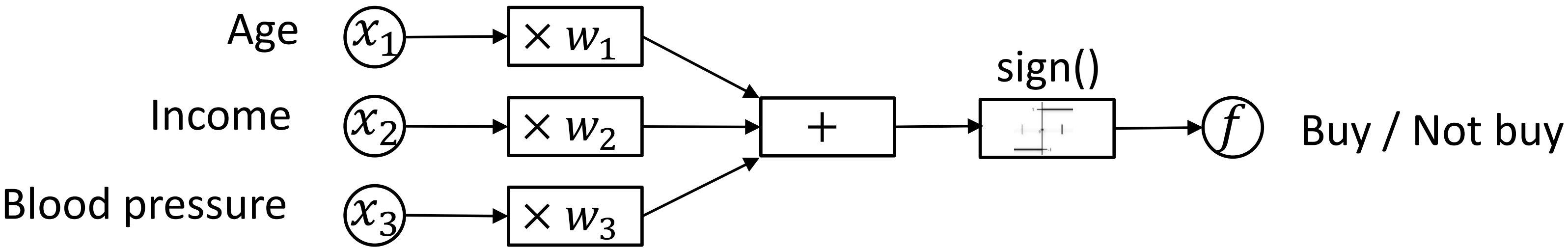


A model for classification: Linear classification model

- Model f takes an input $\mathbf{x} = (x_1, x_2, \ldots, x_D)^\top$ and outputs a value from $\{+1, -1\}$ (class label)

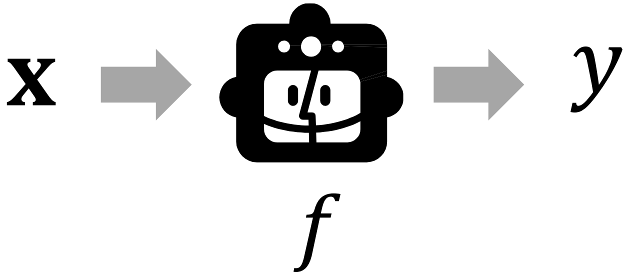
$$\boxed{f(\mathbf{x}) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D)}$$

  - Model parameter $\mathbf{w} = (w_1, w_2, \ldots, w_D)^\top \in \mathbb{R}^D$:
    - w_d : contribution of x_d to the output (if $w_d > 0$, $x_d > 0$ contributes to $+1$, $x_d < 0$ contributes to -1)

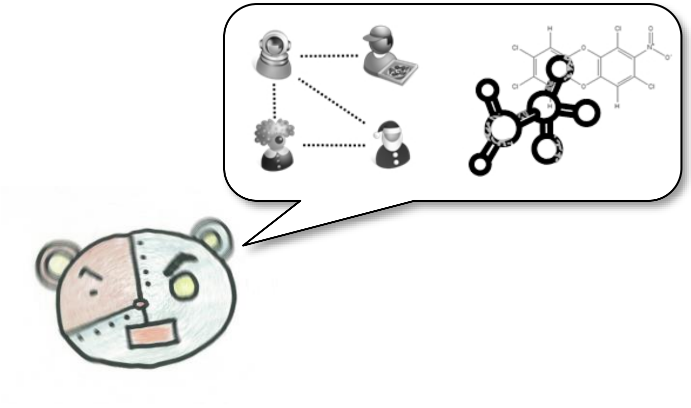


Formulations of machine learning problems: Supervised learning and unsupervised learning

- What we want is the function f, or its parameters $\mathbf{w}$
  - We estimate f (or $\mathbf{w}$) from data
- Two learning problem settings: supervised and unsupervised
  - Supervised learning: input-output pairs are given
    - $\left\{\left(\mathbf{x}^{(1)}, y^{(1)}\right), \left(\mathbf{x}^{(2)}, y^{(2)}\right), \ldots, \left(\mathbf{x}^{(N)}, y^{(N)}\right)\right\}$: N pairs
  - Unsupervised learning: only inputs are given
    - $\left\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\right\}$: N inputs

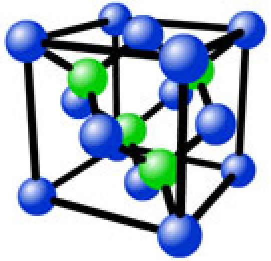


Machine learning applications



Growing ML applications:
Emerging applications from IT areas to non-IT areas

- Recent advances in ML offer:
  - Methodologies to handle uncertain and enormous data
  - Black-box tools
- Not limited to IT-related areas, ML is wide-spreading over non-IT areas
  - Healthcare, airline, automobile, material science, education, …



Various applications of machine learning:
From on-line shopping to system monitoring

- Marketing
  - Recommendation
  - Sentiment analysis
  - Web ads optimization

- Finance
  - Credit risk estimation
  - Fraud detection

- Science
  - Biology
  - Material science

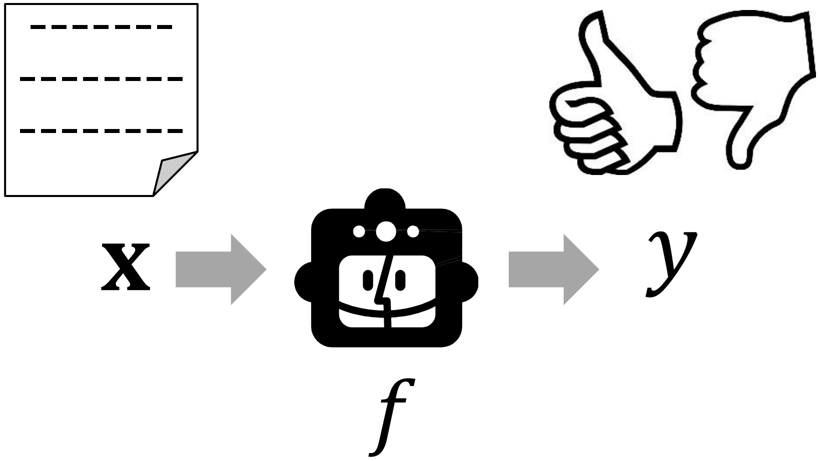
- Web
  - Search
  - Spam filtering
  - Social media

- Healthcare
  - Medical diagnosis

- Multimedia
  - Image/voice understanding
- System monitoring
  - Fault detection

An application of supervised classification learning: Sentiment analysis

- Judge if a document $(\mathbf{x})$ is positive or not $(y \in \{+1, -1\})$ toward a particular product or service
- For example, we want to know reputation of our new product S, and gain marketing insights
- Collect tweets by searching the word "S", and analyze them

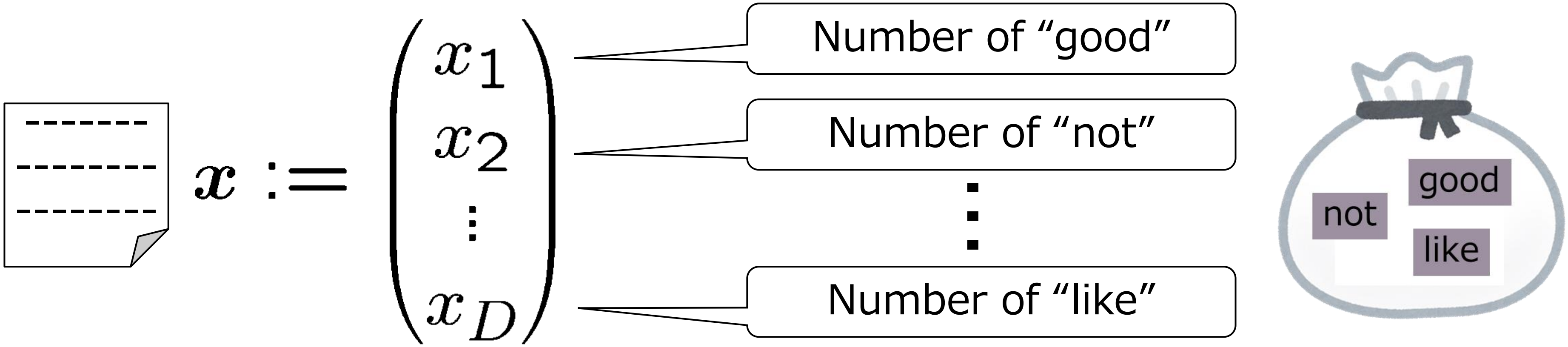


An application of supervised learning:
Some hand labeling followed by supervised learning

- First, give labels to some of the collected documents
  - 10,000 tweets hit the word “S”
  - Manually read 300 of them and give sentiment labels
    - ”I used S, and found it not bad.” → 👍
    - “I gave up S. The power was not on.” → 👎
    - “I like S.” → 👍
- Use the collected 300 labels to train a predictor.
  Then apply the predictor to the rest 9,700 documents

How to represent a document as a vector: bag-of-words representation

- Represent a document $\mathbf{x}$ using words appearing in it



$$\boldsymbol{x} := \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{pmatrix}$$

bag-of-words representation

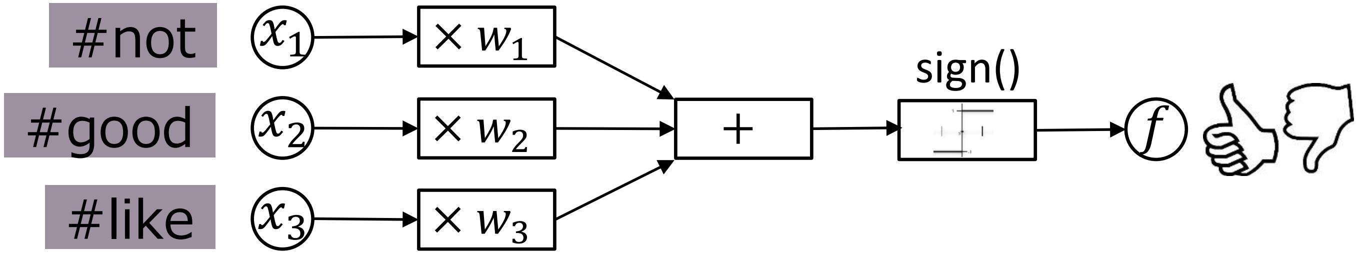
- Note: design of the feature vector is left to users

A simple model for sentiment analysis: Linear binary classification model

- Model f takes a BoW vector $\mathbf{x} = (x_1, x_2, \ldots, x_D)^\top$ and outputs a sentiment label from $\{+1, -1\}$:

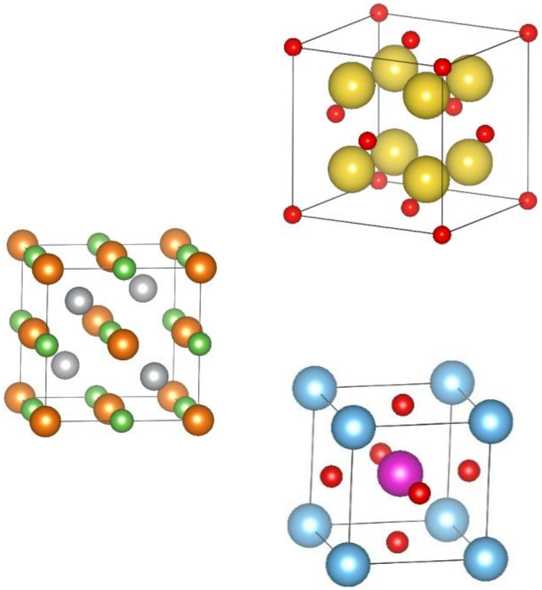
$$f(\mathbf{x}) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D)$$

  - Model parameter $\mathbf{w} = (w_1, w_2, \ldots, w_D)^\top \in \mathbb{R}^D$:
    - w_d : contribution of the d-th word (e.g. “good”) to the sentiment label



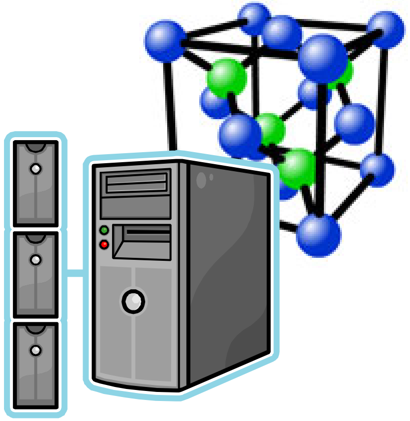
An application of supervised *regression* learning: Discovering new materials

- Material science aims at discovering and designing new materials with desired properties
  - Volume, density, elastic coefficient, thermal conductivity, …
- Traditional approach (try-and-error):
  1. Determine chemical structure
  2. Synthesize the chemical compounds
  3. Measure their physical properties



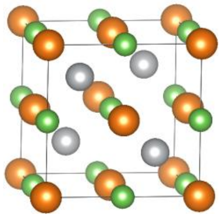
Computational approach to material discovery: Still needs high computational costs

- Computational approach: First-order principle calculations based on quantum physics to run simulation to estimate physical properties
- First-order calculation still requires high computational costs
  - Proportional to the cubic number of atoms
  - Sometimes more than a week or a month…



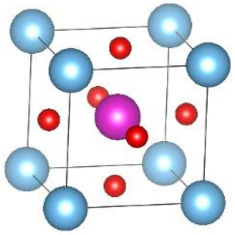
Data driven approach to material discovery:
Regression to predict physical properties

- Predict the result of first-order principle calculation from data



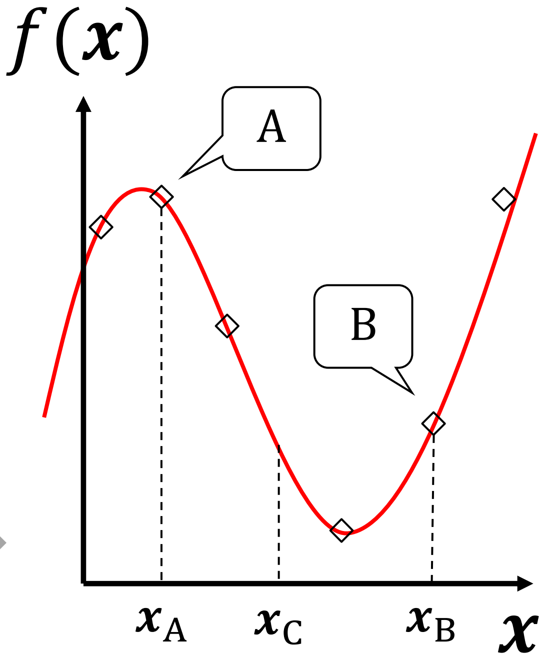
Compound A

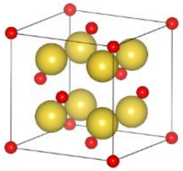
$$\boldsymbol{x}_{\mathrm{A}} = \begin{pmatrix} 1.5 \\ 140 \\ 3 \\ 72 \\ \vdots \\ 0.32 \end{pmatrix}$$



Compound B

$$\boldsymbol{x}_{\mathrm{B}} = \begin{pmatrix} 1.8 \\ 210 \\ 5 \\ 64 \\ \vdots \\ 0.15 \end{pmatrix}$$





New compound C

$$\downarrow f(\boldsymbol{x})$$

Predicted Physical property $\boxed{0.62}$

Feature vector representation of chemical compounds

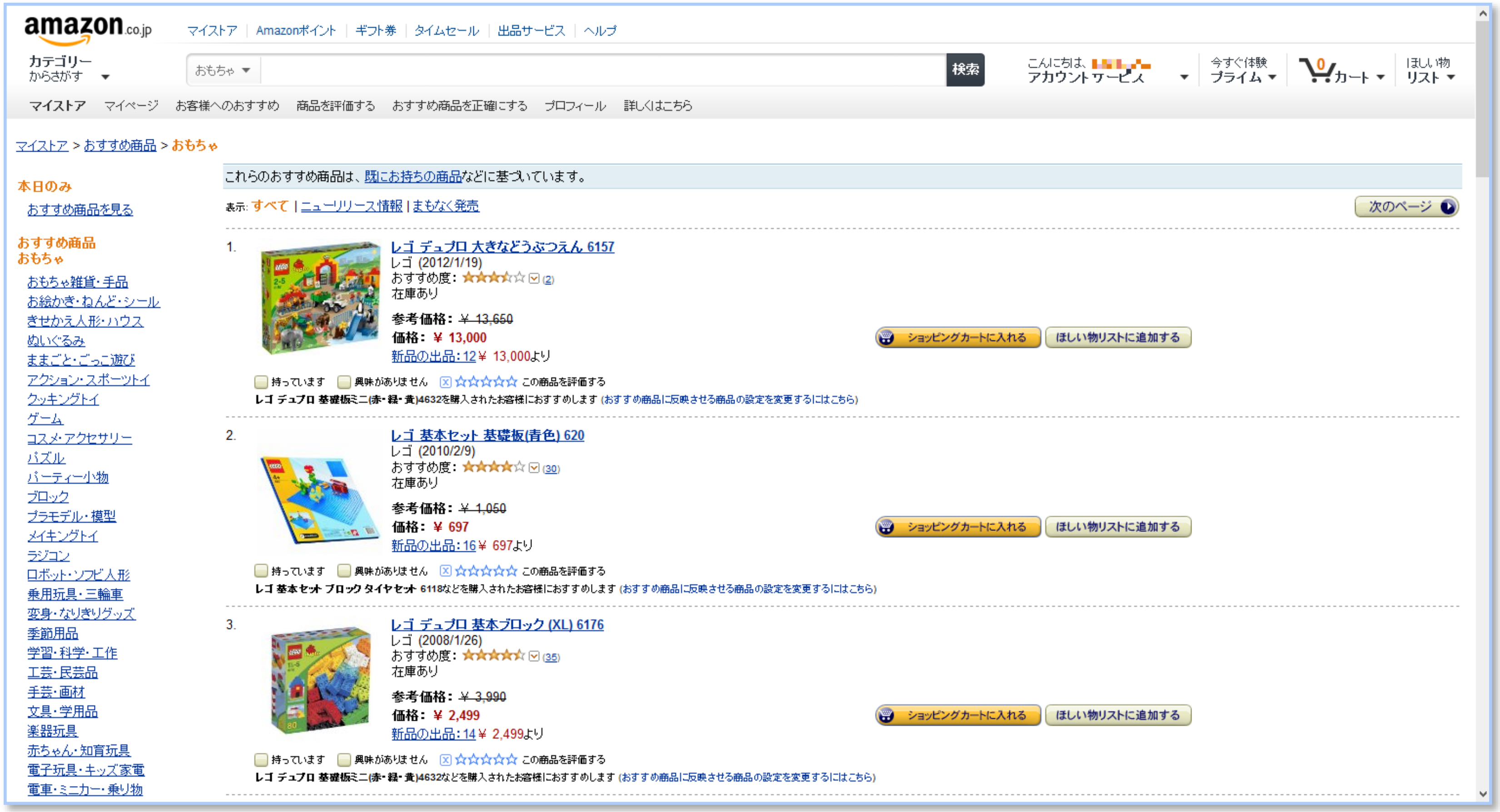
Estimate regression models of physical properties from data

Predict physical properties of new compounds

Recommendation systems

Recommender systems: Personalized information filter

- Amazon offers a list of products I am likely to buy (based on my purchase history)



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Ubiquitous recommender systems:
Recommender systems are present everywhere

- A major battlefield of machine learning algorithms
  - 2006-2009: Netflix challenge (with $100 million prize)
- Recommender systems are present everywhere:
  - Product recommendation in online shopping stores
  - Friend recommendation on SNSs
  - Information recommendation (news, music, …)
  - …

Welcome!

The Netflix Prize seeks to substantially improve the accuracy of predictions about how much someone is going to love a movie based on their movie preferences. Improve it enough and you win one (or more) Prizes. Winning the Netflix Prize improves our ability to connect people to the movies they love.

Read the Rules to see what is required to win the Prizes. If you are interested in joining the quest, you should register a team.

You should also read the frequently-asked questions about the Prize. And check out how various teams are doing on the Leaderboard.

Good luck and thanks for helping!

FAQ | Forum | Netflix Home
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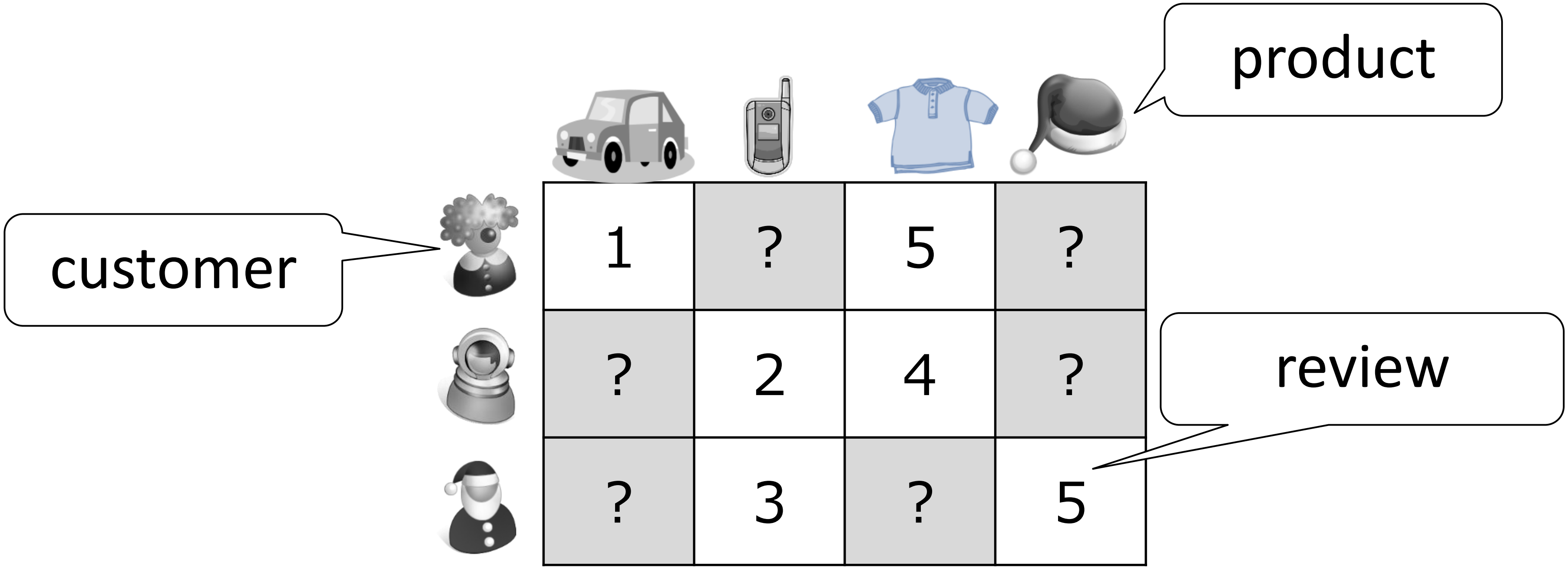
A formulation of recommendation problem: Matrix completion

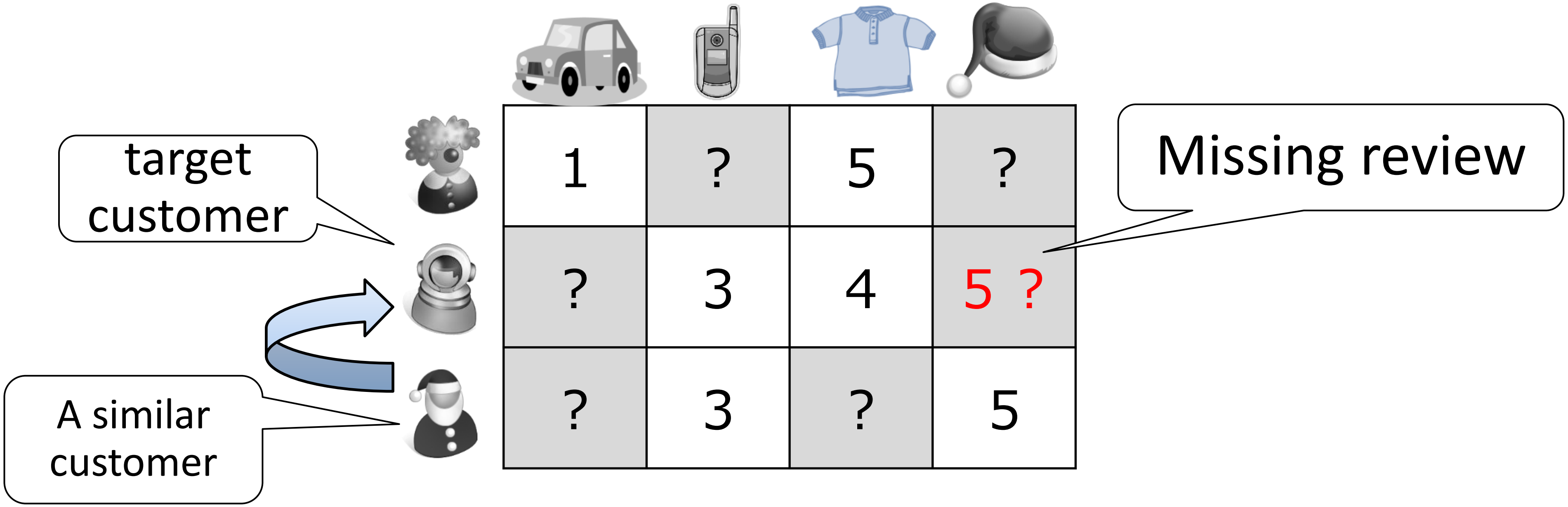
- A matrix with rows (customers) and columns (products)
  - Each element = review score $\in \{1,2,3,4,5,?\}$
- Given observed parts of the matrix, predict the unknown parts ($\boxed{?}$)



1	?	5	?
?	2	4	?
?	3	?	5

Basic idea of recommendation algorithms: “Find people like you”

- GroupLens: an earliest algorithm (for news recommendation)
  - Inherited by MovieLens (for Movie recommendation)
- Find people similar to the target customer, and predict missing reviews with theirs



target customer

A similar customer

Missing review

1	?	5	?
?	3	4	5 ?
?	3	?	5

GroupLens: Weighted prediction using correlations among customers

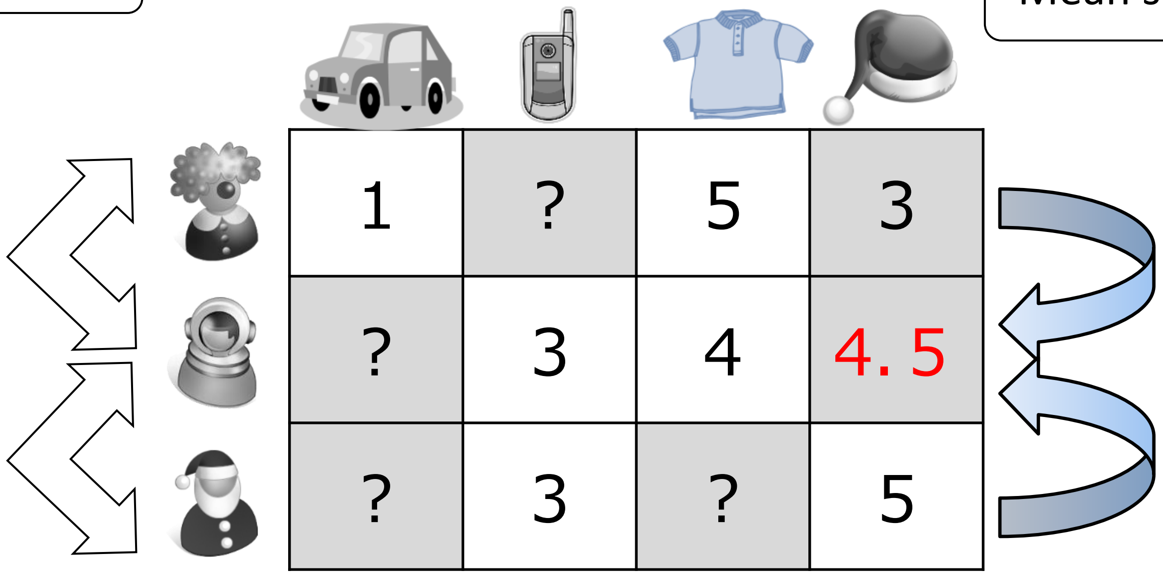
- Define customer similarity by correlation（of observed parts）
- Prediction by weighted averaging with correlations：

$$\hat{y}_{i,j} = \bar{y}_i + \sum_{k\neq i} r_{i,k} \left(y_{k,j} - \bar{y}_k \right) / \sum_{k\neq i} |r_{ij}|$$

Mean score of user i

Pearson correlation between users i and k

Mean score of user k



1	?	5	3
?	3	4	4. 5
?	3	?	5

correlation

correlation

weighted averaging

Low-rank assumption for matrix completion: GroupLens implicitly assumes low-rank matrices

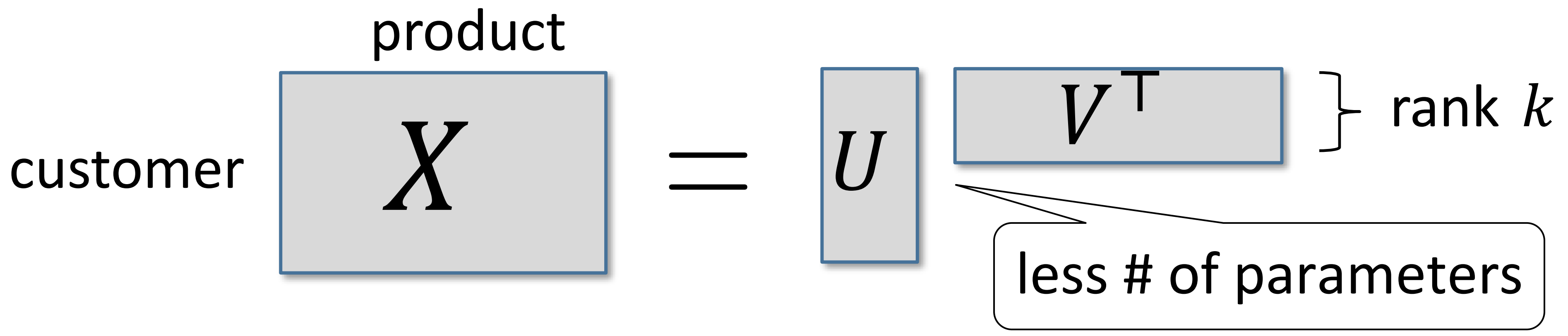
- Assumption of GroupLens algorithm:
  Each row is represented by a linear combination of the other rows (i.e. “linearly dependent”)

⇒ The matrix is not full-rank （≒ low-rank）

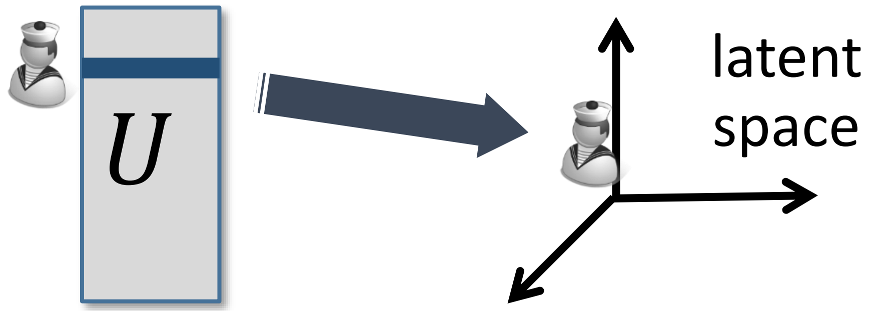
- Low-rank assumption helps matrix completion

Low-rank matrix factorization: Projection onto low-dimensional latent space

- Low-rank matrix: product of two (thin) matrices



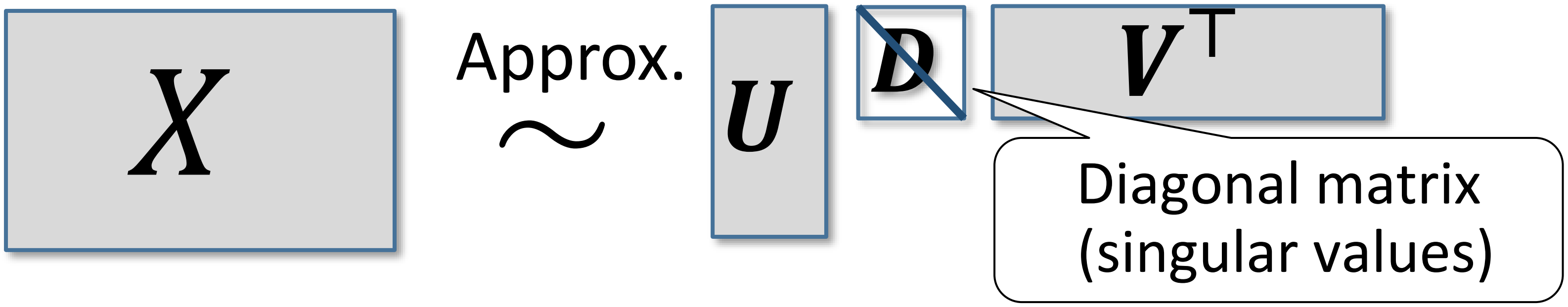
- Each row of $\boldsymbol{U}$ and $\boldsymbol{V}$ is an embedding of each customer (or product) onto low-dimensional latent space
  - Similar users/items are put close to each other



Low-rank matrix decomposition methods: Singular value decomposition (SVD)

- Find a best low-rank approximation of a given matrix

$$\underset{\boldsymbol{Y}}{\text{minimize}} \ \| \boldsymbol{X} - \boldsymbol{Y} \|_{\mathrm{F}}^2 \ \text{ s.t. } \operatorname{rank}(\boldsymbol{Y}) \le k$$

- Singular value decomposition (SVD):
  - 

    Diagonal matrix (singular values)

    w.r.t. the constraints: $\boldsymbol{U}^\top\boldsymbol{U} = \boldsymbol{I}, \ \boldsymbol{V}^\top\boldsymbol{V} = \boldsymbol{I}$
  - The k leading eigenvectors of $\boldsymbol{X}^\top\boldsymbol{X}$ best approximate

Strategies for matrices with missing values: EM algorithm, gradient descent, and trace norm

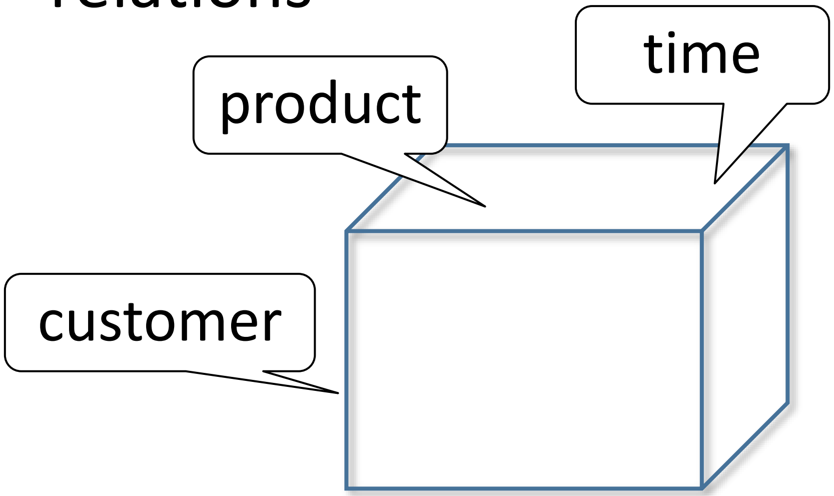
- SVD is not directly applicable to matrices with missing values
  - Our goal is to fill in missing values in a partially observed matrix
- For completion problem:
  - Direct application of SVD to a (somehow) filled matrix
  - Iterative applications: iterations of completion and decomposition
- For large scale data:
  Gradient descent using only observed parts
- Convex formulation: Trace norm constraint

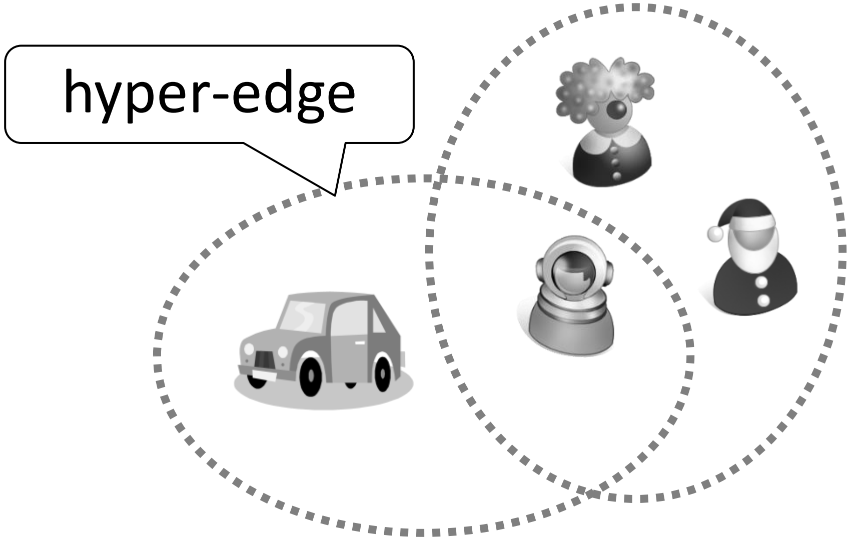
Predicting more complex relations: Multinomial relations

- Matrices can represent only one kind of relations
  - Various kinds of relations (actions):
    Review scores, purchases, browsing product information, …
  - Correlations among actions might help
- Multinomial relations:
  - (customer, product, action)-relation:
    (Alice, iPad, buy) represents “Alice bought an iPad.”
  - (customer, product, time)-relation:
    (John, iPad, July 12th) represents “John bought an iPad on July 12th.”

Multi-dimensional arrays:
Representation of multinomial relations

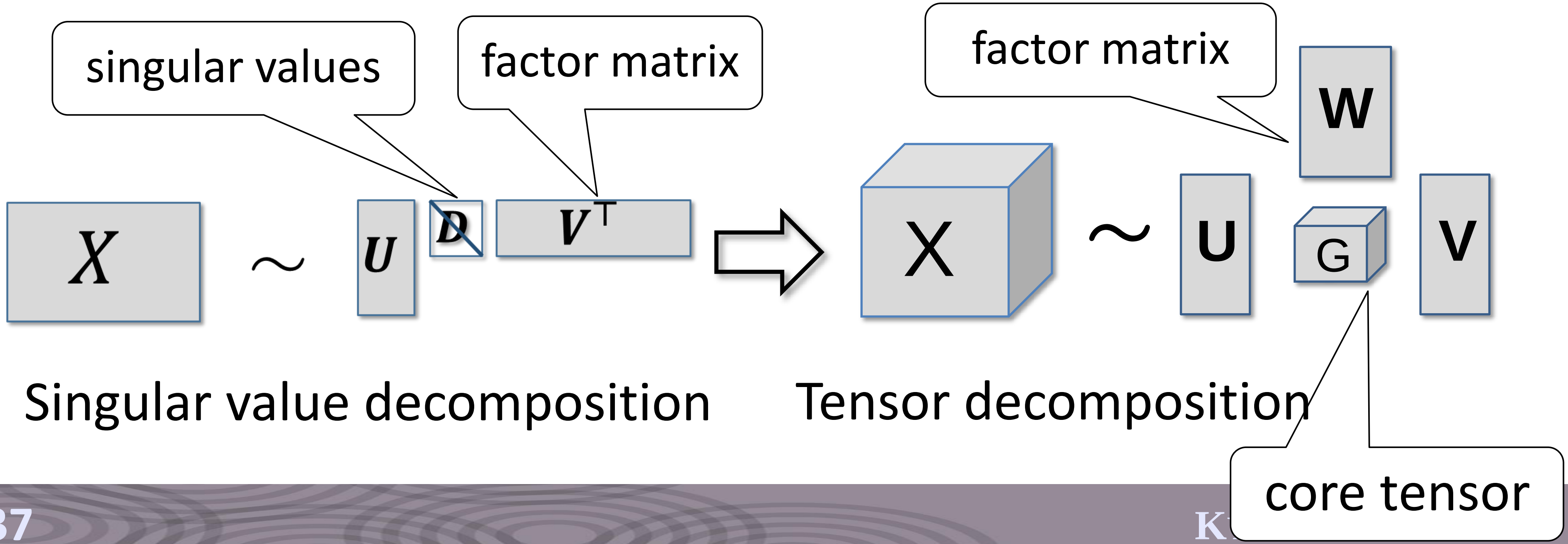
- Multidimensional array: Representation of complex relations among multiple objects
  - Types of relations (actions, time, conditions, …)
  - Relations among more than two objects
- Hypergraph: allows variable number of objects involved in relations





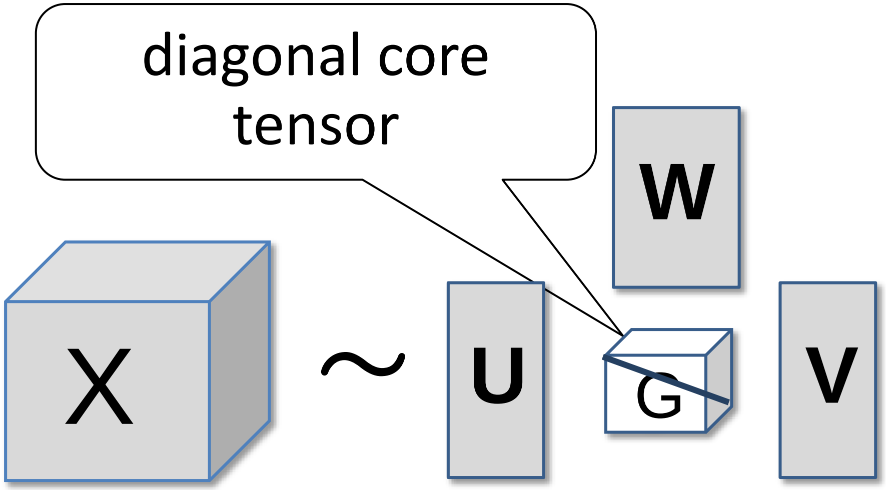
Tensor decomposition:
Generalization of low-rank matrix decomposition

- Generalization of matrix decomposition to multidimensional arrays
  - A small core tensor and multiple factor matrices
- Increasingly popular in machine learning/data mining

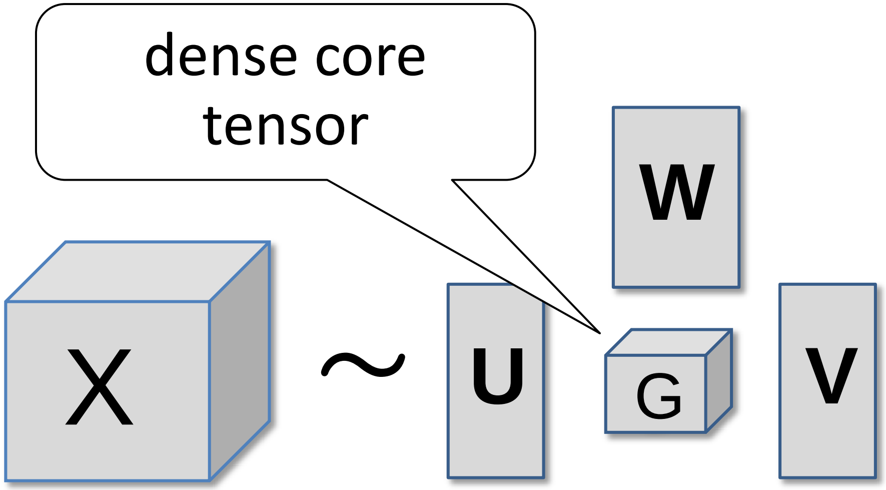


Tensor decompositions:
CP decomposition and Tucker decomposition

- CP decomposition: A natural extension of SVD (with a diagonal core)
- Tucker decomposition: A more compact model (with a dense core)


diagonal core tensor

CP decomposition


dense core tensor

Tucker decomposition

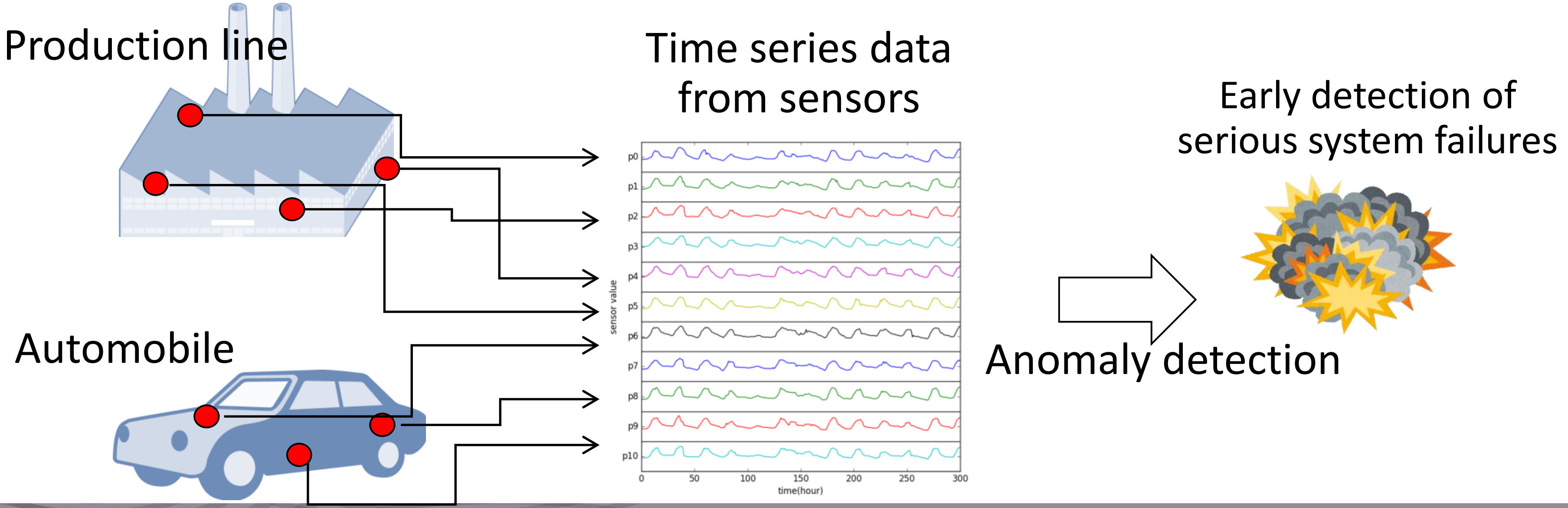
Applications of tensor decomposition: Tag recommendation, social network analysis, …

- Personalized tag recommendation (user×webpage×tag)
  - predicts tags a user gives a webpage
- Social network analysis (user×user×time)
  - analyzes time-variant relationships
- Web link analysis
  (webpage×webpage×anchor text)
- Image analysis (image×person×angle×light×…)

Anomaly detection

Anomaly detection:
Early warning for system failures reduces costs

- A failure of a large system can cause a huge loss
  - Breakdown of production lines in a factory, infection of computer virus/intrusion to computer systems, credit card fraud, terrorism, …
- Modern systems have many sensors to collect data
- Early detection of failures from data collected from sensors



Production line

Automobile

Time series data from sensors

Anomaly detection

Early detection of serious system failures

Anomaly detection techniques: Find “abnormal” behaviors in data

- We want to find precursors of failures in data
  - Assumption: Precursors of failures are hiding in data
- Anomaly: An “abnormal” patterns appearing in data
  - In a broad sense, state changes are also included: appearance of news topics, configuration changes, …
- Anomaly detection techniques find such patterns from data and report them to system administrators

Difficulty in anomaly detection: Failures are rare events

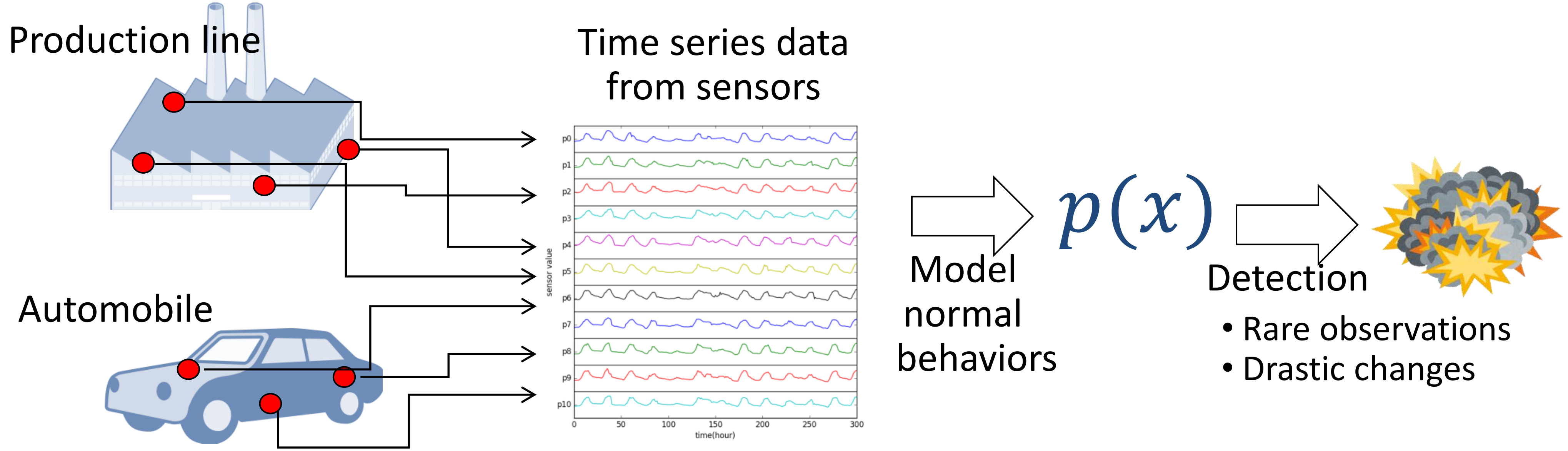
- If target failures are known ones, they are detected by using supervised learning:

  1. Construct a predictive model from past failure data
  2. Apply the model to system monitoring

- However, serious failures are usually rare, and often new ones → (Almost) no past data are available
- Supervised learning is not applicable

An alternative idea:
Model the normal times, detect deviations from them

- Difficult to model anomalies → Model normal times
  - Data at normal times are abundant
- Report “strange” data according to the normal time model
  - Observation of rare data is a precursor of failures



Production line

Automobile

Time series data from sensors

Model normal behaviors

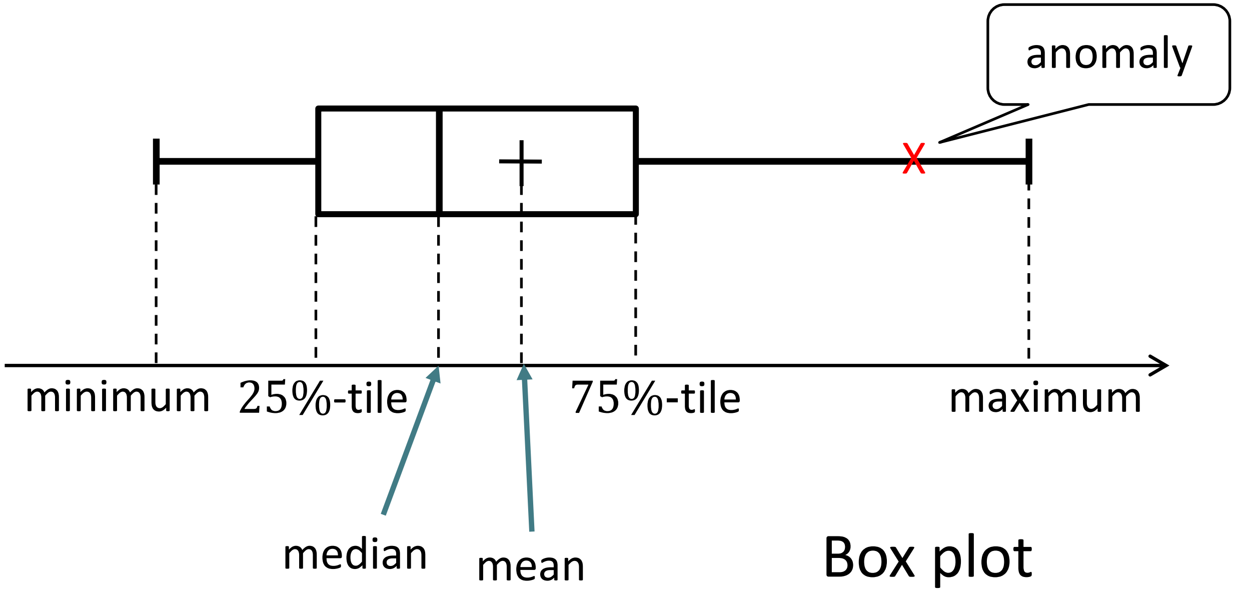
$p(x)$

Detection

- Rare observations
- Drastic changes

A simple unsupervised approach:
Anomaly detection using thresholds

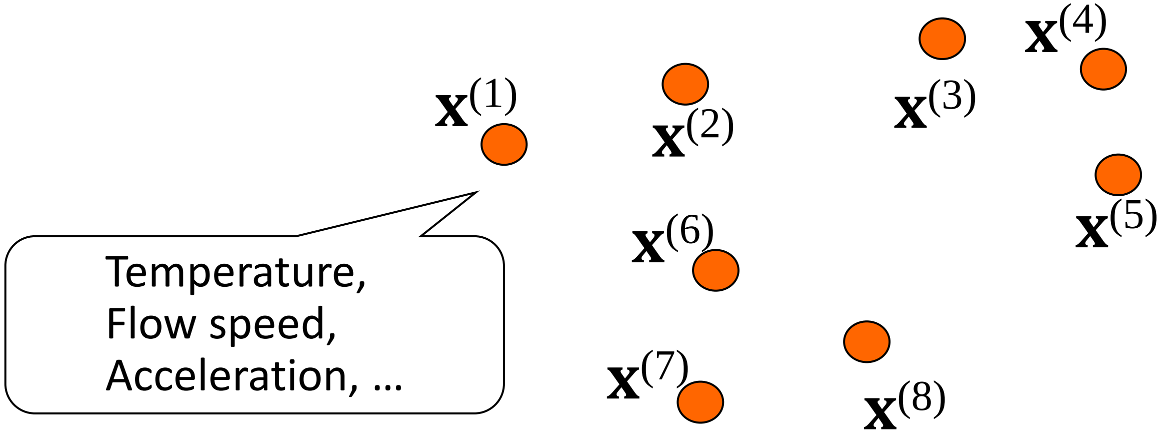
- Suppose a 1-dimensional case (e.g. temperature)
- Find the value range of the normal data (e.g. 20-50 ℃)
- Detect values deviates from the range, and report them as anomalies （e.g. 80℃ is not in the normal range)



Box plot

Clustering for high-dimensional anomaly detection: Model the normal times by grouping the data

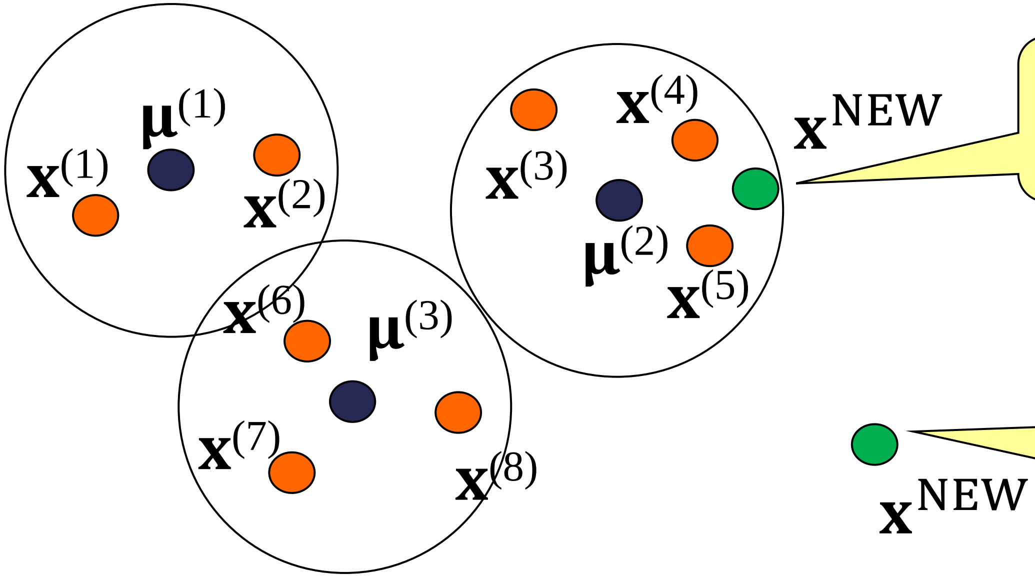
- More complex cases:
  - Multi-dimensional data
  - Several operation modes in the systems
- Divide normal time data $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\}$ into K groups
  - Groups are represented by centers $\{\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \dots, \boldsymbol{\mu}^{(N)}\}$



Clustering for high-dimensional anomaly detection: Find anomalies not belonging to the groups

- Divide normal time data $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\}$ into K groups
  - Groups are represented by centers $\{\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \dots, \boldsymbol{\mu}^{(K)}\}$
- Data $\mathbf{x}$ is an “anomaly” if it lies far from all of the centers

  = system failures, illegal operations, instrument faults



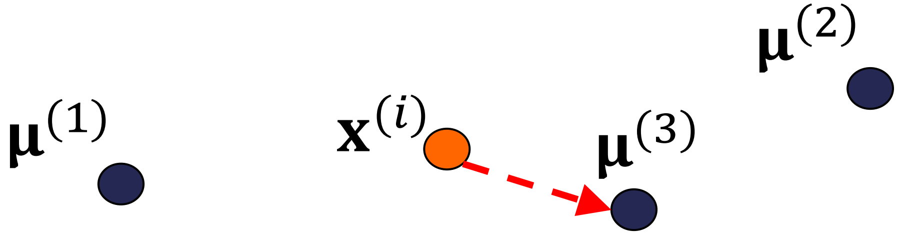
“typical” data

“anomaly”

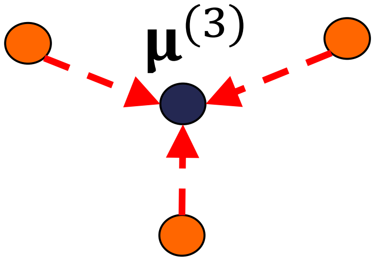
K-means algorithm: Iterative refinement of groups

- Repeat until convergence:

1. Assign each data $\mathbf{x}^{(i)}$ to its nearest center $\boldsymbol{\mu}^{(k)}$



2. Update each center to the center of the assigned data



Anomaly detection in time series:
On-line anomaly detection

- Most anomaly detection applications require real-time system monitoring

- Data instances arrive in a streaming manner:
  - $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(t)}, \ldots$: at each time t, new data $\mathbf{x}^{(t)}$ arrives

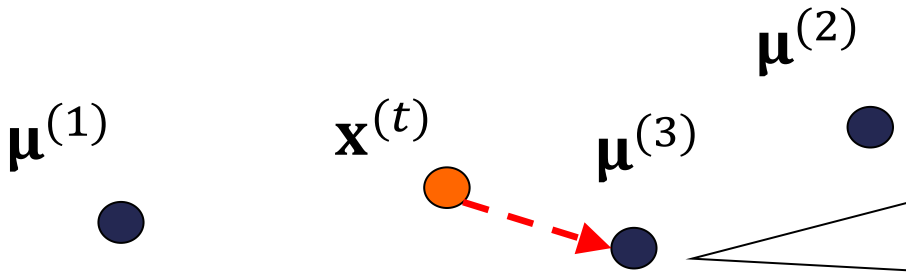
- Each time a new data arrives, evaluate its anomaly

- Also, models are updated in on-line manners:
  - In the one dimensional case, the threshold is sequentially updated
  - In clustering, groups (clusters) are sequentially updated

Sequential K-means: Simultaneous estimation of clusters and outliers

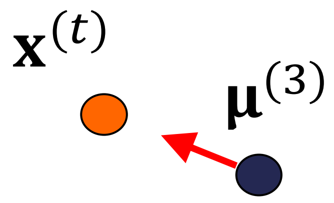
- Data arrives in a streaming manner, and apply clustering and anomaly detection at the same time

1. Assign each data $\mathbf{x}^{(t)}$ to its nearest center $\boldsymbol{\mu}^{(k)}$



If the distance is large, report the data as an anomaly

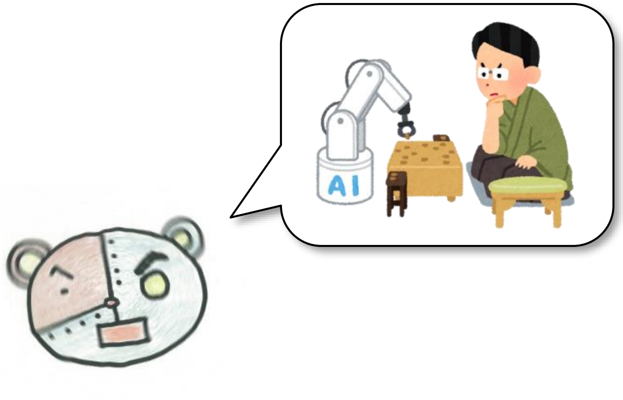
2. Slightly move the center to the data



Limitation of unsupervised anomaly detection: Details of failures are unknown

- In supervised anomaly detection, we know what the failures are
- In unsupervised anomaly detection,
  we can know something is happening in the data,
  but cannot know what it is
  - Failures are not defined in advance
- Based on the reports to system administrators,
  they have to investigate what is happening, what are the reasons, and what they should do

Recent topics: Deep Learning

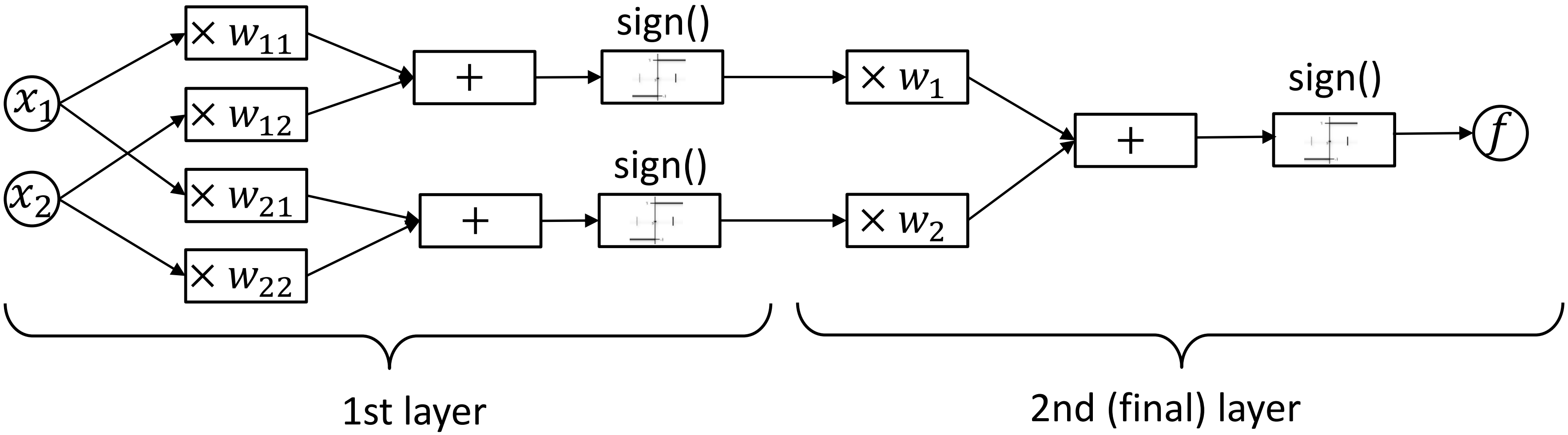


Emergence of deep learning: Significant improvement of prediction accuracy

- Artificial neural networks were hot in 1980s, but burnt low after that…
- In 2012, a deep NN system won in the ILSVRC image recognition competition with 10% improvement
- Major IT companies (such as Google and ~~Facebook~~Meta) invest much in deep learning technologies
- Big trend in machine learning research

Deep neural network:
Deeply stacked NN for high representational power

- Essentially, multi-layer neural networks
  - Regarded as stacked linear classification models
    - First to semi-final layers bear feature extraction
    - Final layer makes predictions
- Deep stacking introduces high non-linearity in the model and ensures high representational power



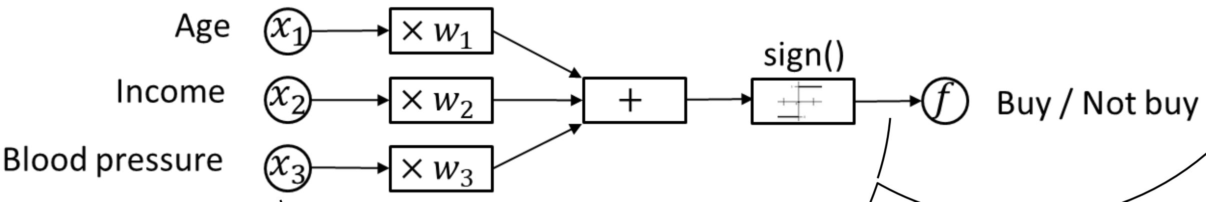
A model for classification:
Linear classification model

- Model f takes an input $\mathbf{x} = (x_1, x_2, \dots, x_D)^\top$ and outputs a value from $\{+1, -1\}$

$$\boxed{f(\mathbf{x}) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D)}$$

– Model parameter $\mathbf{w} = (w_1, w_2, \dots, w_D)^\top \in \mathbb{R}^D$:

- w_d : contribution of x_d to the output
  ($x_d > 0$ contributes to $+1$, $x_d < 0$ contributes to -1)



What is the difference from the past NN?: Deep structures and new techniques with modern flavors

- Differences from the ancient NNs:
  - Far more computational resources are available now
  - Deep network structure: from wide-and-shallow to narrow-and-deep
  - New techniques and model architectures: Dropout, batch normalization, adversarial learning, ReLU, graph neural networks, attention, …
- We will look at some of the key ideas in this lecture