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KYOTO UNIVERSITY

Statistical Learning Theory

- Introduction -

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Statistical learning theory:

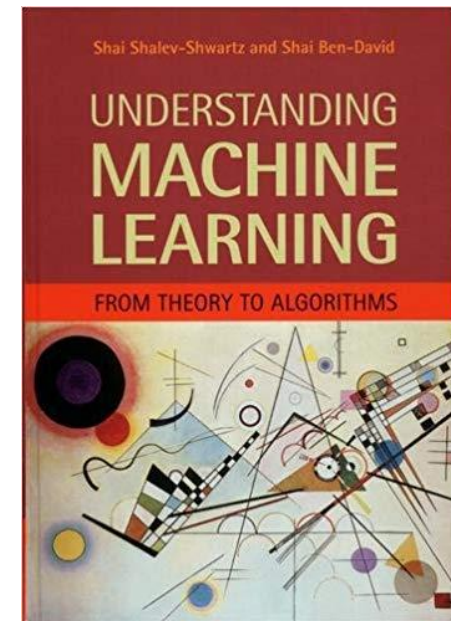
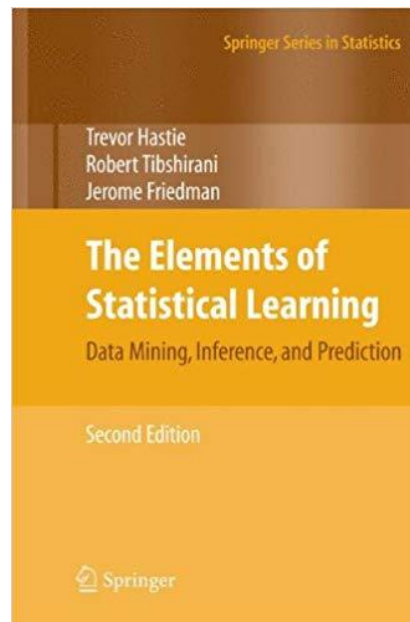
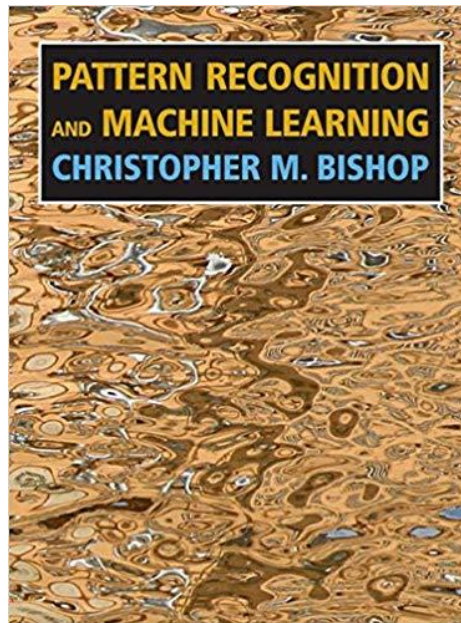
Foundations of recent data analysis technologies

- 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 (using Python)
- Advanced topics

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



Evaluations:

Final Exam is All You Need

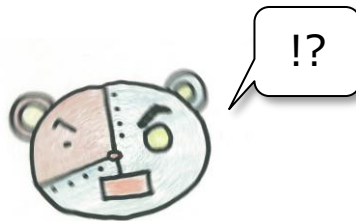
- Evaluation is based on the final exam
 - The examination is a standard written exam and does not allow the use of reference materials
- No attendance checks. No homework.

Introduction:

Basic ideas of machine learning and applications

1. What is machine learning?
2. Learning machines
3. Machine learning applications:
 1. Applications of supervised learning
 2. Applications of unsupervised learning: Anomaly detection

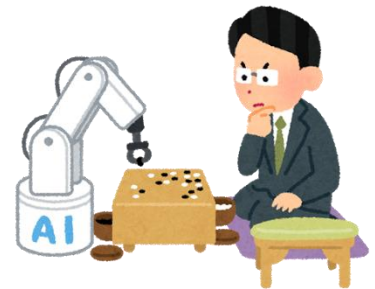
What is machine learning?



“The third A.I. boom”:

Machine learning is a core technology behind the boom

- 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

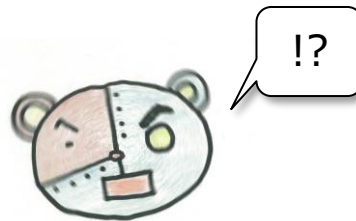
2. Discovery

- “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

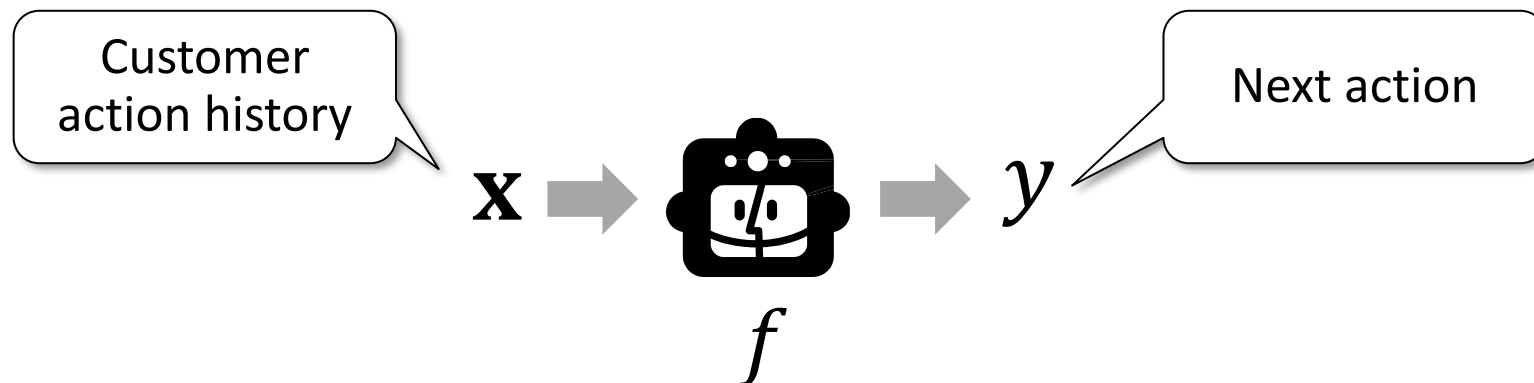
Learning Machines



Prediction machine:

A function from a vector to a scalar

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



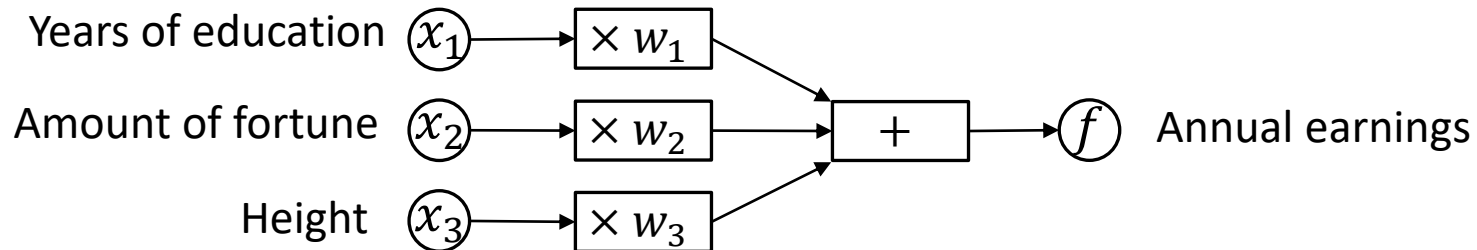
A model for regression:

Linear regression model

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

$$f(\mathbf{x}) = w_1x_1 + w_2x_2 + \dots + w_Dx_D$$

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



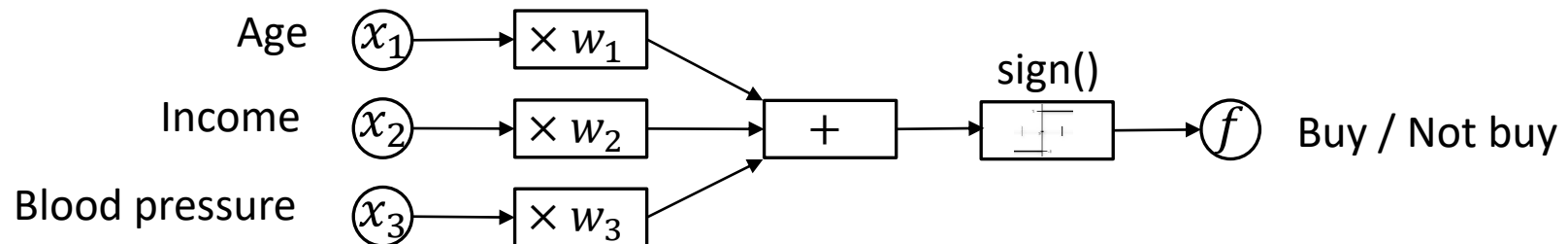
A model for classification:

Linear classification model

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

$$f(\mathbf{x}) = \text{sign}(w_1x_1 + w_2x_2 + \dots + w_Dx_D)$$

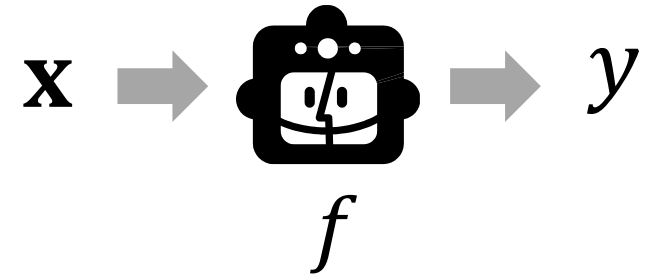
- Model parameter $\mathbf{w} = (w_1, w_2, \dots, w_D)^\top \in \mathbb{R}^D$:
 - w_d : contribution of x_d to the output (if $w_d > 0$, $x_d > 0$ contributes to $+1$, $x_d < 0$ contributes to -1)



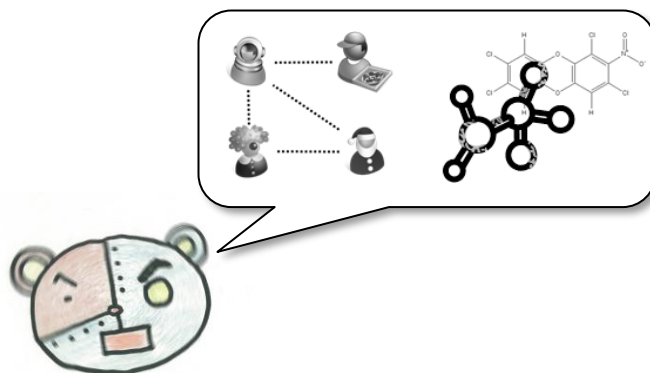
Formulations of machine learning problems:

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
 - $\{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \dots, (\mathbf{x}^{(N)}, y^{(N)})\} : N \text{ pairs}$
 - Unsupervised learning: only inputs are given
 - $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\} : N \text{ inputs}$



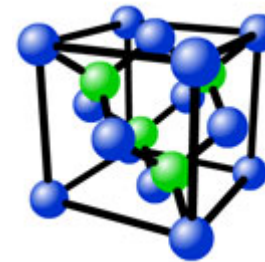
Machine learning applications



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

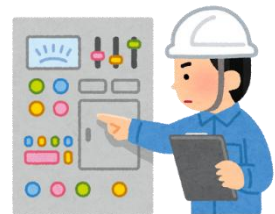


■ Multimedia

- Image/voice understanding

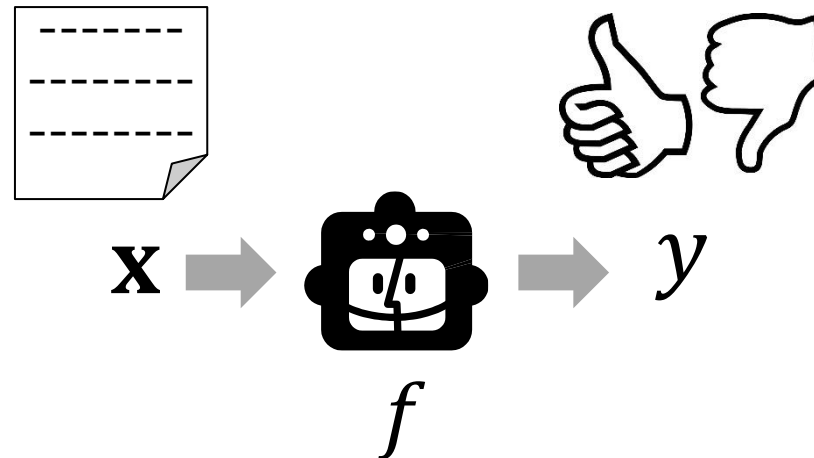
■ System monitoring

- 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/posts by searching the word “ S ”, and analyze them



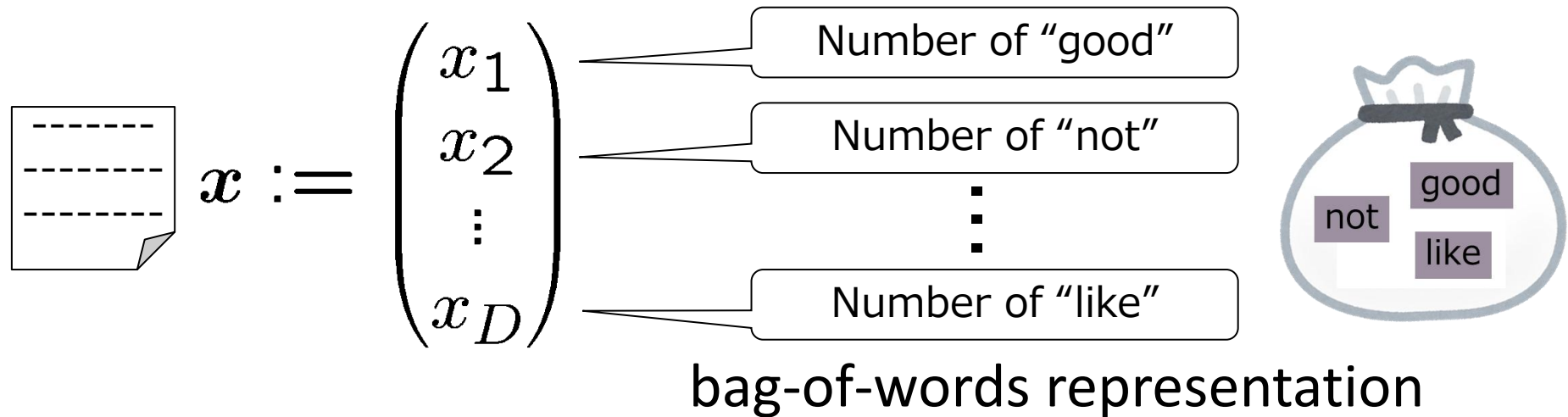
An application of supervised learning:

Some hand labeling followed by supervised learning

- First, give labels to some of the collected documents
 - 10,000 posts 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 posts

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

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



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

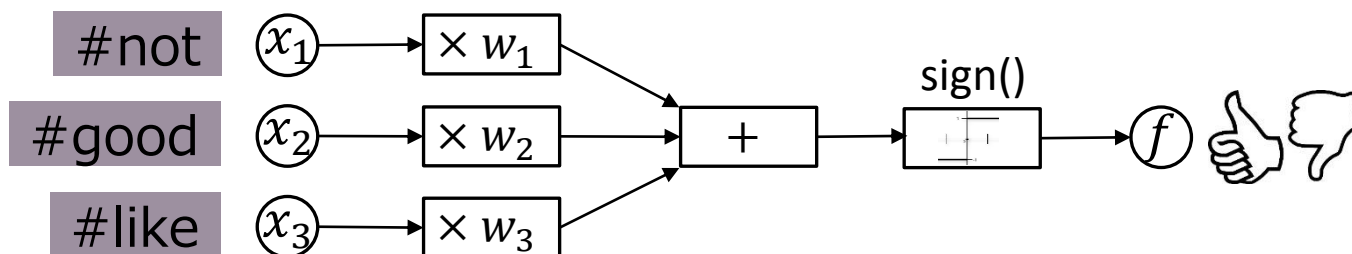
A simple model for sentiment analysis:

Linear binary classification model

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

$$f(\mathbf{x}) = \text{sign}(w_1x_1 + w_2x_2 + \dots + w_Dx_D)$$

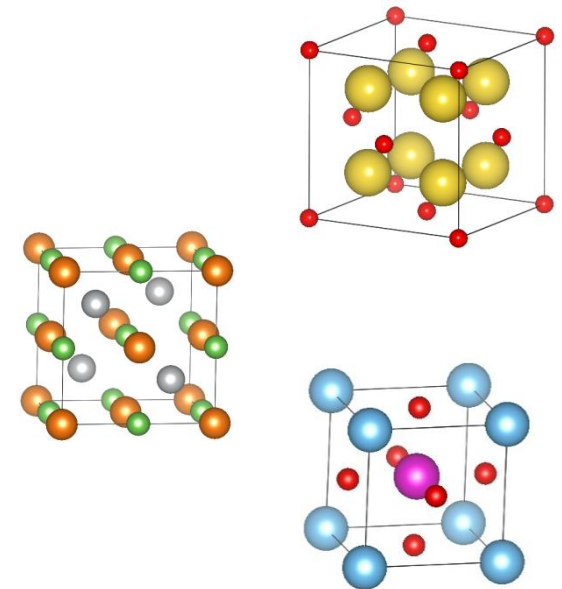
- Model parameter $\mathbf{w} = (w_1, w_2, \dots, w_D)^\top \in \mathbb{R}^D$:
 - w_d : contribution of the d -th word (e.g. “good”) to the sentiment label



An application of supervised *regression* learning:

Discovering new materials

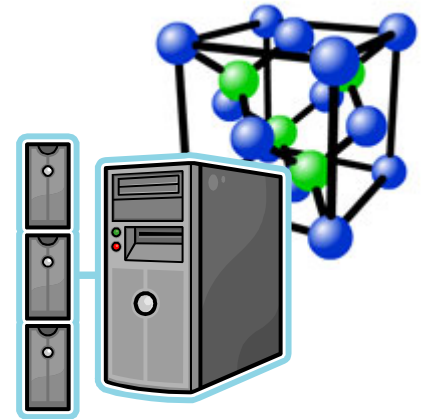
- Material science aims at discovering and designing new materials with desired properties
 - Volume, density, elastic coefficient, thermal conductivity, ...
- Traditional approach (try-and-error):
 1. Determine chemical structure
 2. Synthesize the chemical compounds
 3. Measure their physical properties
 4. If not satisfied, return to 1



Computational approach to material discovery:

Still needs high computational costs

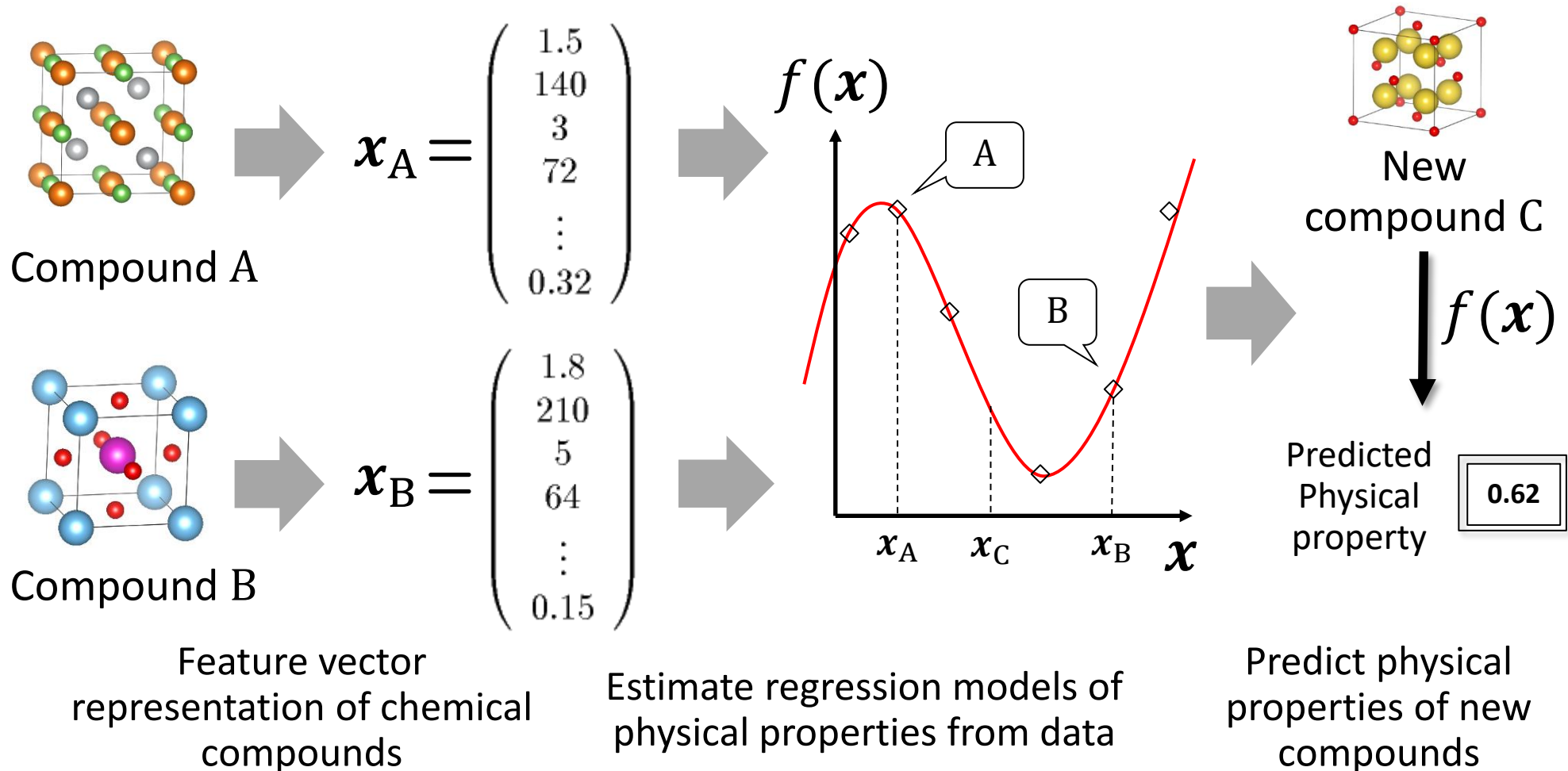
- Computational approach: First-order principle calculations based on quantum physics to run simulation to estimate physical properties
- First-order principle calculation still requires high computational costs
 - Proportional to the cubic number of atoms
 - Sometimes more than a week or a month...



Data driven approach to material discovery:

Regression to predict physical properties

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



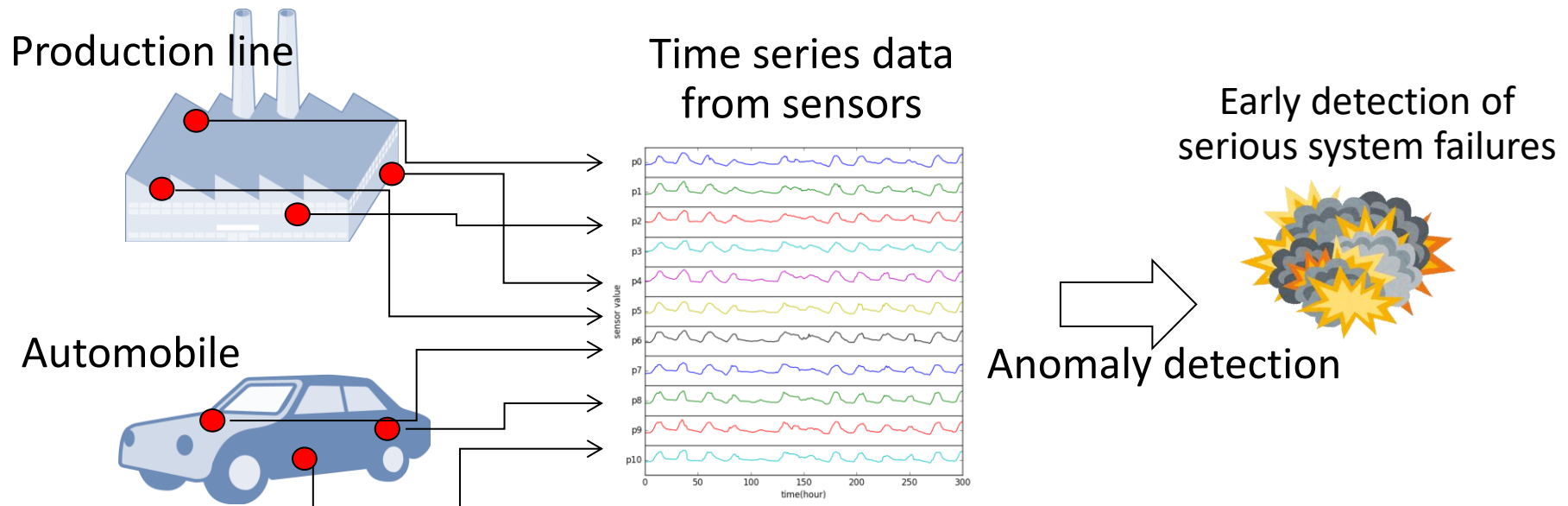
Anomaly detection



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



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:

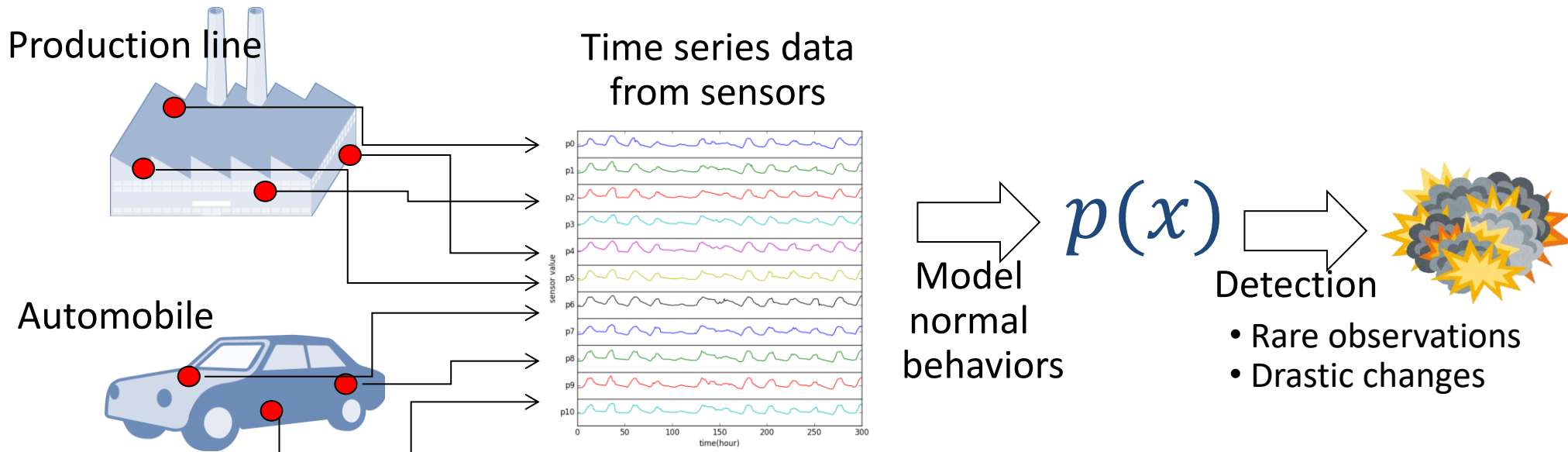
Failures are rare events

- 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 in most cases

An alternative idea:

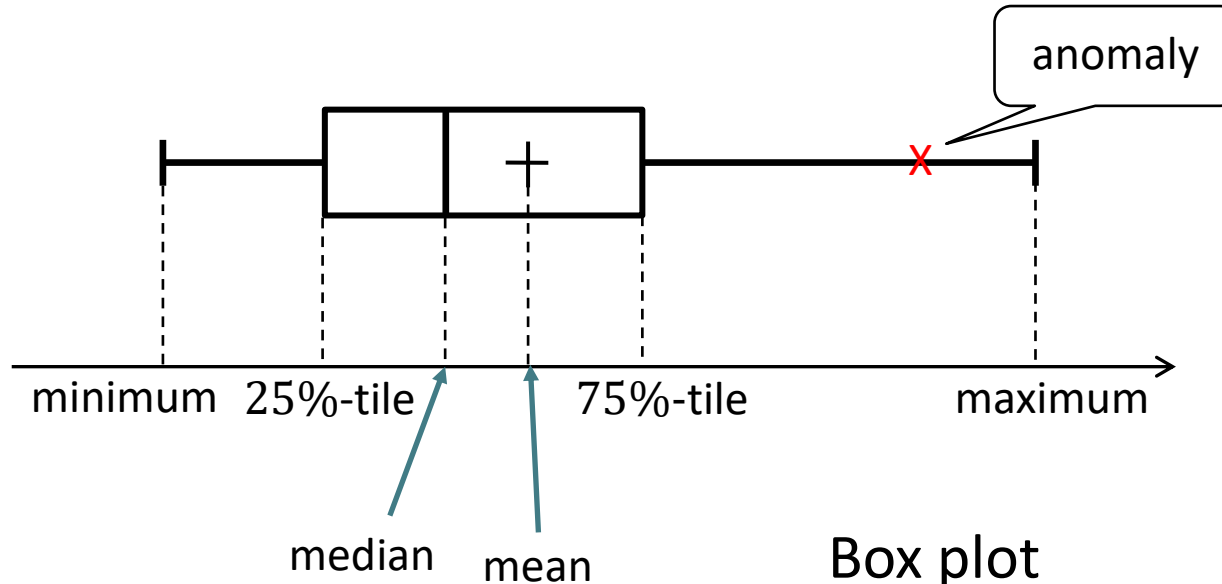
Model the normal times, detect deviations from them

- 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



A simple unsupervised approach: Anomaly detection using thresholds

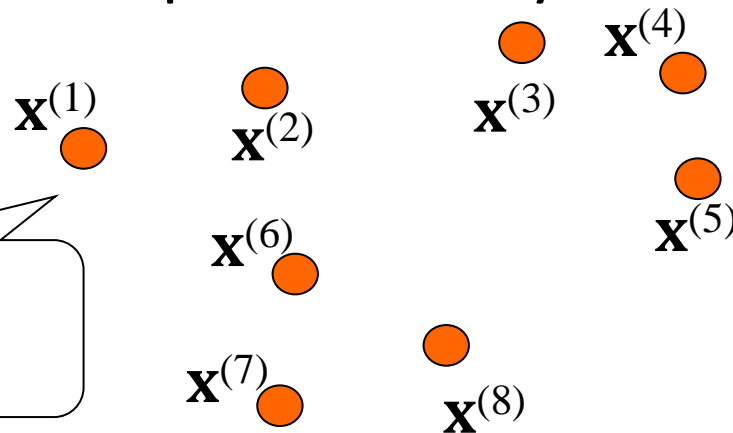
- Suppose a 1-dimensional case (e.g. temperature)
- Find the value range of the normal data (e.g. 20-50 °C)
- Detect values deviates from the range, and report them as anomalies (e.g. 80°C is not in the normal range)



Clustering for high-dimensional anomaly detection:

Model the normal times by grouping the data

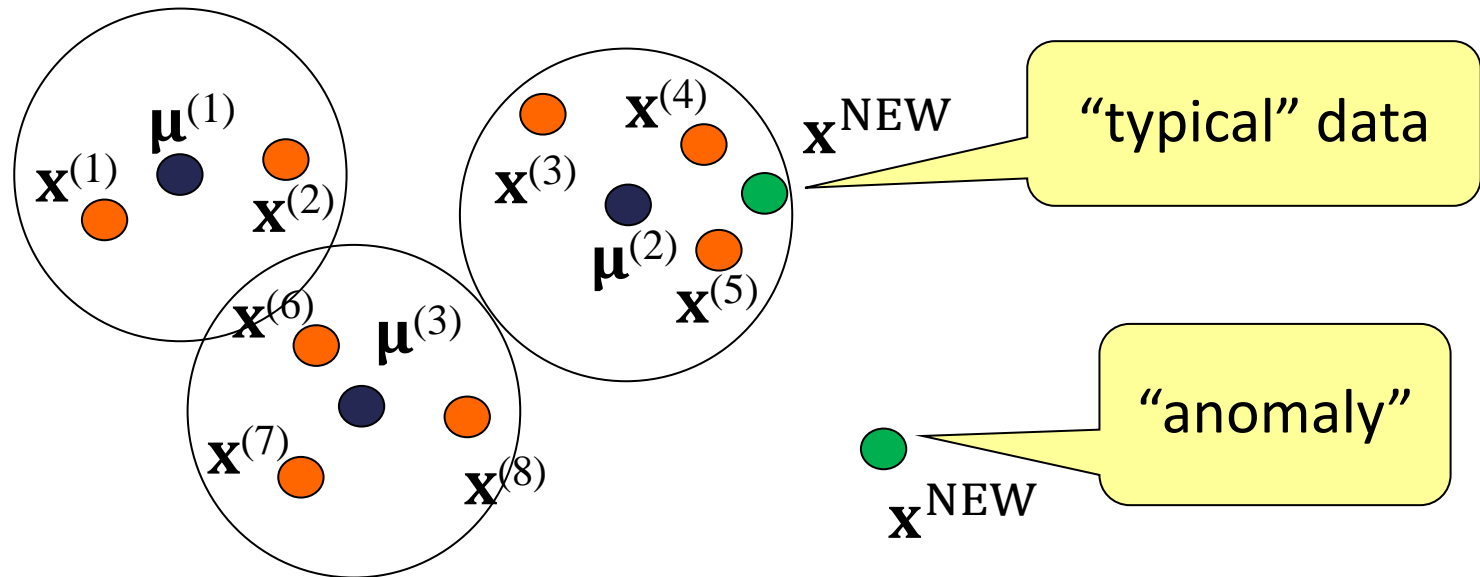
- More complex cases:
 - Multi-dimensional data
 - Several operation modes in the systems
- Divide normal time data $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\}$ into K groups
 - Groups are represented by centers $\{\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \dots, \boldsymbol{\mu}^{(N)}\}$



Clustering for high-dimensional anomaly detection:

Find anomalies not belonging to the groups

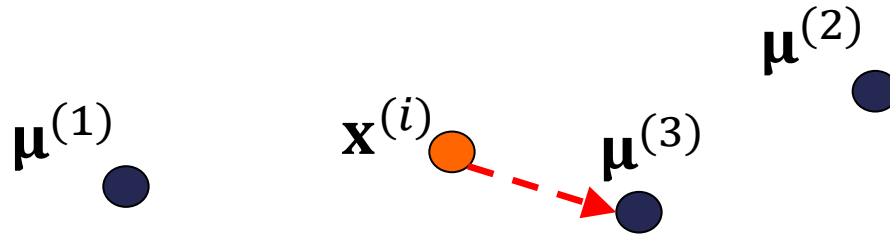
- Divide normal time data $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(N)}\}$ into K groups
 - Groups are represented by centers $\{\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \dots, \boldsymbol{\mu}^{(K)}\}$
- Data \mathbf{x} is an “anomaly” if it lies far from all of the centers
=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



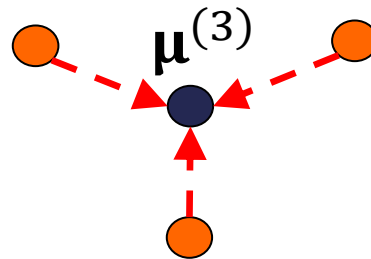
K-means algorithm: Iterative refinement of groups

- Repeat until convergence:

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



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



Anomaly detection in time series:

On-line anomaly detection

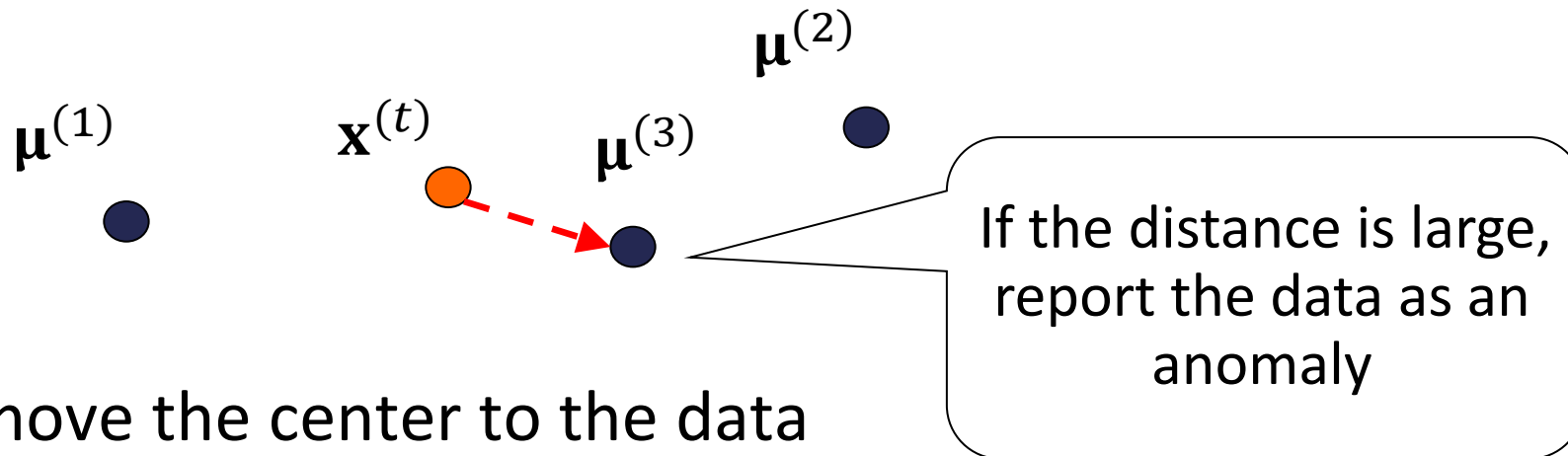
- Most anomaly detection applications require real-time system monitoring
- Data instances arrive in a streaming manner:
 - $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots, \mathbf{x}^{(t)}, \dots$: at each time t , new data $\mathbf{x}^{(t)}$ arrives
- Each time a new data arrives, evaluate its anomaly
- 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:

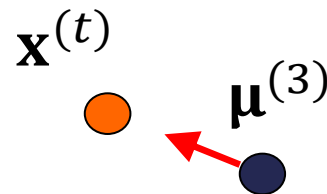
Simultaneous estimation of clusters and outliers

- 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 $\mu^{(k)}$



2. Slightly move the center to the data

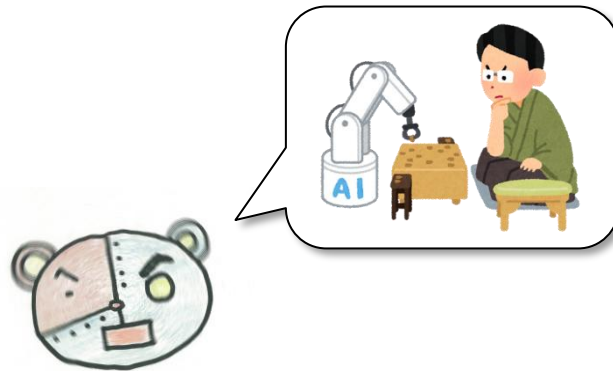


Limitation of unsupervised anomaly detection:

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:

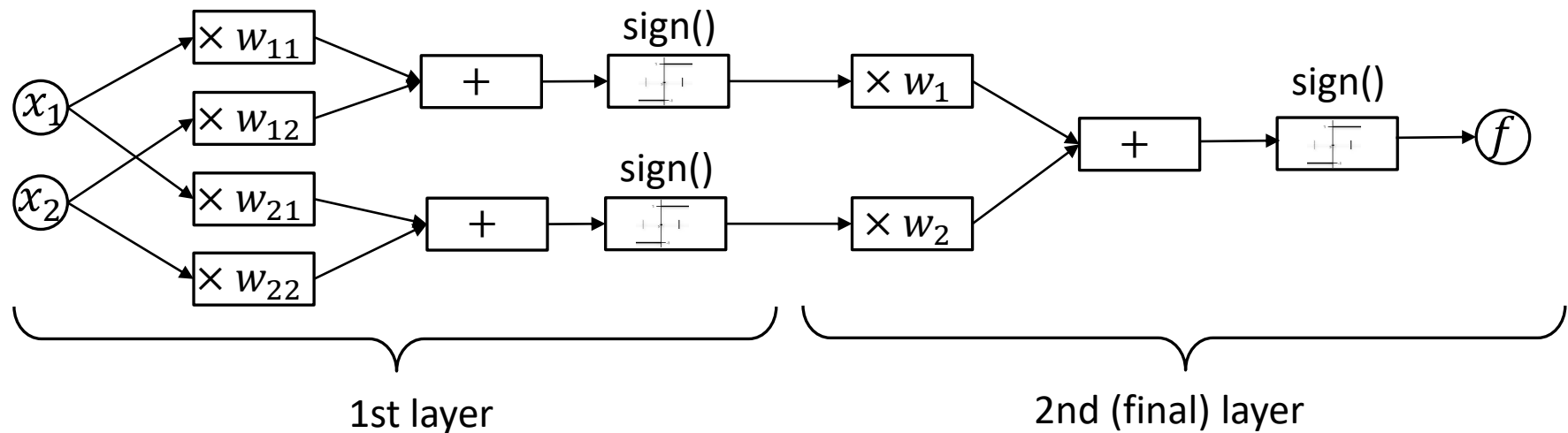
Significant improvement of prediction accuracy

- 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 invest much in deep learning technologies
- A 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



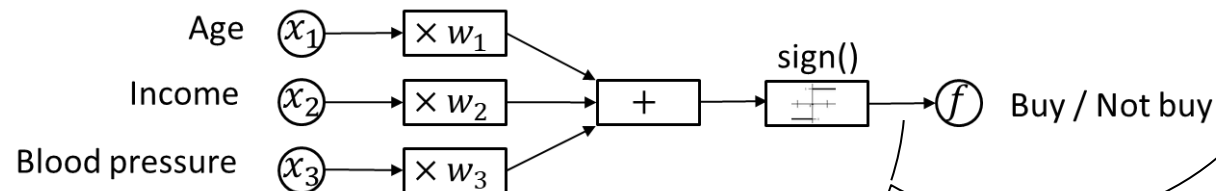
A model for classification: Linear classification model

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

$$f(\mathbf{x}) = \text{sign}(w_1x_1 + w_2x_2 + \dots + w_Dx_D)$$

–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