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KYOTO UNIVERSITY

Statistical Learning Theory
- Introduction -

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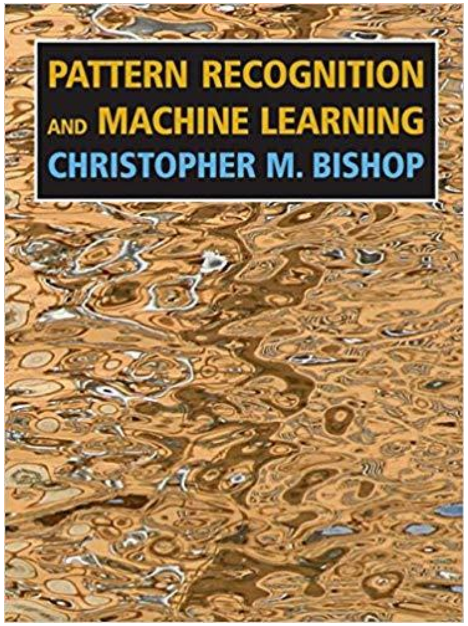
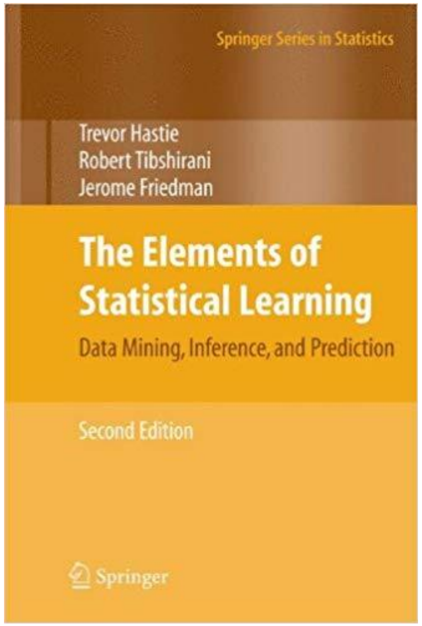
Statistical learning theory: Foundations of recent data analysis technologies

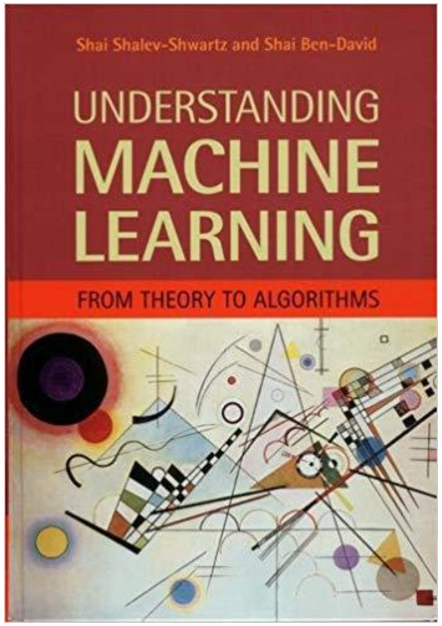
- This lecture will cover:
  - Basic ideas, problems, solutions, and applications of statistical machine learning
    - Supervised & unsupervised learning
    - Models & algorithms: linear regression, SVM, neural nets, …
  - Statistical learning theory
    - Theoretical foundation of statistical machine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

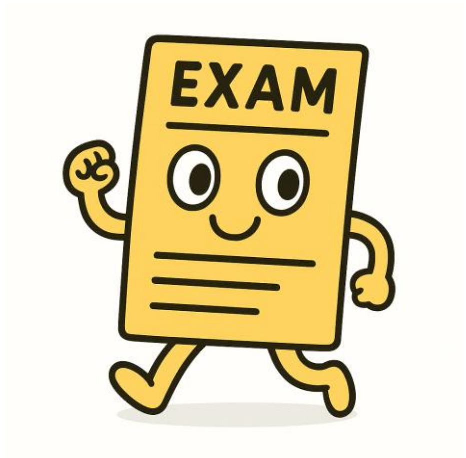






Evaluations:
Final Exam is All You Need

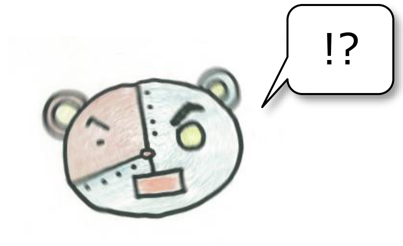
- Evaluation is solely based on the final exam
  - The examination is a standard written exam
  - You are allowed to use any reference materials
- No attendance checks. No homework.



Contents:
Basic ideas of machine learning and applications

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

What is machine learning?

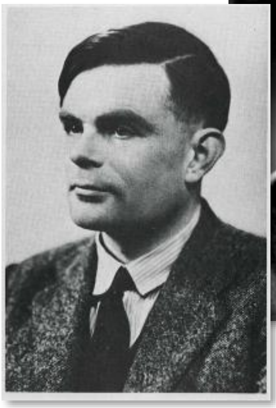


“The third A.I. boom”:
Machine learning is a core technology behind the boom

- 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



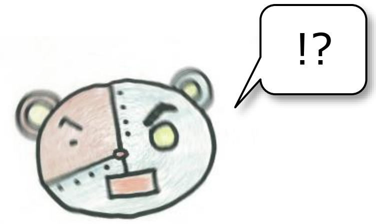

What is machine learning? ：
A data analytics technology

- Rise of “statistical” machine learning
  - Successes in bioinformatics, natural language processing, and other business areas
- Technically, it can be 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

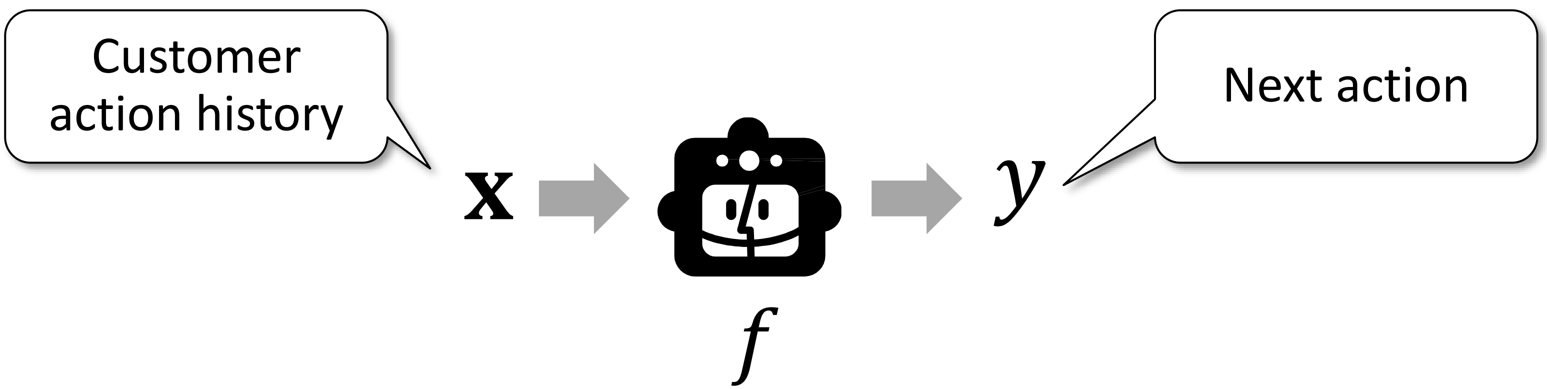
1. Prediction
   - "What will happen in future data?"
   - Given past data, predict about future data
2. Discovery
   - "What is happening in data in hand?"
   - Given past data, find insights in them
3. Data generation
   - "Generate new data satisfying certain properties"
   - Given past data, generate 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 $f: \mathbf{x} \to y$
  - 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 $y \in \{C_1, C_2, \dots, C_M\}$

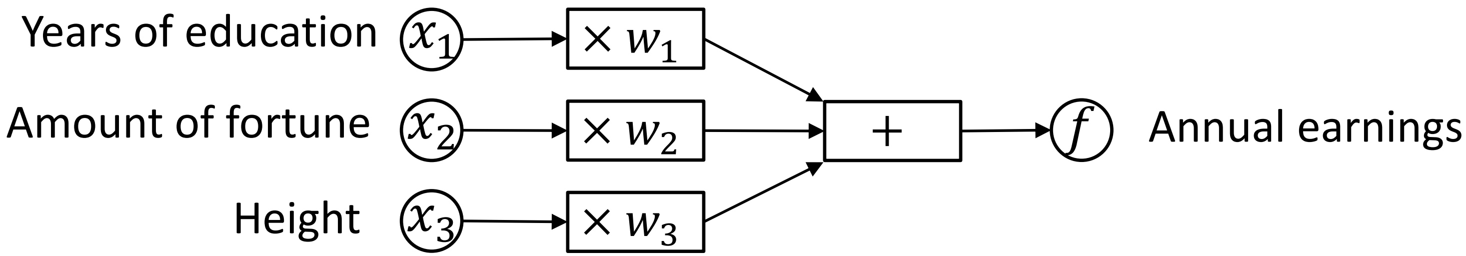


A model for regression: Linear regression model

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

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

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

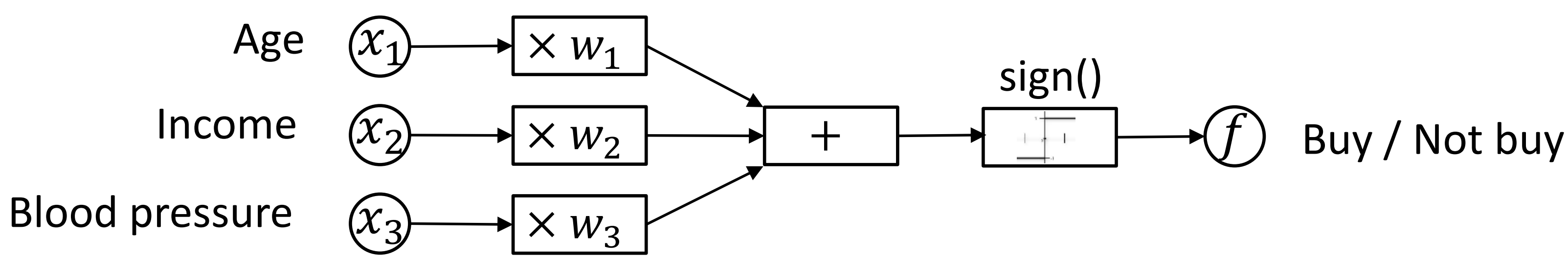


A model for classification:
Linear classification model

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

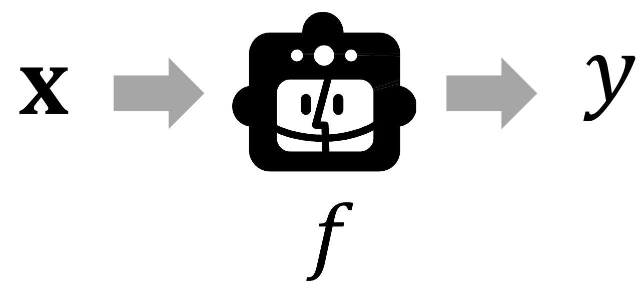
$$f(\mathbf{x}) = \mathrm{sign}(w_1 x_1 + w_2 x_2 + \cdots + w_D x_D)$$

  – 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)

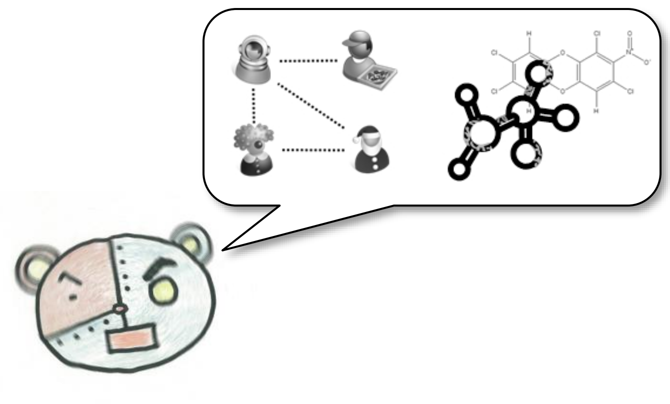


Formulations of machine learning problems: Supervised learning and unsupervised learning

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



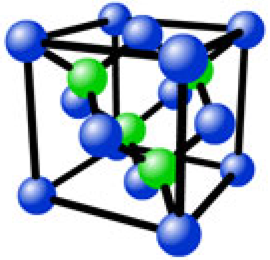
Machine learning applications



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

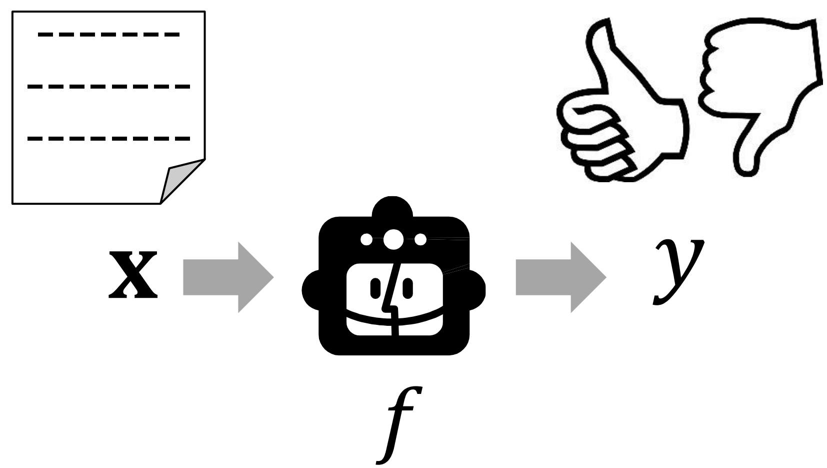
- Web
  - Search
  - Spam filtering
  - Social media

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

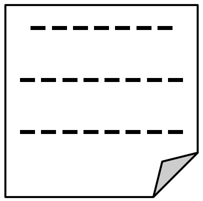


An application of supervised learning:
Some hand labeling followed by supervised learning

- 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



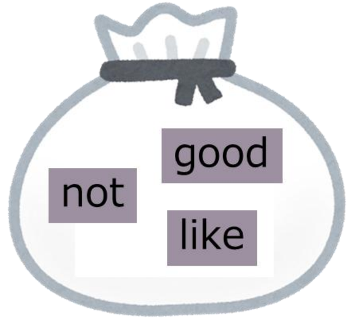
$$\boldsymbol{x} := \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{pmatrix}$$

Number of "good"

Number of "not"

⋮

Number of "like"



bag-of-words representation

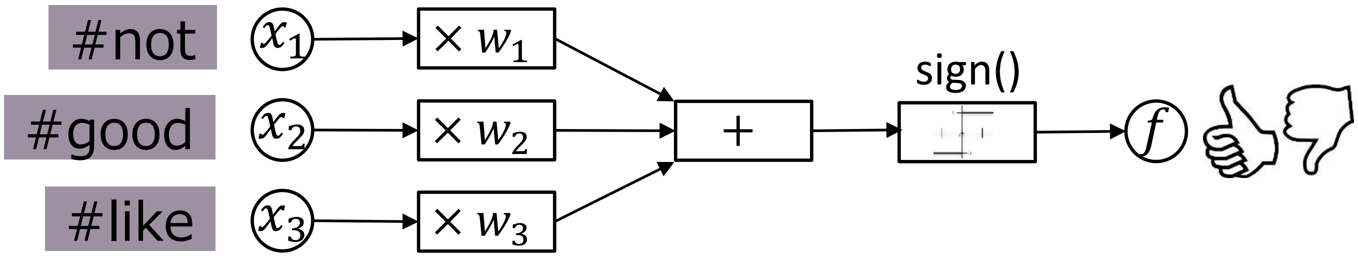
- Note: design of the feature vector is left to users

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 $\{+1, -1\}$:

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

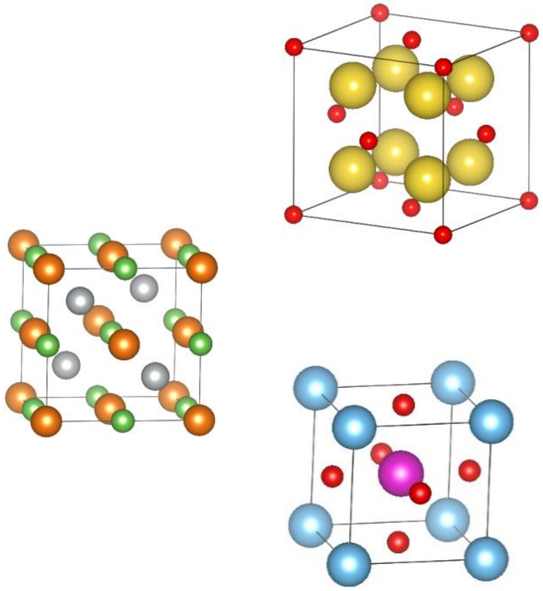
  - Model parameter $\mathbf{w} = (w_1, w_2, \ldots, w_D)^\top \in \mathbb{R}^D$:
    - w_d : contribution of the d-th word (e.g. “good”) to the sentiment label



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):

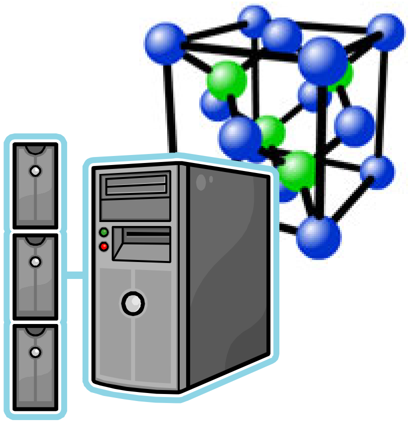
1. Determine chemical structure
2. Synthesize the chemical compounds
3. Measure their physical properties
4. If not satisfied, return to 1



Computational approach to material discovery: Still needs high computational costs

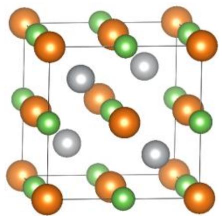
- Computational approach: First-principle calculations based on quantum physics to run simulation to estimate physical properties

- First-order principle calculation still requires high computational costs
  - Proportional to the cubic number of atoms
  - Sometimes more than a week or a month…



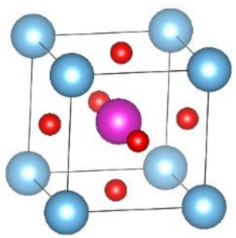
Data driven approach to material discovery: Regression to predict physical properties

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



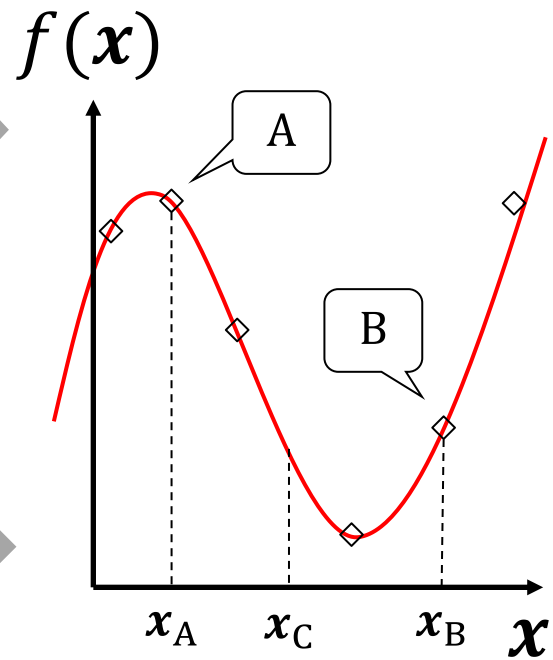
Compound A

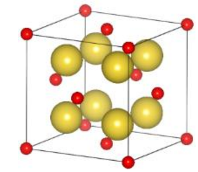
$$\boldsymbol{x}_\mathrm{A} = \begin{pmatrix} 1.5 \\ 140 \\ 3 \\ 72 \\ \vdots \\ 0.32 \end{pmatrix}$$



Compound B

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





New compound C

$f(\boldsymbol{x})$

Predicted Physical property: **0.62**

Feature vector representation of chemical compounds

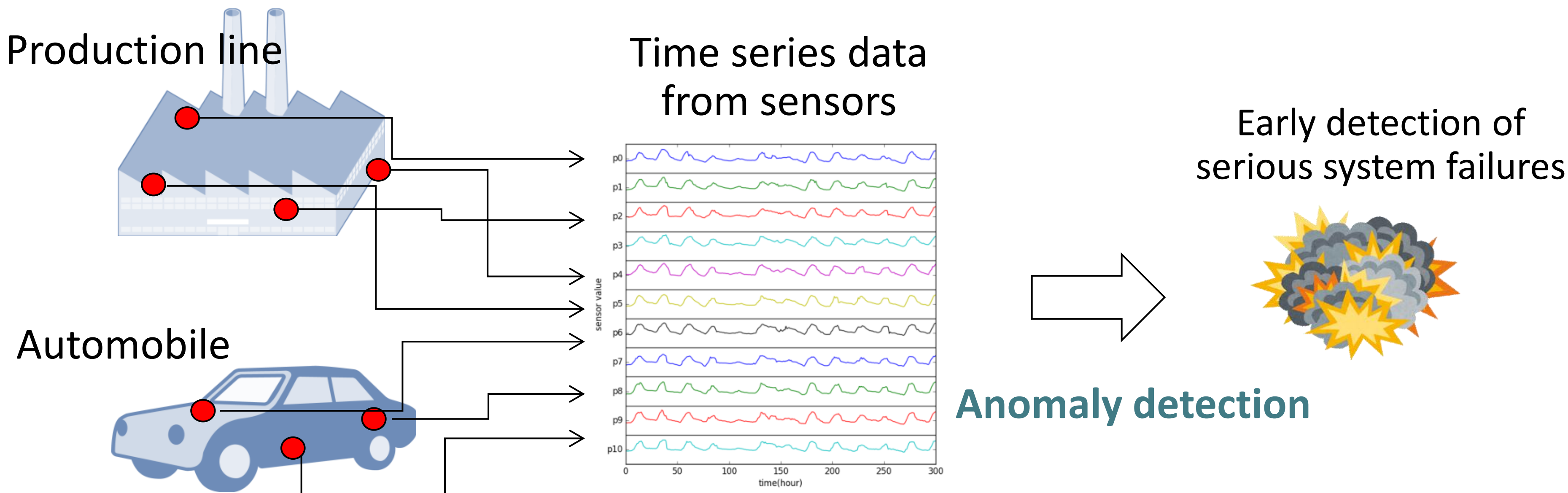
Estimate regression models of physical properties from data

Predict physical properties of new compounds

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

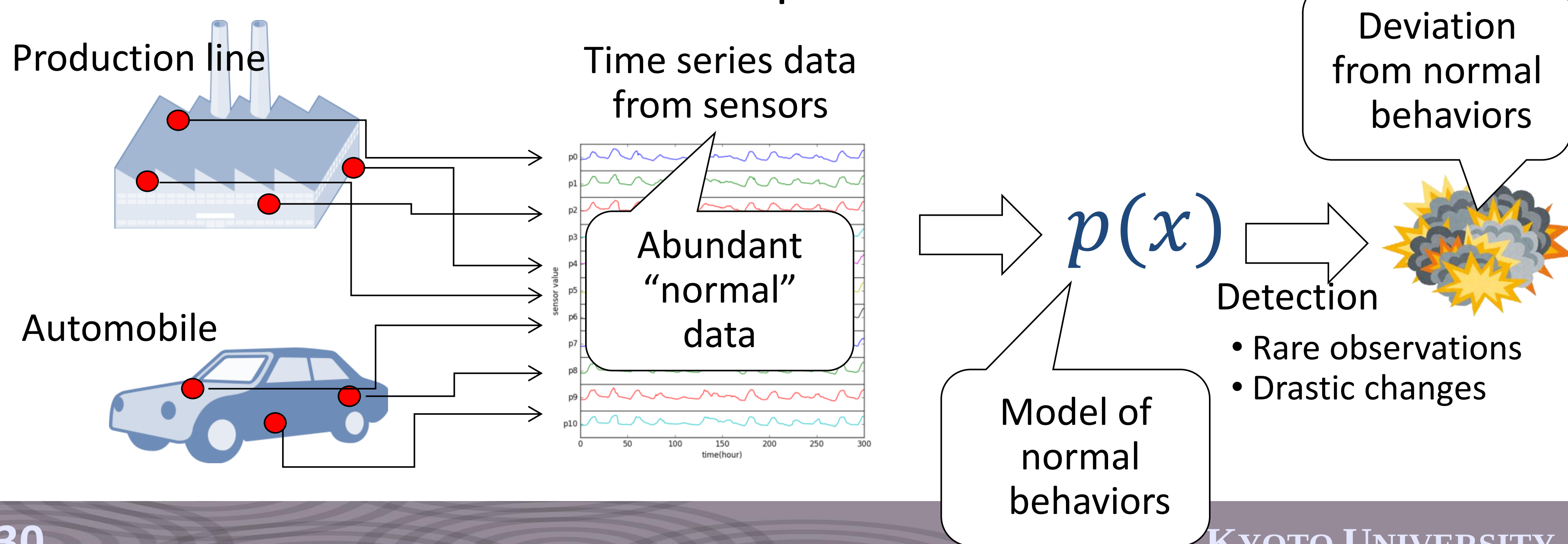
- We want to find precursors of failures in data
  - Assumption: Precursors of failures are hiding in data
- Anomaly: An “abnormal” patterns appearing in data
  - In a broad sense, state changes are also included: appearance of news topics, configuration changes, …
- Anomaly detection techniques find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

Difficulty in anomaly detection: Failures are rare events

- If target failures are known ones and many data are available, 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

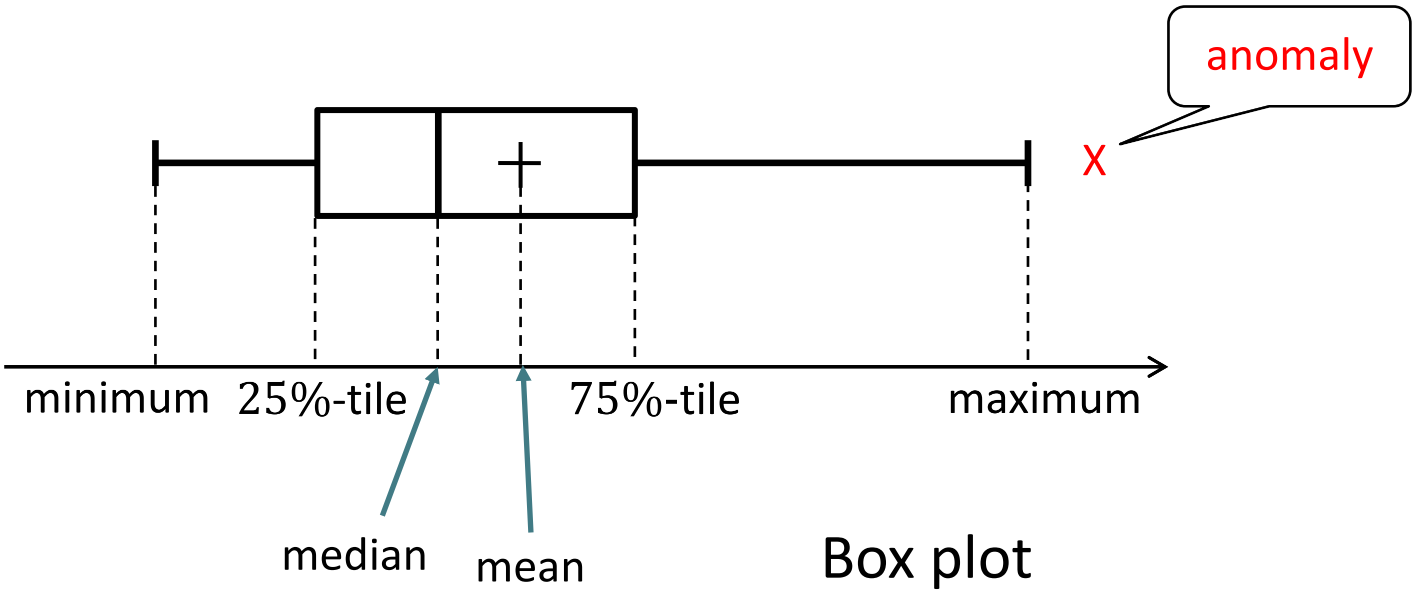
An alternative idea:
Model the normal times, detect deviations from them

- 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

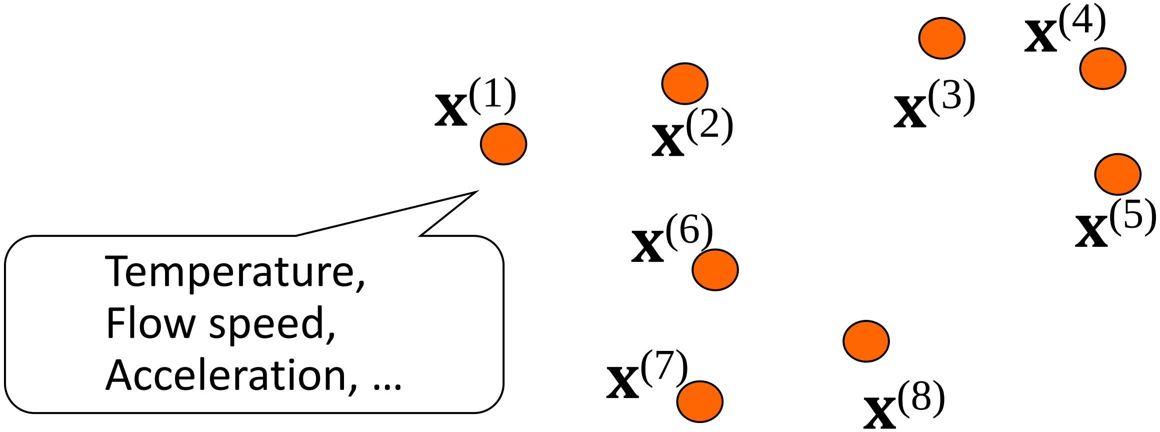
- Suppose a 1-dimensional case (e.g. temperature)
- Find the value range of the normal data (e.g. 20-50 ℃)
- Detect values deviates from the range, and report them as anomalies （e.g. 80℃ is not in the normal range)



Box plot

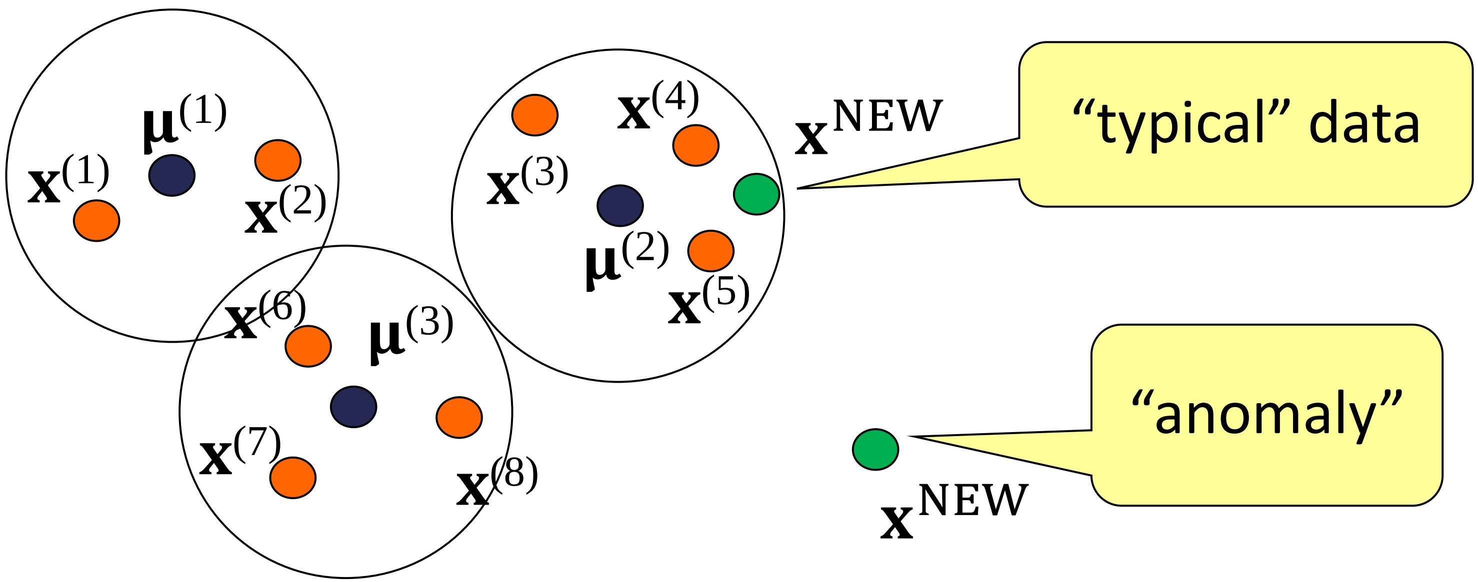
Clustering for high-dimensional anomaly detection: Model the normal times by grouping the data

- 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

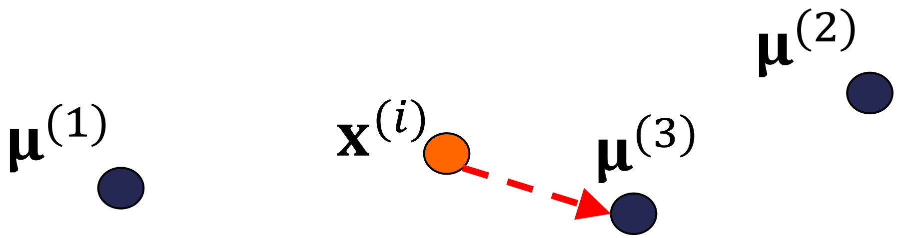
- Divide normal data $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(N)}\}$ into K groups
  - Groups are represented by centers $\{\boldsymbol{\mu}^{(1)}, \boldsymbol{\mu}^{(2)}, \ldots, \boldsymbol{\mu}^{(K)}\}$
- Data $\mathbf{x}$ is an "anomaly" if it lies far from all of the centers
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



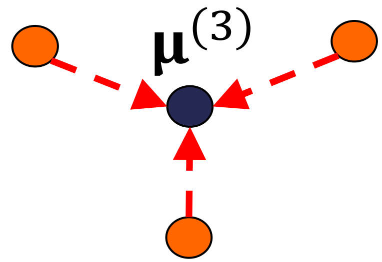
K-means algorithm: Iterative refinement of groups

- 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



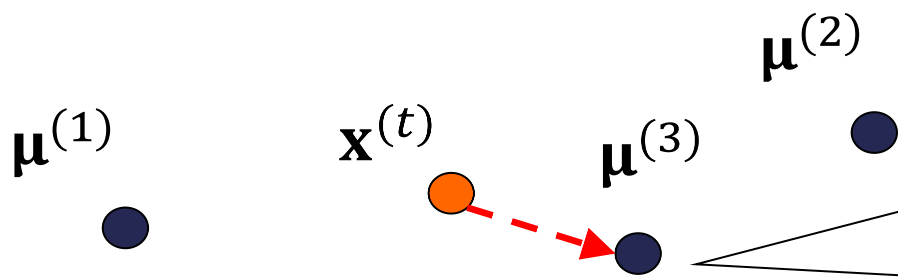
Anomaly detection in time series: On-line anomaly detection

- Most anomaly detection applications require real-time system monitoring
- Data instances arrive in a streaming manner:
  - $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(t)}, \ldots$: 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

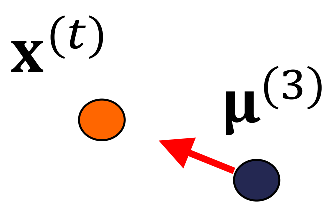
- Data arrives in a streaming manner, and apply clustering and anomaly detection at the same time

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

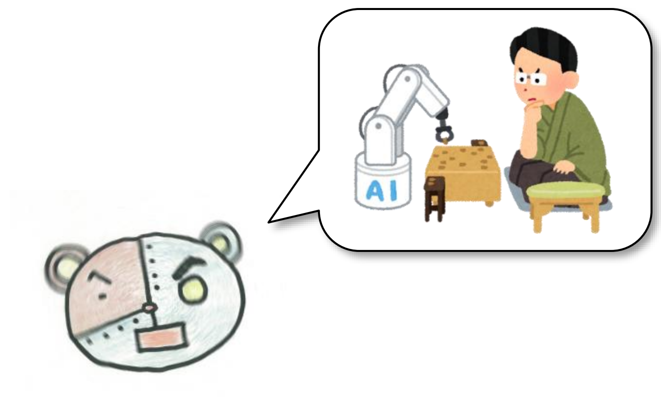
2. Slightly move the center to the data



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

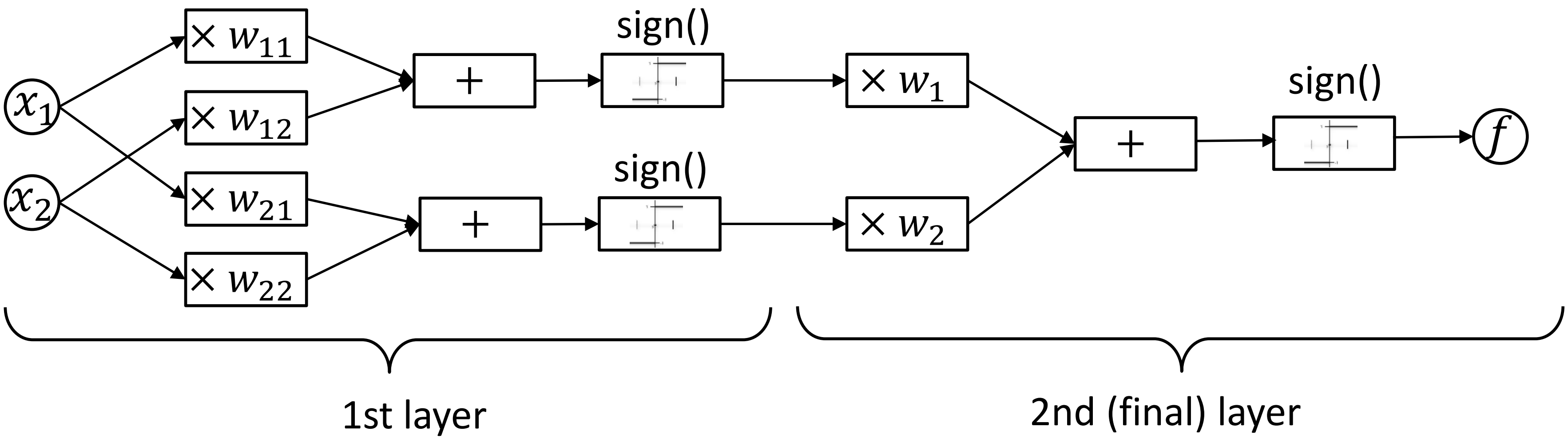


Emergence of deep learning: Significant improvement of prediction accuracy

- 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 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
- Stacking many layers makes the model highly non-linear, and gives it strong power to represent complex patterns.

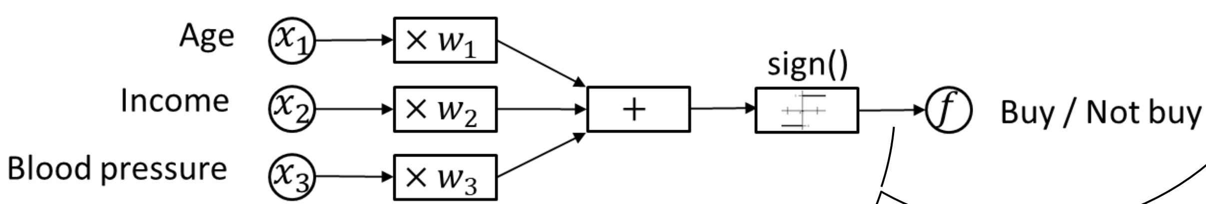


A model for classification: Linear classification model

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

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

– 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

Summary:
Introduction to statistical learning theory

- Machine learning is a data-driven approach to prediction, discovery, and generation
- Applications are expanding from IT to various fields: healthcare, finance, materials, and more
- Learning = estimating a model (function) from data: supervised & unsupervised learning
- Anomaly detection finds irregular patterns by modeling normal behavior
- Deep learning leverages stacked neural networks with modern techniques and large-scale data