Linear Regression and Gradient Descent

Prof. Mingkui Tan

SCUT Machine Intelligence Laboratory (SMIL)

Contents

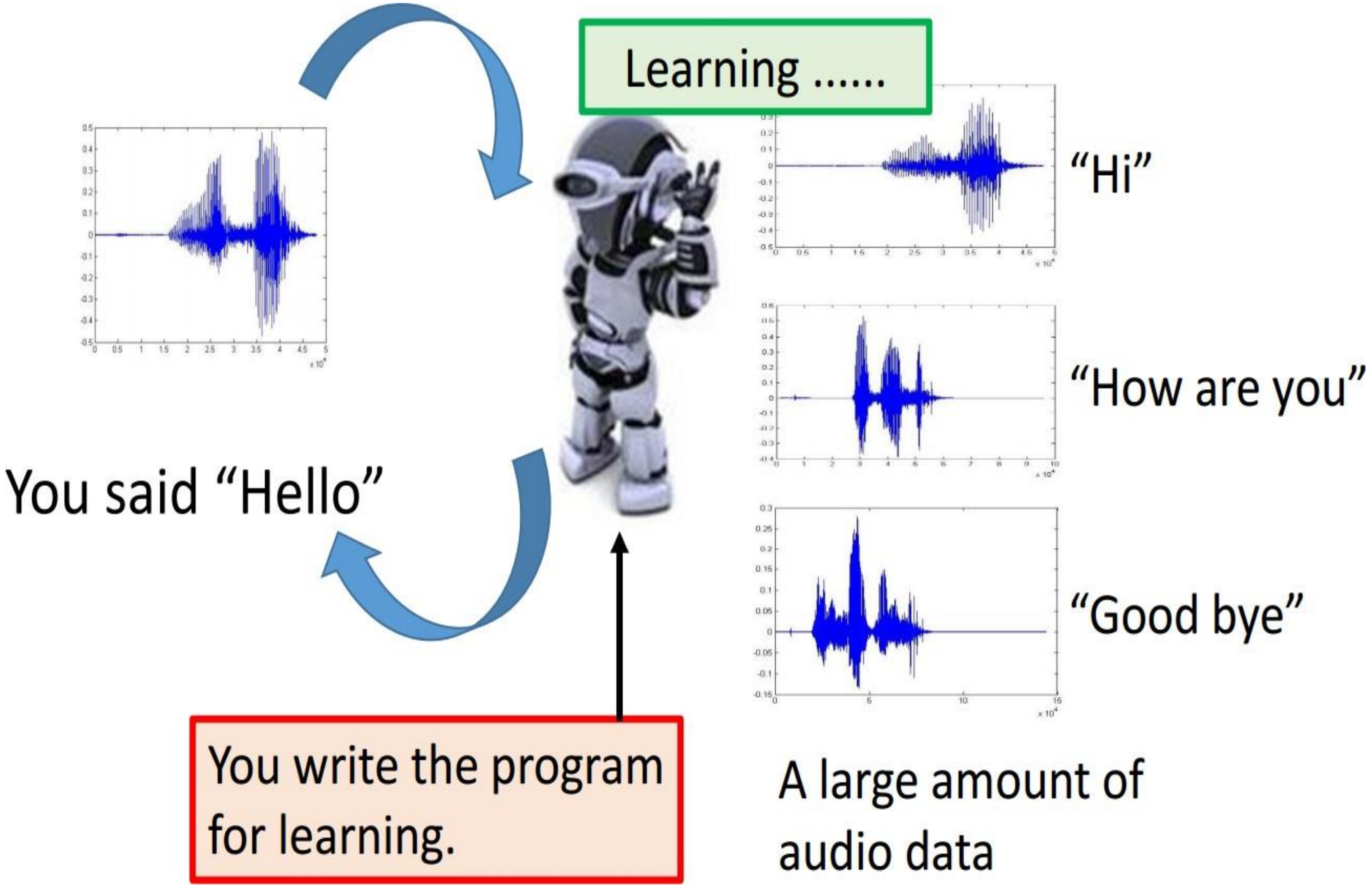
Contents

What is Machine Learning?

Machine Learning composes of three parts:

- Data
- Model
- Loss Function

Introduction to Machine Learning



Speech Recognition

Introduction to Machine Learning

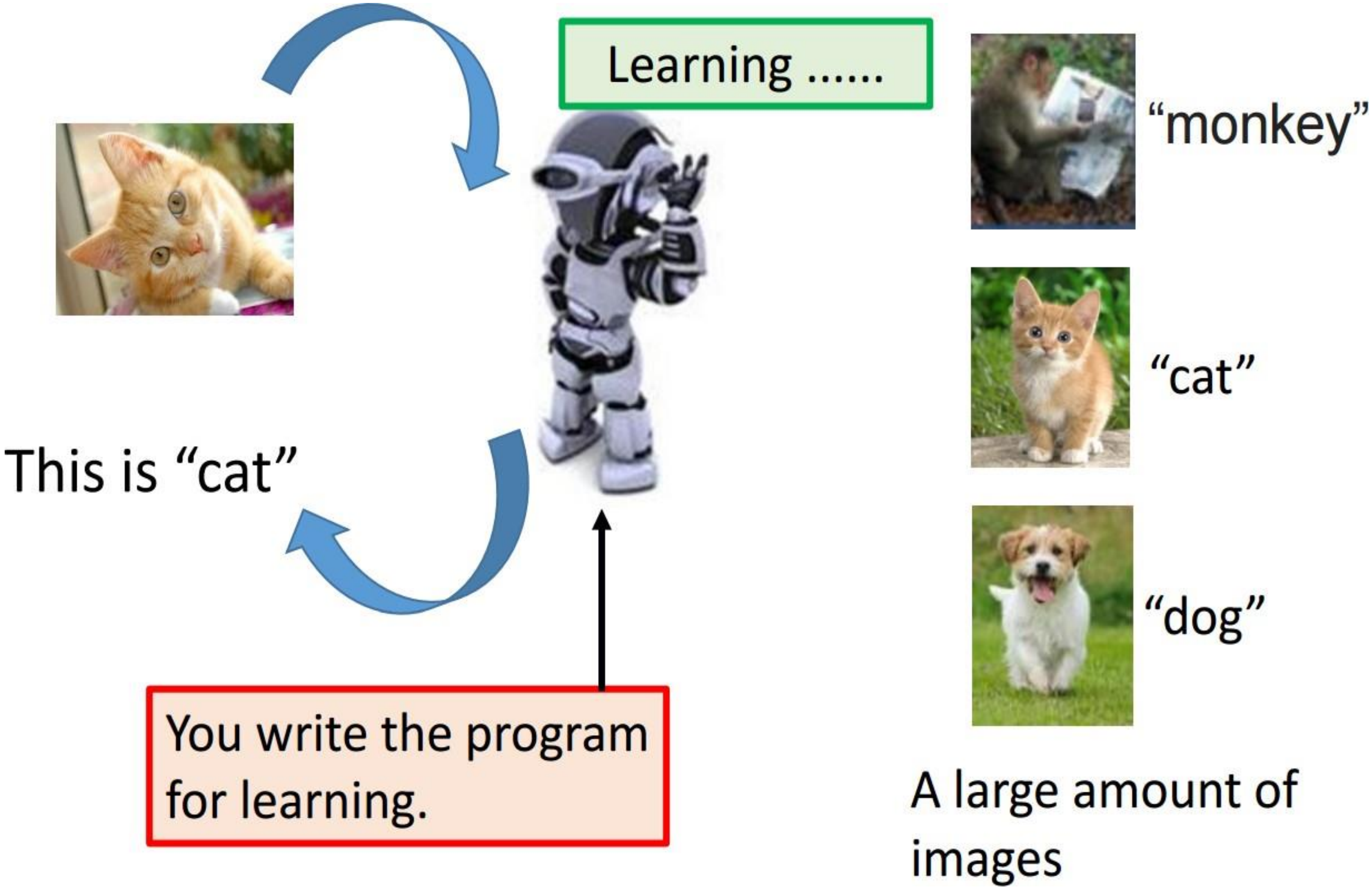
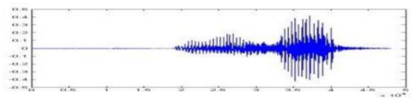


Image Recognition

Machine Learning ≈ Looking for a Function

- Speech Recognition

$f($  $)=$ "How are you"

- Image Recognition

$f($  $)=$ "Cat"

- Playing Go

$f($  $)=$ "5-5" (next move)

- Dialogue System

$f($ "Hi" $)=$ "Hello"

(what the user said) (system response)

Introduction to Machine Learning

A set of function

Model

$f_1, f_2 \cdots$

$f_1($  $) =$ "cat"

$f_2($  $) =$ "money"

$f_1($  $) =$ "dog"

$f_2($  $) =$ "snake"

Image Recognition

Three Main Elements of Machine Learning

Data

Different application have different data
Such as face detection, financial application

Model

Define the model according to specific problem
Such as recommendation system

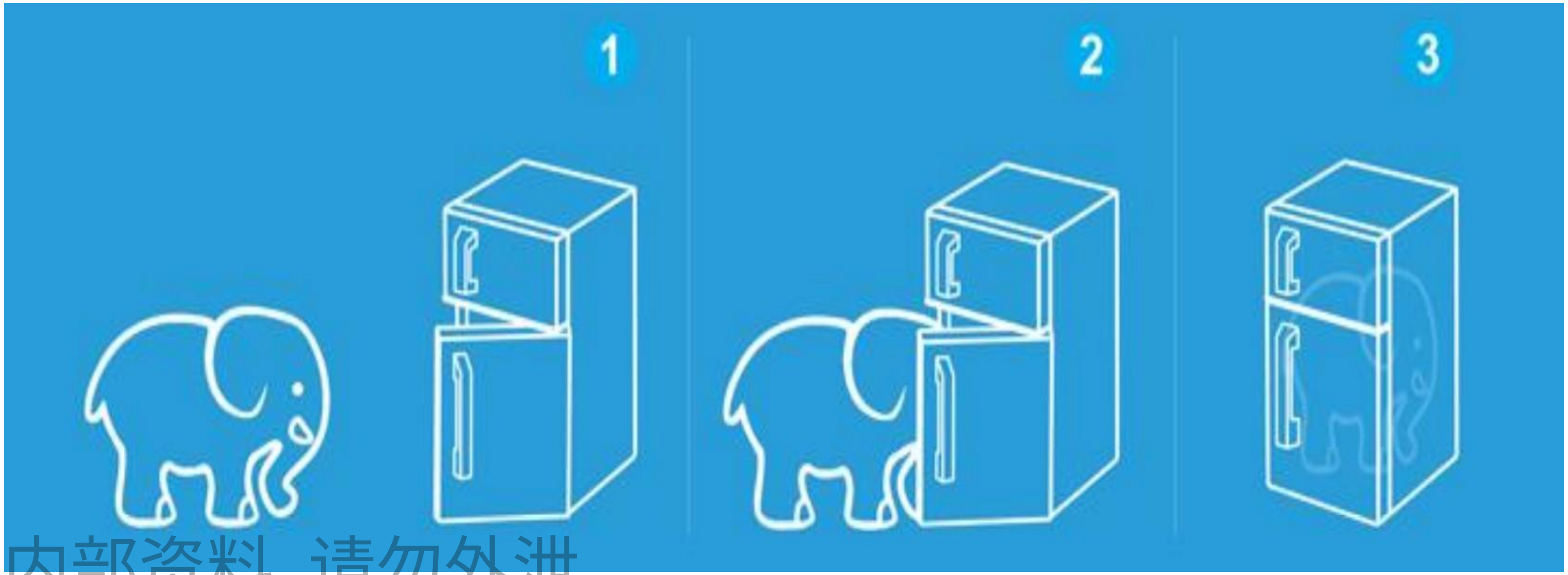
Model evaluation

Use loss function (Hinge loss) (Logistic loss) (Softmax loss)

Machine Learning is so simple…

Step 1: Define a set of functions → Step 2: Goodness of function → Step 3: Pick the best function

Just like putting an elephant into the fridge…



Introduction to Machine Learning

- Use a function to predict y:

$$\hat{y} = f(x)$$

- However, the prediction may be inconsistent with the ground-truth
- Calculate the difference by loss function:

$$\mathcal{L}_{\mathcal{D}}(\mathbf{W}) = \sum_{i=1}^{n} l(\hat{y}_i, y_i)$$

where $\mathcal{D}$ refers to data and $\mathbf{W}$ refers to parameter

Introduction to Machine Learning

- Machine Learning = Regression?
  - Unsupervised Learning
    - Dimension Reduction (PCA)
    - Matrix Completion
Recommender Systems
    - Image Painting, Restoration,
Super-resolution
    - K-Means Clustering
    - Naive GAN
  - Supervised Learning
    - Function f is known
      - Linear Regression
      - Nonlinear Regression
      - Linear Classification
    - Function f is unknown
      - Kernel Methods
      - Adaboost, GBDT,
XGBoost
      - Deep Learning
      - Advanced GANs

Supervised Machine Learning

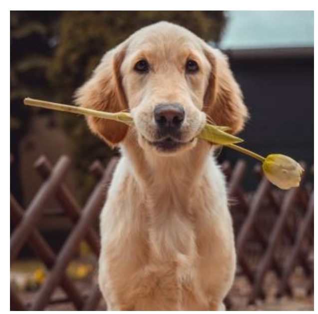
Supervised learning is the machine learning task of inferring a function from labeled training data

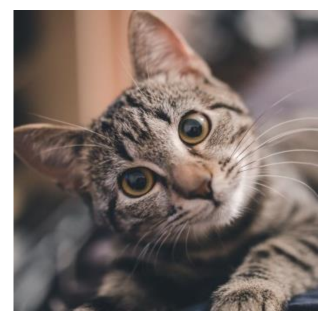
Labeled data

cat

dog

Unlabeled data





Dataset for Supervised Learning

Libsvm dataset

- It contains many classification, regression, multi-label and string data sets
  https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
- You can use LIBSVM, a package, with these sets
  http://www.csie.ntu.edu.tw/~cjlin/libsvm
- You can also use LIBLINEAR, a linear classifier, with the sets
  https://www.csie.ntu.edu.tw/~cjlin/liblinear/#document
- Other tutorials you can read are as follows:

Tools: https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/

Guide: https://www.csie.ntu.edu.tw/~cjlin/papers/guide/guide.pdf

Column Vector

Data:

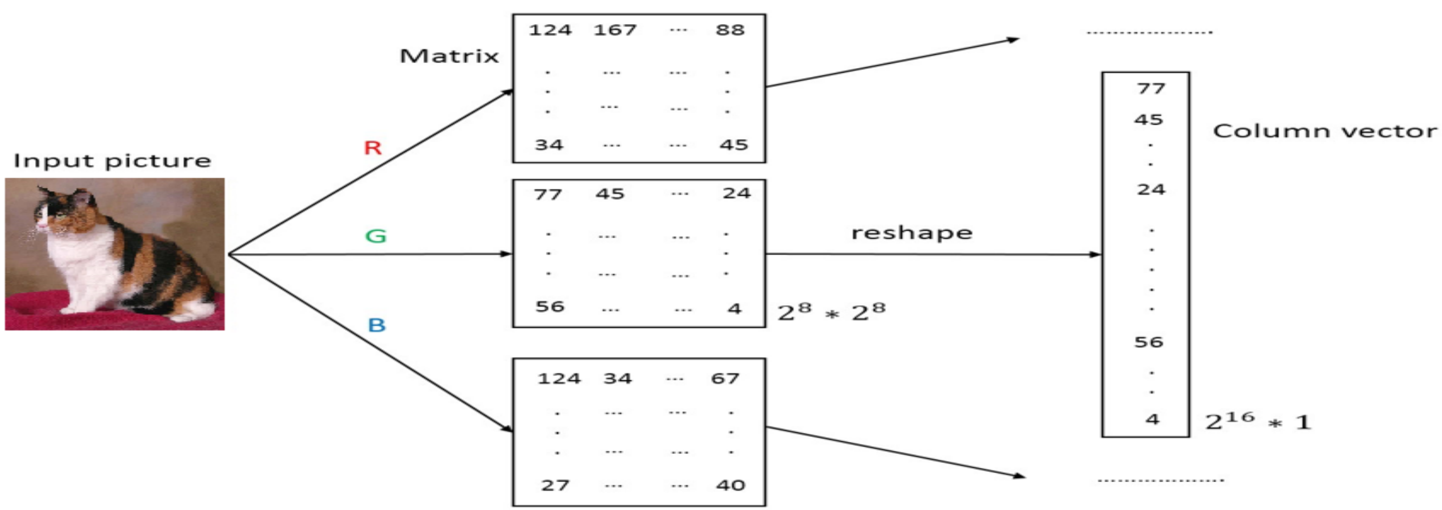
$$\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$$

$\mathbf{x}$ is the input, which is usually presented as a column vector

y is the output, for example, a person's name

n is the number of samples

For example, $\mathbf{x}$ can be a picture stored as a matrix:



Introduction to the Format of LIBSVM

Two properties of data:

- The number of features is large
- Each instance is sparse for most feature values are zero

Sparse format:

<label1> <index1>:<value1> <index2>:<value2> …
<label2> <index1>:<value1> <index2>:<value2> …

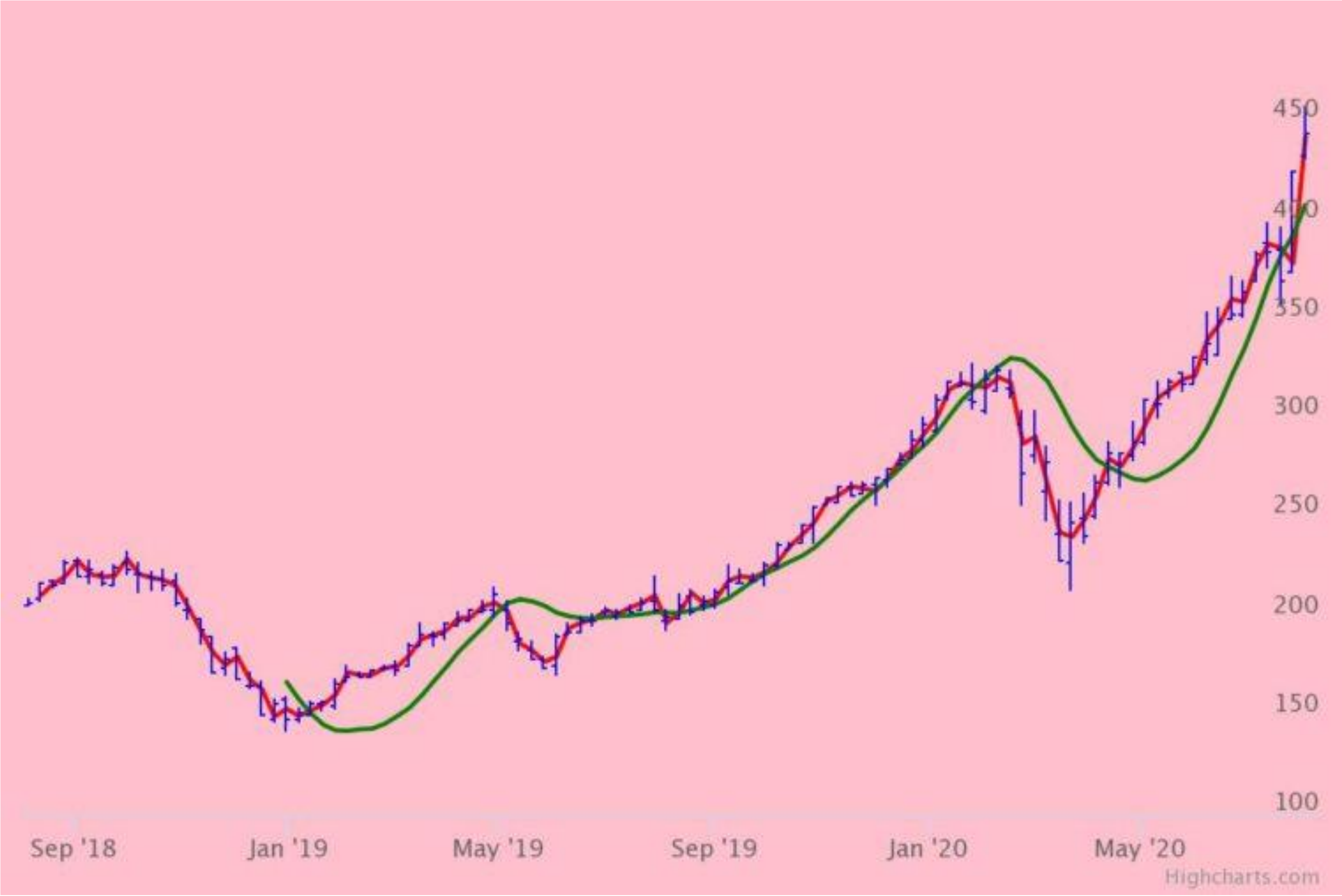
- An example for classification:

  +1 1:2 4:5 \n-1 2:4 \n

  translate to: The points (2,0,0,5) and (0,4,0,0) are assigned to class +1 and class -1 respectively

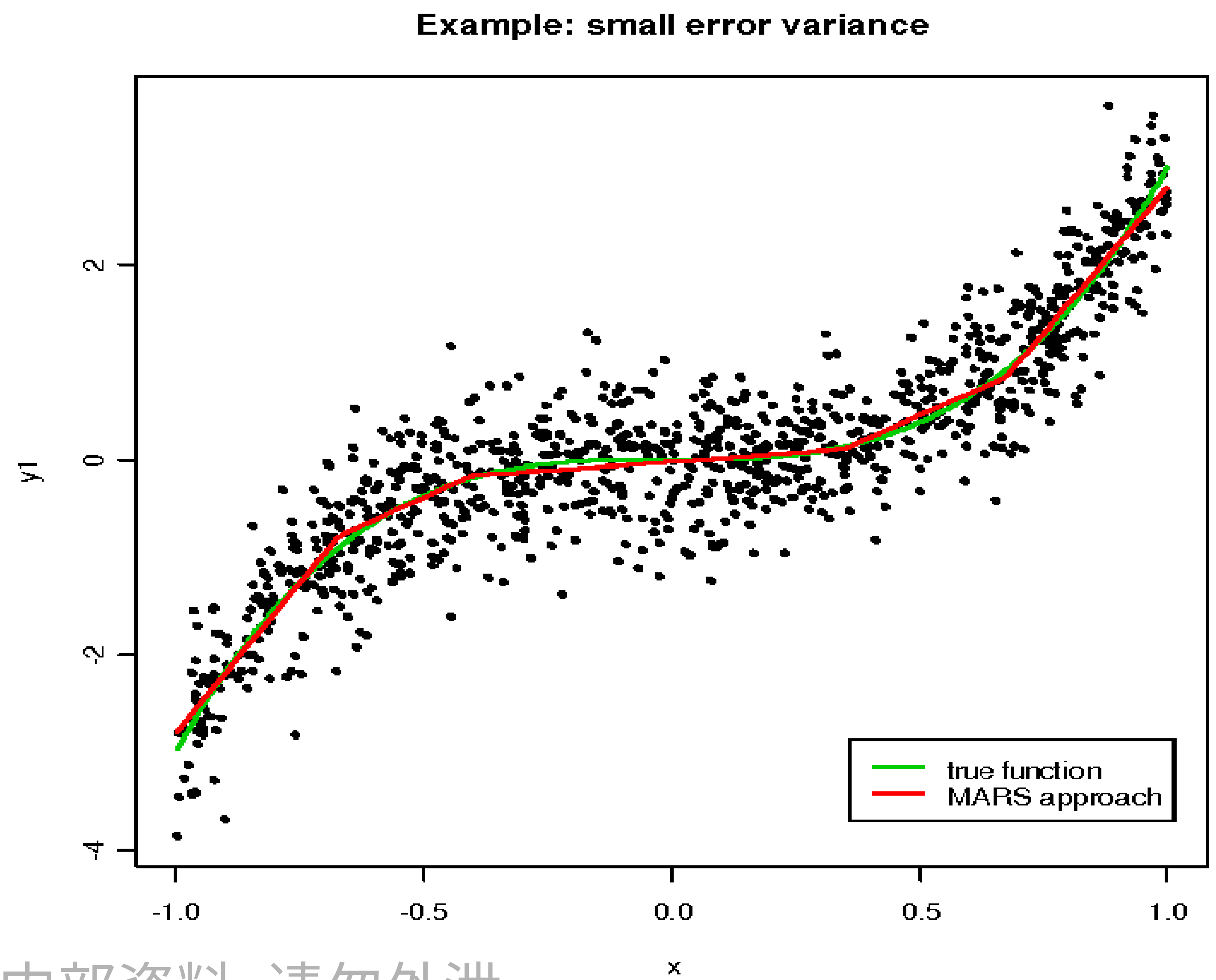
Contents

Regression

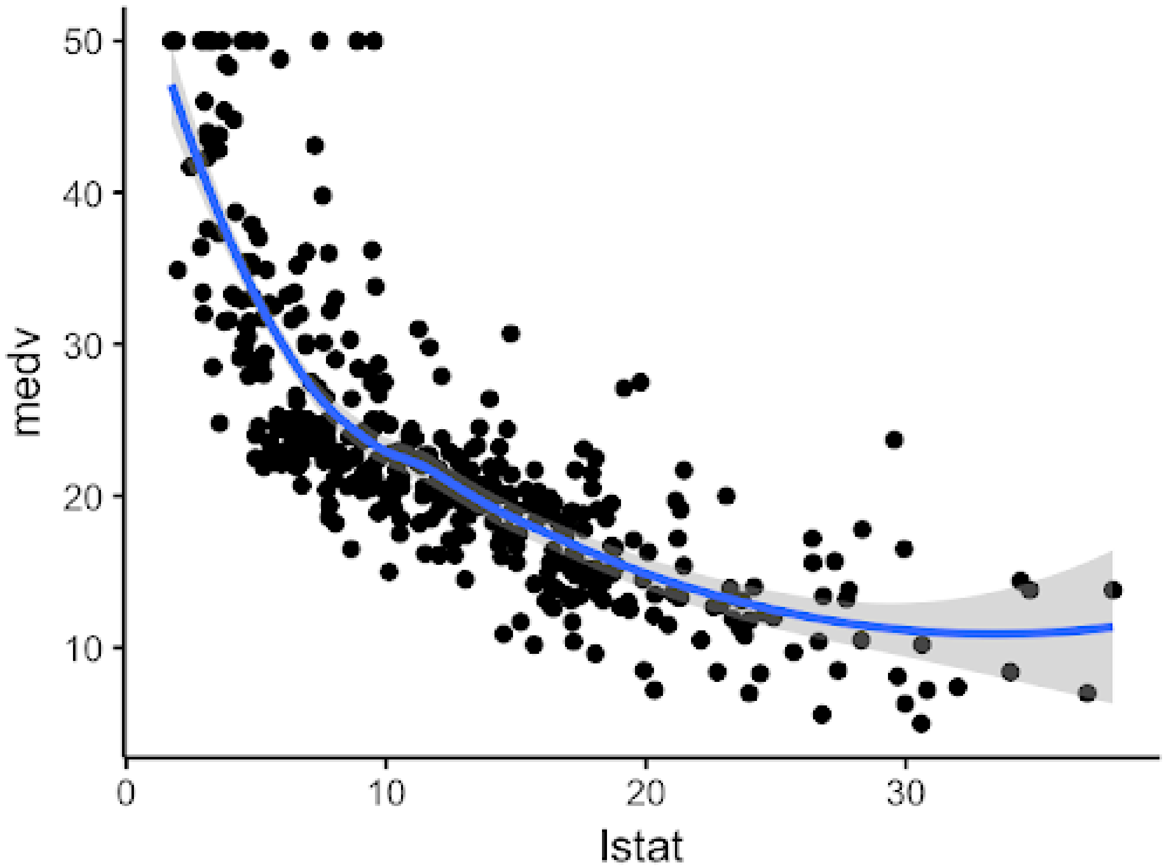


450
400
350
300
250
200
150
100
Sep '18
Jan '19
May '19
Sep '19
Jan '20
May '20
Highcharts.com

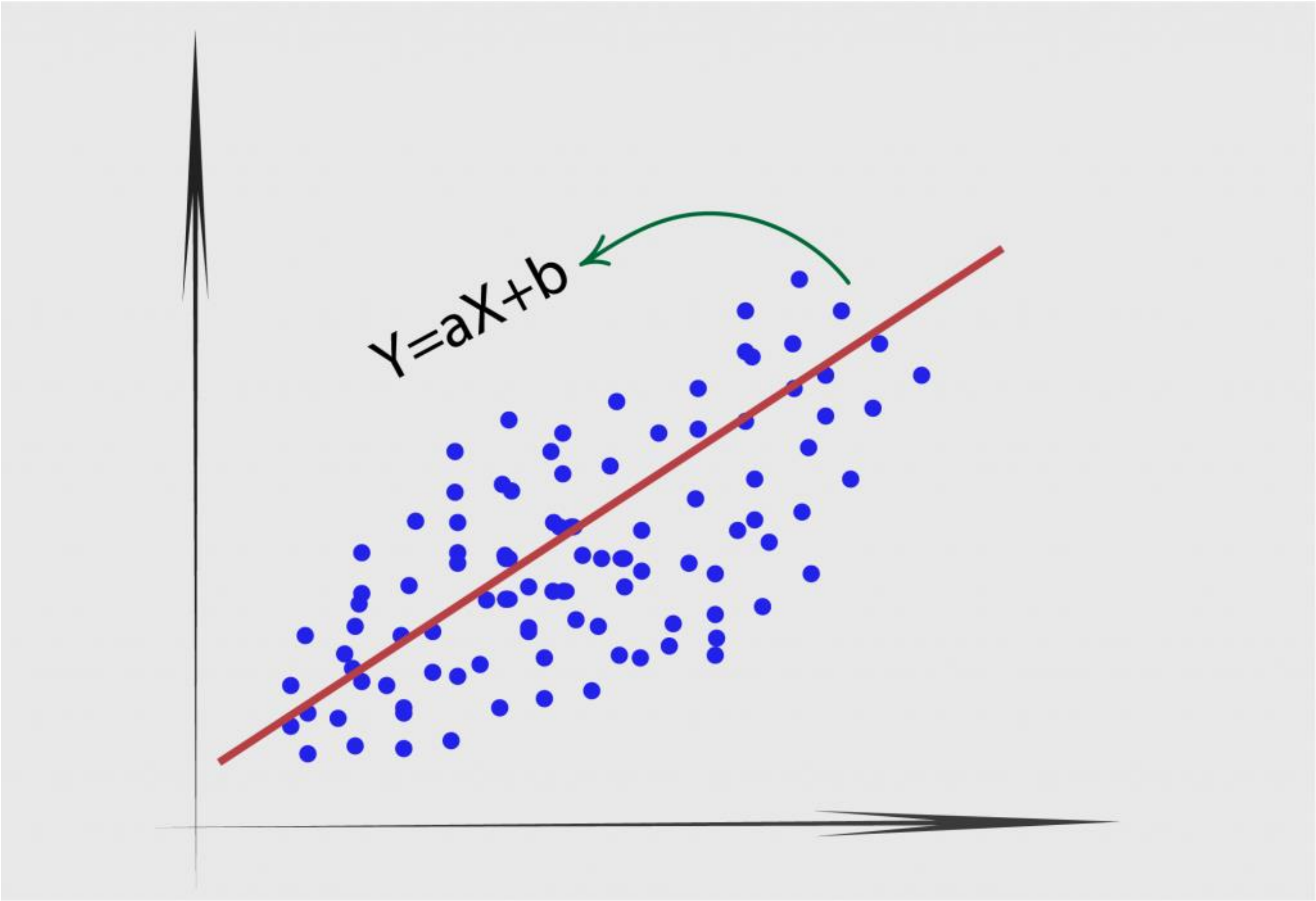
Regression


Example: small error variance
y1
2
0
-2
-4
-1.0
-0.5
0.0
0.5
1.0
x
true function
MARS approach

Regression



Regression



Problem Setup for Regression

- **Inputs**

  Input space: $\mathcal{X} = \{\mathbf{x}_i\}_{i=1}^{N}, \mathbf{x}_i \in \mathbb{R}^m$

  N is the number of data samples

  $\mathbf{x}_i$ includes m features

- **Outputs**

  Output space: $\mathcal{Y} = \{y_i\}_{i=1}^{N}, y_i \in \mathbb{R}$

- **Goal**

  Learn a hypothesis / model $f: \mathcal{X} \to \mathcal{Y}$

Regression

Loss:

- Absolute value loss:

$$l(\hat{y}_i, y_i) = |\hat{y}_i - y_i|$$

- Least squares loss:

$$l(\hat{y}_i, y_i) = \frac{1}{2}(\hat{y}_i - y_i)^2$$

Total loss function:

$$\mathcal{L}_{\mathcal{D}}(\mathbf{W}) = \sum_{i=1}^{n} l(\hat{y}_i, y_i)$$

Regression

- The smaller value of $\mathcal{L}_{\mathcal{D}}$ is better, and loss function $\mathcal{L}_{\mathcal{D}}$ plays a major role in machine learning

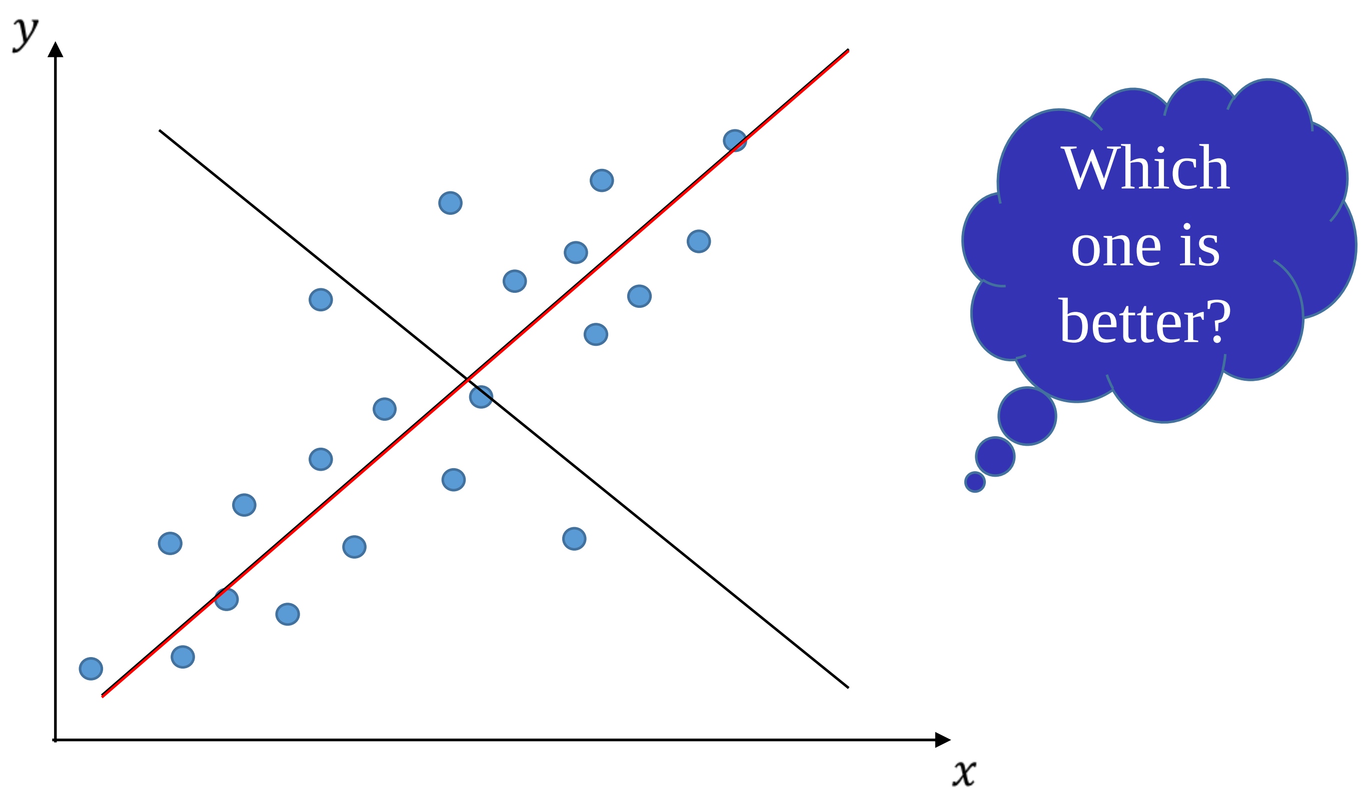
Target:

- Find the best f by solving the following optimization problem:

$$f^* = \underset{f}{\operatorname{argmin}} \sum_{i=1}^{n} l(f(x), y_i)$$

Linear Regression

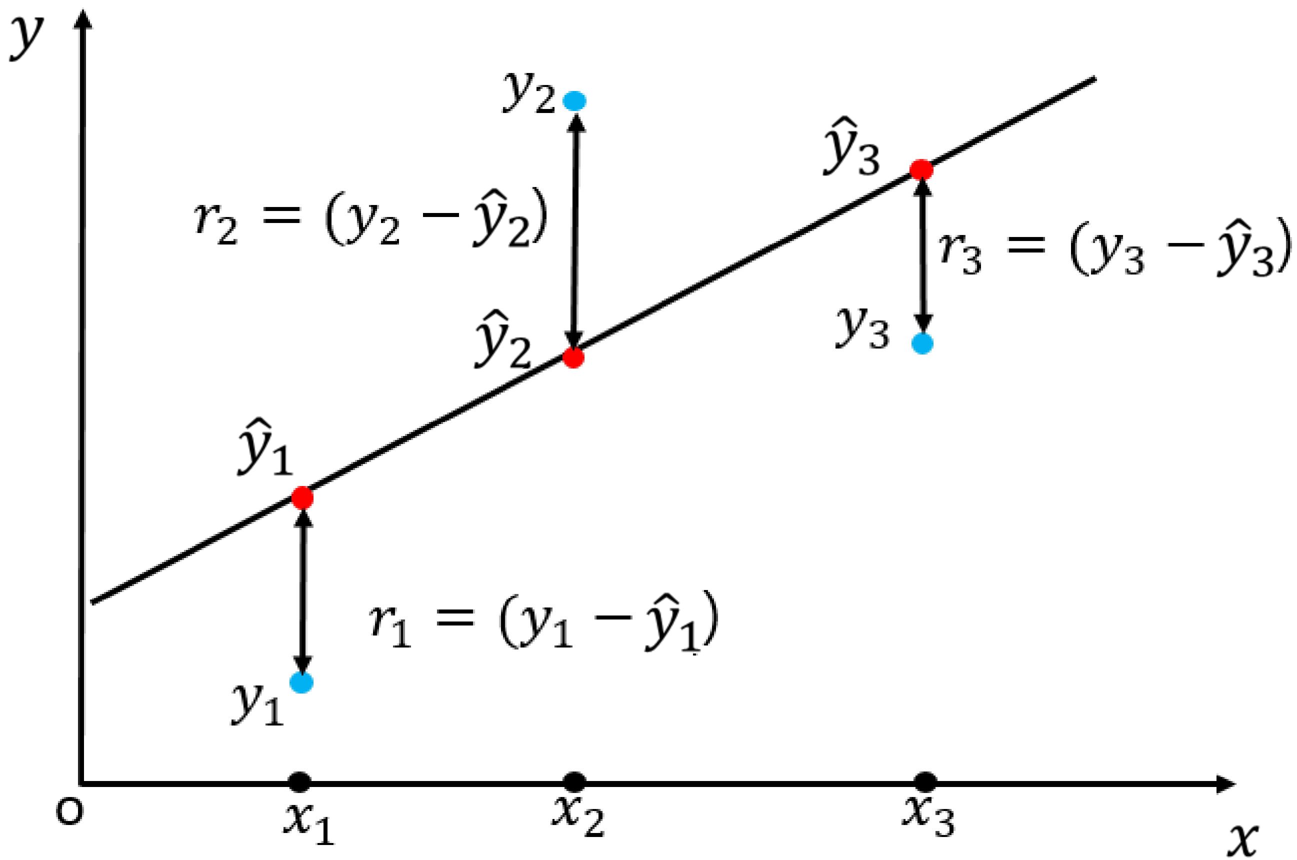
Simple linear regression describes the linear relationship between a variable x and a response variable y



Simple linear 1-D regression

Linear Regression

- **What makes a good model?**



Linear Regression

Learn $f(\mathbf{x}; \mathbf{w}, b)$ with

- Parameters: $\mathbf{w} \in \mathbb{R}^m, b \in \mathbb{R}$
- Input: $\mathbf{x}$ where $x_i \in \mathbb{R}$, features for $i \in \{1, \cdots, m\}$
- Model Function:

$$f(\mathbf{x}; \mathbf{w}, b) = w_1 x_1 + \cdots + w_m x_m + b$$

$$= \sum_{i=1}^{m} w_i x_i + b$$

$$= \mathbf{w}^{\mathrm{T}} \mathbf{x} + b$$

Performance Measure for Regression

- Least squared loss

$$\mathcal{L}_{\mathcal{D}}(\mathbf{w}, b) = \frac{1}{2}\sum_{i=1}^{n}(y_i - f(\mathbf{x}_i; \mathbf{w}, b))^2$$

$$= \frac{1}{2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

Training: find minimizer of least squared loss

$$\mathbf{w}^*, b^* = \underset{\mathbf{w}, b}{\operatorname{argmin}}\, \mathcal{L}_{\mathcal{D}}(\mathbf{w}, b)$$

Contents

Matrix Presentation for Loss Function

In order to simplify our proof, we introduce augmented matrix and augmented vector and still represent them by $\mathbf{w}$ and $\mathbf{X}$.

i.e.

$$\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_i, \dots, \mathbf{x}_n)^{\mathrm{T}}$$

$$\mathbf{x}_i = (1, x_{i1}, x_{i2}, \dots, x_{in})$$

$$\mathbf{w} = (b, w_1, w_2, \dots, w_n)^{\mathrm{T}}$$

Loss function:

$$\mathcal{L}_D(w) = \frac{1}{2} \|Y - Xw\|_2^2$$

$$where\ X = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nm} \end{pmatrix},\quad Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Matrix Presentation for Loss Function

- Proof:

$$\mathcal{L}_D(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n}(y_i - \mathbf{x}_i\mathbf{w})^2$$

$$= \frac{1}{2}\begin{bmatrix} y_1 - \mathbf{x}_1^{\mathrm{T}}\mathbf{w} \\ \vdots \\ y_n - \mathbf{x}_n^{\mathrm{T}}\mathbf{w} \end{bmatrix}^{\mathrm{T}} \begin{bmatrix} y_1 - \mathbf{x}_1^{\mathrm{T}}\mathbf{w} \\ \vdots \\ y_n - \mathbf{x}_n^{\mathrm{T}}\mathbf{w} \end{bmatrix}$$

$$= \frac{1}{2}\left(\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{x}_n^{\mathrm{T}} \end{bmatrix}\mathbf{w}\right)^{\mathrm{T}} \left(\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}} \\ \vdots \\ \mathbf{x}_n^{\mathrm{T}} \end{bmatrix}\mathbf{w}\right)$$

$$= \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\mathbf{w})$$

$$= \frac{1}{2}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2$$

Analytical Solution

How to address the linear regression question?

- Closed-form solution to linear regression:

$$\mathcal{L}_D(\mathbf{w}) = \frac{1}{2}(\mathbf{y} - \mathbf{X}\mathbf{w})^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\mathbf{w}) \text{ , Let } \mathbf{a} = \mathbf{y} - \mathbf{X}\mathbf{w},$$

$$\begin{aligned}
\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}} &= \frac{\partial \mathbf{a}}{\partial \mathbf{w}} \frac{\partial(\frac{1}{2}\mathbf{a}^T\mathbf{a})}{\partial \mathbf{a}} \\
&= \frac{1}{2}\frac{\partial \mathbf{a}}{\partial \mathbf{w}}(2\mathbf{a}) \\
&= \frac{\partial(\mathbf{y} - \mathbf{X}\mathbf{w})}{\partial \mathbf{w}}(\mathbf{y} - \mathbf{X}\mathbf{w}) \\
&= -\mathbf{X}^{\mathrm{T}}(\mathbf{y} - \mathbf{X}\mathbf{w})
\end{aligned}$$

Since $\mathcal{L}_D(\mathbf{w})$ is a convex function, $\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}} = 0$ derive $\mathbf{w}^*$

Analytical Solution

- Assuming $|\mathbf{X}^{\mathrm{T}}\mathbf{X}| \neq 0$
- Let $$\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}} = -\mathbf{X}^{\mathrm{T}}\mathbf{y} + \mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{w} = 0$$

$$\Longrightarrow \mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{w} = \mathbf{X}^{\mathrm{T}}\mathbf{y}$$

$$\Longrightarrow \mathbf{w} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

- Solve the optimal parameter $\mathbf{w}^*$

$$\mathbf{w}^* = \underset{w}{\operatorname{argmin}}\, \mathcal{L}_{\mathcal{D}}(\mathbf{w}) = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$$

Challenges about Analytical Solution

There are two challenges left to address about the analytical solution $\mathbf{w}^* = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$:

- Many matrices are not invertible

  Necessary and Sufficient Condition:

  If $\mathbf{X}$ is a matrix of m rows and n columns $(n \leq m)$,

$$|\mathbf{X}^{\mathrm{T}}\mathbf{X}| \neq 0 \Leftrightarrow rank(\mathbf{X}) = n$$

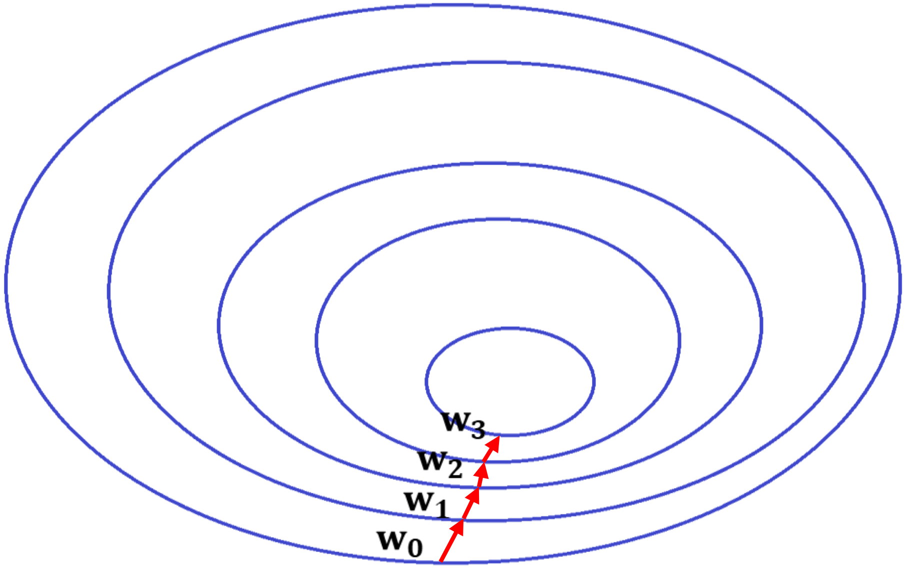
- The inverse of a large matrix needs huge memory, which takes $O(m^3)$ to compute.

Contents

Gradient Descent

- Get the best $\mathbf{w}$ by minimizing a loss function $\mathcal{L}_{\mathcal{D}}(\mathbf{w})$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \mathcal{L}_{\mathcal{D}}(\mathbf{w})$$



- Do we have other optimization methods in addition to closed-form solution ?

General Optimization Scheme

- General optimization scheme contains 3 iterative steps：

Algorithm 1: General Iterative Optimization Scheme

---

for $k = 0, 1, \ldots$ **do**
    Find a feasible search direction $\mathbf{d}_k$;
    Find a good step size η_k;
    Set $\mathbf{w}_{k+1} = \mathbf{w}_k + \eta_k \mathbf{d}_k$.
end

- The core questions are:
  - How to find a feasible search direction d ?
  - How to find a good step size η ?
- No matter what kind of problems are, we do just care the above two questions
- The construction of feasible search direction d is problem dependent and can be very complex

Descent Direction

- We use $\mathbf{d} = -\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}$ as the direction of optimization
- Gradient (vector of partial derivatives)

$$\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}} = \begin{bmatrix} \frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial w_1} \\ \frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial w_2} \\ \vdots \\ \frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial w_m} \end{bmatrix}$$

(We always write a vector into column form)

- Why $\mathcal{L}_{\mathcal{D}}(\mathbf{w}') = \mathcal{L}_{\mathcal{D}}(\mathbf{w} + \eta\mathbf{d}) \leq \mathcal{L}_{\mathcal{D}}(\mathbf{w}), \ \eta \to 0^+$?

Descent Direction

Proof:

By Taylor expansion, when $\eta \to 0^+$:

$$\mathcal{L}_{\mathcal{D}}(\mathbf{w} + \eta\mathbf{d}) = \mathcal{L}_{\mathcal{D}}(\mathbf{w}) + \left(\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}\right)^{\mathrm{T}} \eta\mathbf{d} + o(\eta\mathbf{d})$$

$$= \mathcal{L}_{\mathcal{D}}(\mathbf{w}) + \eta' \left(\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}\right)^{\mathrm{T}} \mathbf{d}$$

Note that $\eta' > 0$ and

$$\eta' \left(\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}\right)^{\mathrm{T}} \mathbf{d} = -\eta' \mathbf{d}^{\mathrm{T}}\mathbf{d} \le 0$$

We have:

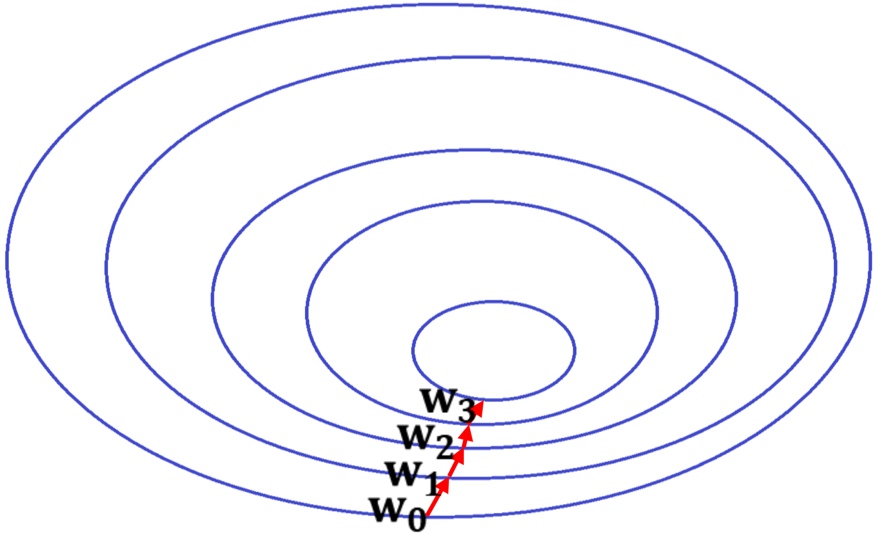
$$\mathcal{L}_{\mathcal{D}}(\mathbf{w}') = \mathcal{L}_{\mathcal{D}}(\mathbf{w} + \eta\mathbf{d}) \le \mathcal{L}_{\mathcal{D}}(\mathbf{w})$$

Gradient Descent: Update Parameters

Minimize loss by repeated gradient steps (when no closed form):

- Compute gradient of loss with respect to parameters $\frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}$
- Update parameters with learning rate η

$$\mathbf{w}' = \mathbf{w} - \eta \frac{\partial \mathcal{L}_{\mathcal{D}}(\mathbf{w})}{\partial \mathbf{w}}$$



General Gradient Decent Scheme

- General gradient decent scheme contains 3 iterative steps：

Algorithm 2: General Gradient Decent Scheme

Set $\mathbf{w}_0 = \mathbf{0}$

for $k = 0, 1, \ldots$ **do**

  Find a feasible search direction $\mathbf{d}_k = -\frac{\partial L_D(\mathbf{w}_k)}{\partial \mathbf{w}_k}$;

  Find a good learning rate η_k;

  Set $\mathbf{w}_{k+1} = \mathbf{w}_k + \eta_k \mathbf{d}_k$

end

- Why a good learning rate is necessary?

Appropriate Value of Learning Rate

Learning rate η has a large impact on convergence

- Too large $\eta \Rightarrow$ oscillate and may even diverge
- Too small $\eta \Rightarrow$ too slow to converge

Adaptive learning rate (For example) :

- Set larger learning rate at the beginning
- Use relatively smaller learning rate in the later epochs
- Decrease the learning rate:

$$\eta_{k+1} = \frac{\eta_k}{k+1}$$

Thank You