Prof. Mingkui Tan

South China University of Technology Southern Artificial Intelligence Laboratory(SAIL)

October 13, 2017





#### Content

- Basic Concepts about Machine Learning
- 2 Linear Regression
- Closed-form solution
- **Gradient Descent**

#### Contents

- Basic Concepts about Machine Learning

#### What is Machine Learning?

Mchine Learning compose of three parts:

- Data
- Model(function)
- Loss(prediction)

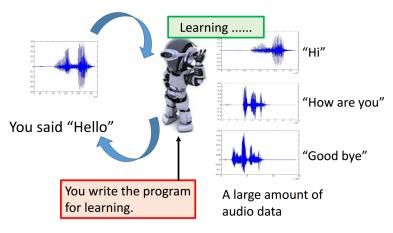


Figure: Speech Recognition

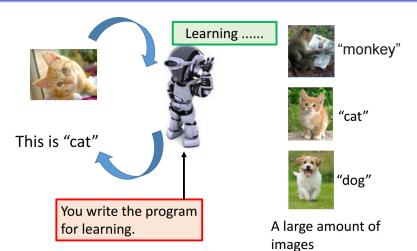


Figure: Image Recognition

#### Machine Learning $\approx$ Looking for a Function

Speech Recognition

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

Image Recognition



Playing Go



Dialogue System

$$f($$
 "Hi"  $)=$  "Hello" (what the user said) (system response)



#### Basic Concepts about Machine Learning Framework

A set of function

Model  $f_1, f_2 \cdots$ 

$$f_1($$



$$)=$$
 "money"

$$f_1$$



Figure: Image Recognition

# Three Main Elements of Machine Learning

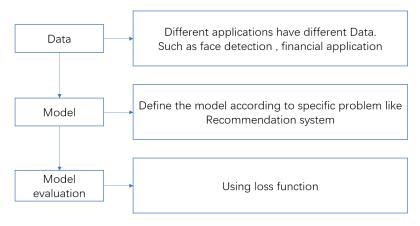


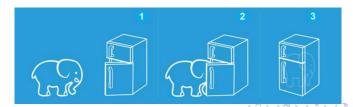
Figure: Three main elements of machine learning

#### Basic Concepts about Machine Learning Framework

#### Machine Learning is so simple ...



Just like putting an elephant into the fridge . . .

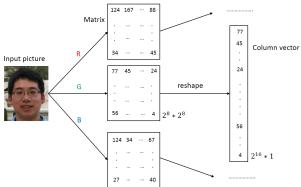


#### Column Vector

• Data:

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

- $\bullet \ \mathbf{x}$  is input,and we usually present it as column vector
- ullet For example,  ${f x}$  may be a picture stored as a matrix:



- y is output (for example: name of a person)
- n is number
- We want to use a function predicting y:

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

 However, the prediction may be inconsistent with the groundtruth. We calculate the differences by loss function:

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

# 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(loss function):

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

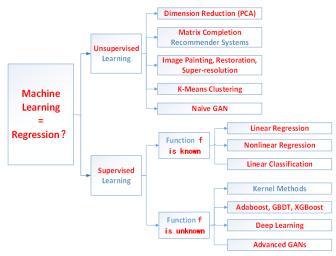
# Regression

• The smaller value of  $\mathcal{L}_D$  the better, and loss function( $\mathcal{L}_D$ ) plays a major role in machine learning

Find the best f by solving the following optimization problem:

$$f^* = \min_{f} \sum_{i=1}^{n} l(f(\mathbf{x}), y_i)$$

# Supervised Optimization for Deep Learning Learning Map



# Supervised Optimization for Deep Learning Learning Map

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

Labelled data





Unlabeled data





Figure: Images of cats and dogs

# Data Sets for Supervised Learning

#### Libsym dataset

http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/

#### LIBSVM Data: Classification, Regression, and Multi-label

This page contains many classification, regression, multi-label and string data sets stored in LIBSVM format. Many are from UCI, Statlog, StatLib and other col scale each attribute to [-1,1] or [0,1]. The testing data (if provided) is adjusted accordingly. Some training data are further separated to "training" (tr) and "vali each data set. To read data via MATLAB, you can use "libsymread" in LIBSYM package.

A summary of all data sets is in the following. If you have used LIBSVM with these sets, and find them useful, please cite our work as: Chih-Chung Chang and Chih-Jen Lin, LIBSVM: a library for support vector machines, ACM Transactions on Intelligent Systems and Technology, 2:27:1--27:27. http://www.csie.ntu.edu.tw/~cilin/libsvm.

Please also cite the source of the data sets (references given below).

Go to pages of classification (binary, multi-class), regression, multi-label, and string. Those interested in hierarchical data with many classes can visit LSHTC pages.

Some sets are large and the connection may fail. On Linux you can use

> wget -t inf URL address of data

to retry infinitely many times. If it still fails, add -c to continuely get a partially-downloaded set. You can also use

> 1ftp -c 'pget -c URL address of data'

to have several connections for reducing the downloading time.

name		source	type	class	training size	testing size	feature	
<u>a1a</u>	UCI		classification	2	1,605	30,956	123	
a2a	UCI		classification	2	2,265	30,296	123	
a3a	LICT		classification	2	3 185	29 376	123	

### Contents

- 2 Linear Regression

## Linear Regression

Simple linear regression describes the linear relationship between a predictor variable, plotted on the x-axis, and a response variable, plotted on the y-axis

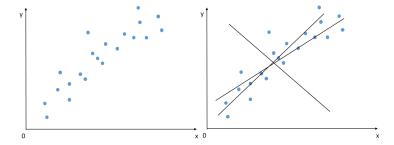


Figure: Simple linear 1D regression

# Machine Learning Setup

- Inputs Input space  $\mathbf{X} = \mathbb{R}^m$ feature, covariants, predictors, etc.
- Outputs Output space: Y many different types of predictions.
- Goal:Learn a hypothesis/model  $f: \mathbf{X} \mapsto \mathbf{Y}$

# Supervised Learning

• Given set of input, output pairs

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

- Learn the "best" model based on D
- Predict  $\hat{y}$  for unseen x based on f(x)

Closed-form solution

# Linear Regression:Common

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

- Parameters:  $\mathbf{w} \in \mathbb{R}^m, w_0 \in \mathbb{R}$
- Input:x where  $x_j \in \mathbb{R}$  for  $j \in 1,...m$  features
- Model Function:

$$f(\mathbf{x}; w_0, \mathbf{w}) = w_0 + w_1 x_1 + \dots + w_m x_m$$
$$= \sum_{j=1}^m w_j x_j + w_0$$
$$= \mathbf{w}^\top \mathbf{x} + w_0$$

# Linear Regression

• What makes a good model?

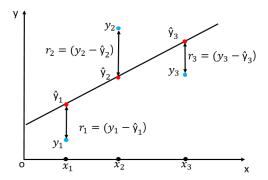


Figure: Contributing loss terms for 1D regression

# Performance Measure for Regression

Least squared loss

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

Training: find minimizer of least squared loss

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

### Contents

- 2 Linear Regression
- Closed-form solution

#### Matrix Presentation

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

## Matrix Presentation

Proof:

$$\frac{1}{2} (\mathbf{y} - \mathbf{X} \mathbf{w})^{\top} (\mathbf{y} - \mathbf{X} \mathbf{w})$$

$$= \frac{1}{2} \begin{pmatrix} \begin{bmatrix} y_1 \\ \dots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^{\top} \\ \dots \\ \mathbf{x}_n^{\top} \end{bmatrix} \mathbf{w} \end{pmatrix}^{\top} \begin{pmatrix} \begin{bmatrix} y_1 \\ \dots \\ y_n \end{bmatrix} - \begin{bmatrix} \mathbf{x}_1^{\top} \\ \dots \\ \mathbf{x}_n^{\top} \end{bmatrix} \mathbf{w} \end{pmatrix}$$

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

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

# **Analytical Solution**

• Closed-form of linear regression:

$$\mathcal{L}_{D}(\mathbf{w}) = \frac{1}{2} (\mathbf{y} - \mathbf{X} \mathbf{w})^{\top} (\mathbf{y} - \mathbf{X} \mathbf{w})$$

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

$$\frac{\partial \mathcal{L}_{D}(\mathbf{w})}{\partial \mathbf{w}} = \frac{1}{2} (\frac{\partial \mathbf{y}^{\top} \mathbf{y}}{\partial \mathbf{w}} - \frac{\partial 2 \mathbf{w}^{\top} \mathbf{X}^{\top} \mathbf{y}}{\partial \mathbf{w}} + \frac{\partial \mathbf{w}^{\top} \mathbf{X}^{\top} \mathbf{X} \mathbf{w}}{\partial \mathbf{w}})$$

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

$$= -\mathbf{X}^{\top} \mathbf{v} + \mathbf{X}^{\top} \mathbf{X} \mathbf{w}$$

# **Analytical Solution**

$$\frac{\partial \mathcal{L}(\mathbf{w})}{\partial \mathbf{w}} = -\mathbf{X}^{\top} \mathbf{y} + \mathbf{X}^{\top} \mathbf{X} \mathbf{w} = 0$$
$$\Rightarrow \mathbf{X}^{\top} \mathbf{X} \mathbf{w} = \mathbf{X}^{\top} \mathbf{y}$$
$$\Rightarrow \mathbf{w} = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}$$

Solve for optimal parameters w\*

$$\mathbf{w}^* = (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y} = \arg \min_{\mathbf{w}} \mathcal{L}_D(\mathbf{w})$$

# Problem about The Analytical Solution

Issues about the analytical solution  $\mathbf{w}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ :

- Many matrices are not invertible
- The inverse of a large matrix needs huge memory
- The inverse takes  $O(m^3)$  to compute

Any solutions? Gradient Descent!!

#### Contents

- 2 Linear Regression
- 4 Gradient Descent

# Machine Learning

#### Training Procedure

- ullet Identify a set of hypotheses  $f(\mathbf{x}; \mathbf{w})$
- ullet Define a loss criterion  ${\cal L}_D$
- ullet Pick the best  $\mathbf{w}^*$  by minimizing a loss function  $\mathcal{L}_D(\mathbf{w})$

$$\arg\min_{\mathbf{w}} \mathcal{L}_D(\mathbf{w})$$

Learning is done through optimization

## Main Tool: Gradients

Typical case (with possibly parameterized g)

$$\mathcal{L}_D(\mathbf{w}): \mathbb{R}^n \mapsto \mathbb{R}$$

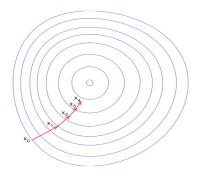
Gradient (vector of partial derivatives)

$$\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}} = \begin{bmatrix} \frac{\partial \mathcal{L}_D(w_1)}{\partial w_1} \\ \frac{\partial \mathcal{L}_D(w_2)}{\partial w_2} \\ \vdots \\ \frac{\partial \mathcal{L}_D(w_n)}{\partial w_n} \end{bmatrix}$$

(We will always write as column vectors)

## **Decent Direction**

We use  $\mathbf{d} = -\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}$  as the direction of optimization



Why 
$$\mathcal{L}_D(\mathbf{w}') = \mathcal{L}_D(\mathbf{w} + \eta \mathbf{d}) \le \mathcal{L}_D(\mathbf{w}) \qquad (\eta \to 0 \& \eta > 0)$$

#### **Decent Direction**

• By Taylor expansion, when  $\eta \to 0$ :

$$\mathcal{L}_D(\mathbf{w} + \eta \mathbf{d}) = \mathcal{L}_D(\mathbf{w}) + \left[\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}\right]^{\top} \eta \mathbf{d} + o(\eta \mathbf{d})$$
$$= \mathcal{L}_D(\mathbf{w}) + \eta \left[\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}\right]^{\top} \mathbf{d}$$

We have:

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

Note that  $\eta > 0$  and

$$\eta \left[\frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}\right]^{\top} \mathbf{d} = -\eta \mathbf{d}^{\top} \mathbf{d} \leq 0$$

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

- ullet Compute gradient of loss with respect to parameters  $rac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}$
- ullet Update parameters with rate  $\eta$

$$\mathbf{w}' \to \mathbf{w} - \eta \frac{\partial \mathcal{L}_D(\mathbf{w})}{\partial \mathbf{w}}$$

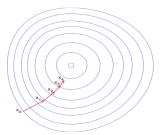


Figure: Gradient steps on a simple m = 2 loss function.

Find out an appropriate size of step

#### Learning rate $\eta$ has a large impact on convergence

- Too large  $\eta \to \text{oscillatory}$  and may even diverge
- Too small  $\eta \to \text{too slow to converge}$

#### Adaptive learning rate(For example):

- Set larger learning rate at the begining
- Use relatively smaller learning rate in the later epochs
- Decrease the learning rate:  $\eta^{t+1} = \frac{\eta^t}{t+1}$

# THANK YOU!