

Machine Learning Basics





























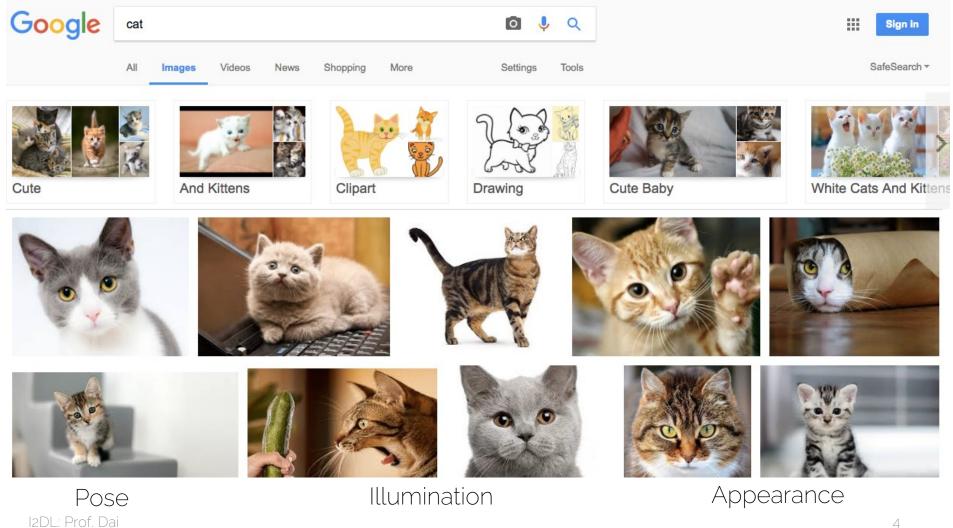


















Occlusions



Background clutter



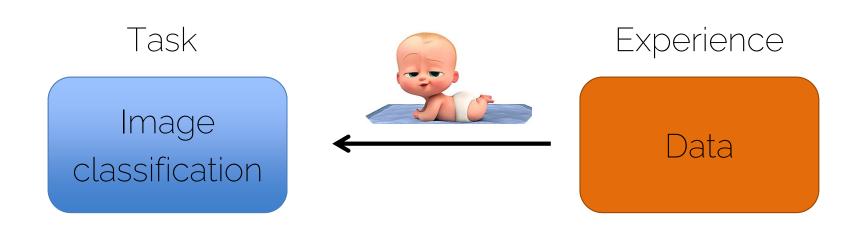




Representation



How can we learn to perform image classification?

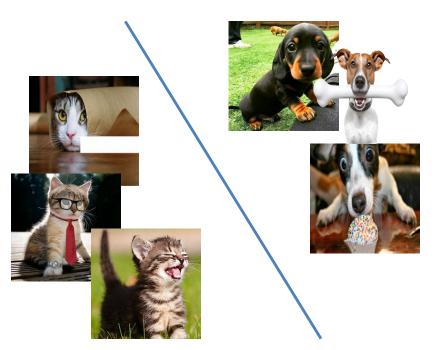


Unsupervised learning

- No label or target class
- Find out properties of the structure of the data
- Clustering (k-means, PCA, etc.)

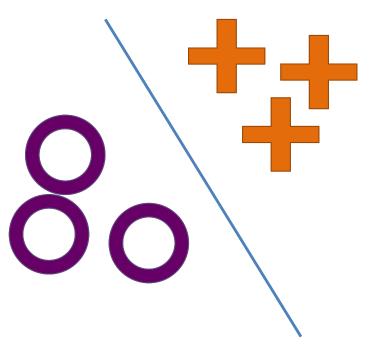
Supervised learning

Unsupervised learning



Supervised learning

Unsupervised learning



Supervised learning

Labels or target classes

Unsupervised learning

Supervised learning

CAT







CAT



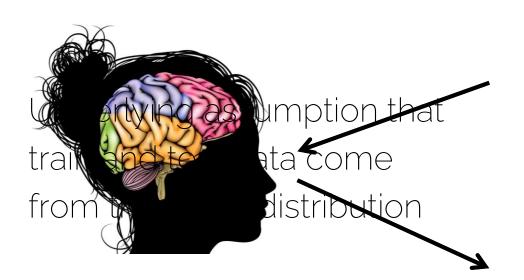


DOG

I2DL: Prof. Dai

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How can we learn to perform image classification?



Experience

Test data

How can we learn to perform image classification?

Task Experience Performance Image Data measure classification Accuracy

Unsupervised learning



Supervised learning



Reinforcement learning



Unsupervised learning



Supervised learning



Reinforcement learning



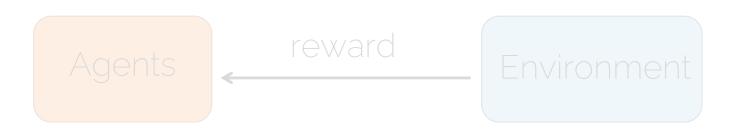
Unsupervised learning



Supervised learning



Reinforcement learning





A Simple Classifier













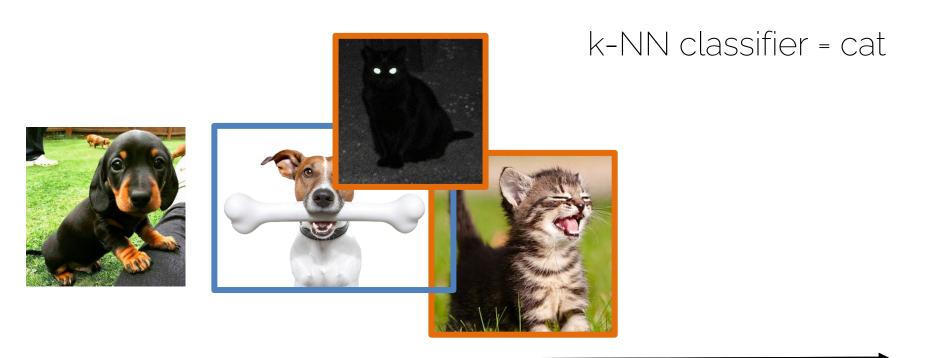




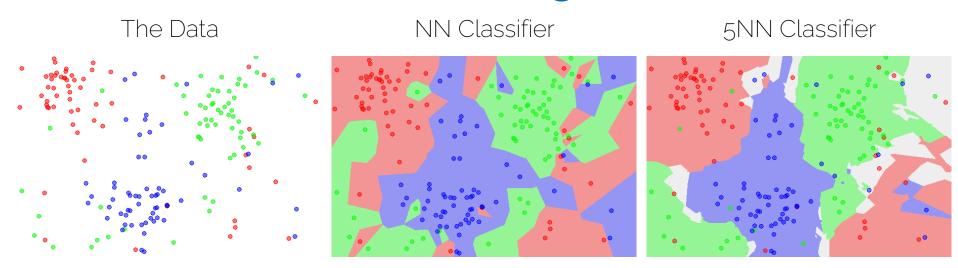




distance



distance



How does the NN classifier perform on training data?

What classifier is more likely to perform best on test data?

Source: https://commons.wikimedia.org/wiki/File:Data3classes.png

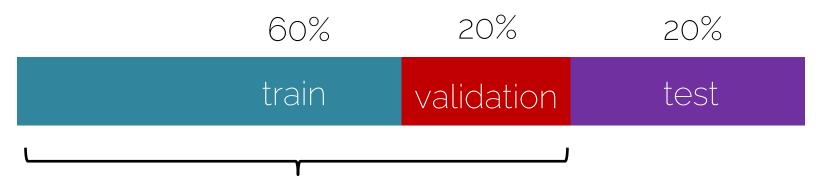
• Hyperparameters \leftarrow L1 distance : |x-c|• L2 distance : |x-c|No. of Neighbors: k

• These parameters are problem dependent.

How do we choose these hyperparameters?

Basic Recipe for Machine Learning

Split your data



Find your hyperparameters

Other splits are also possible (e.g., 80%/10%/10%)

Basic Recipe for Machine Learning

Split your data



Cross Validation

train validation

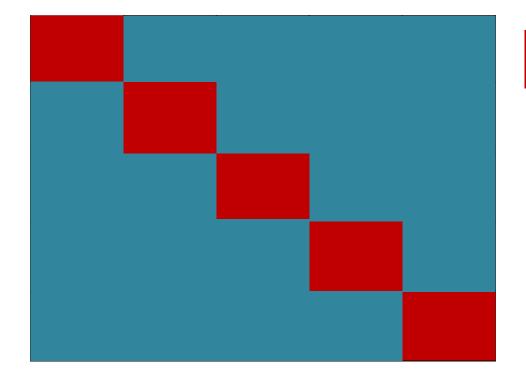


Run 2

Run 3

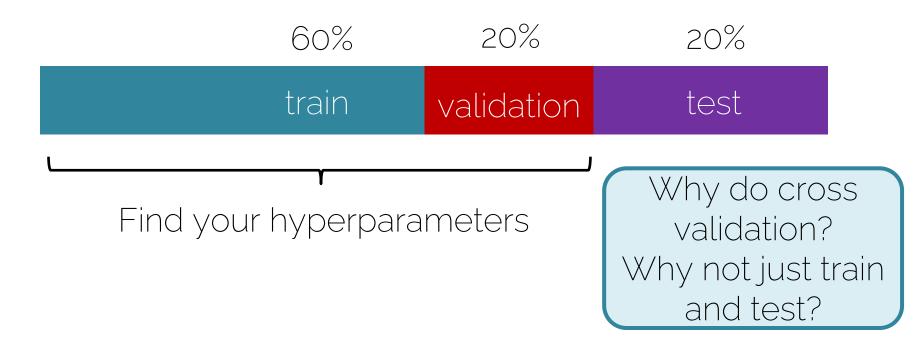
Run 4

Run 5



Split the training data into N folds

Cross Validation

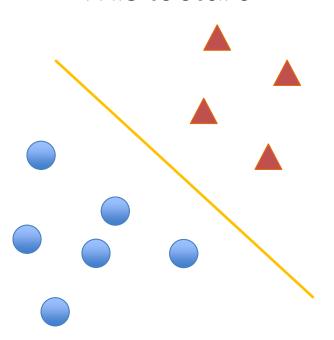


Cross Validation



Linear Decision Boundaries

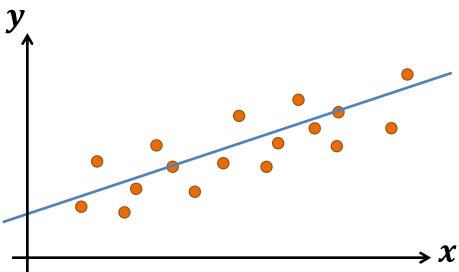
This lecture



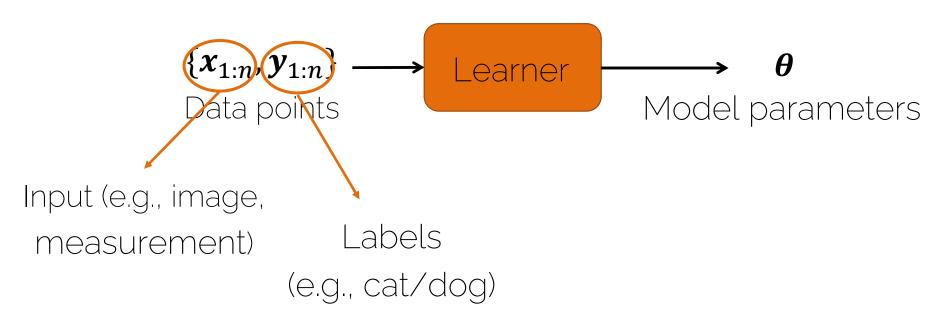
What are the pros and cons for using linear decision boundaries?

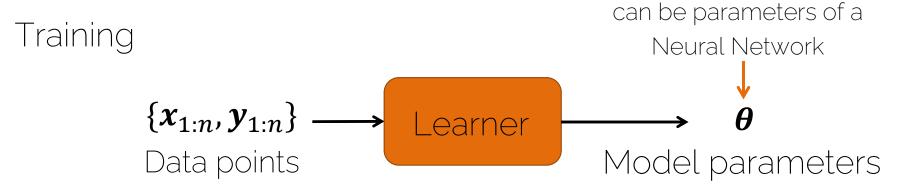


- Supervised learning
- Find a linear model that explains a target ${m y}$ given inputs ${m x}$



Training



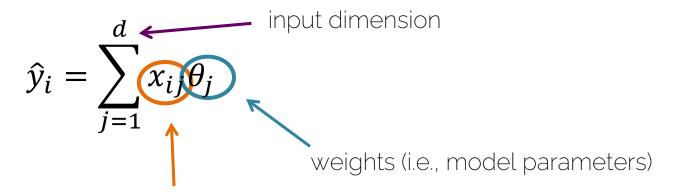


Testing



Linear Prediction

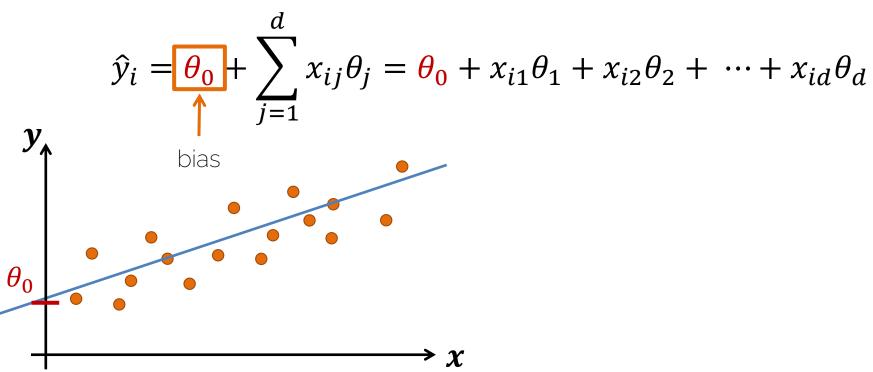
• A linear model is expressed in the form



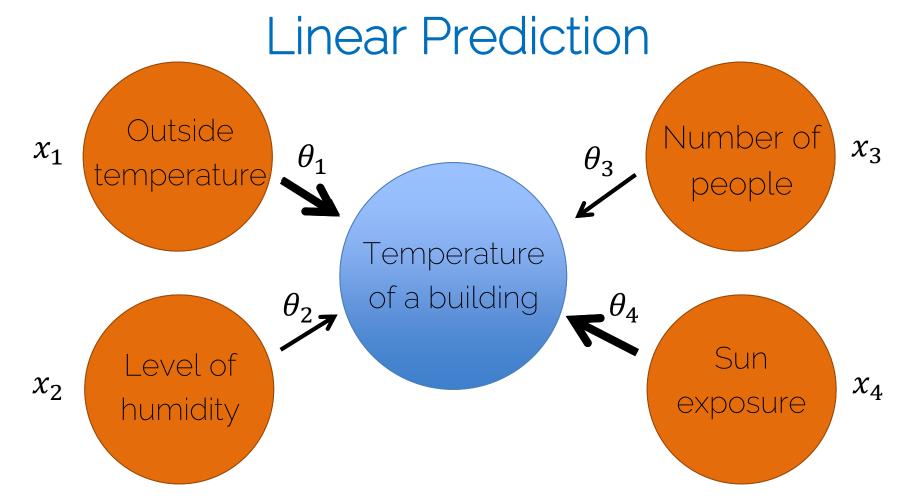
Input data, features

Linear Prediction

A linear model is expressed in the form

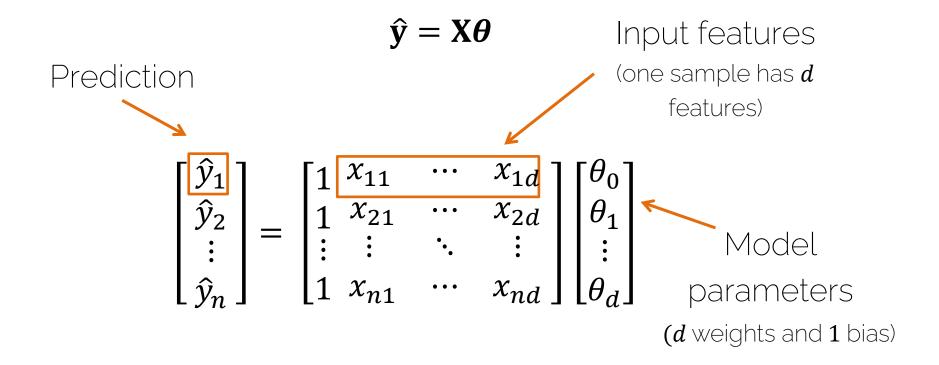


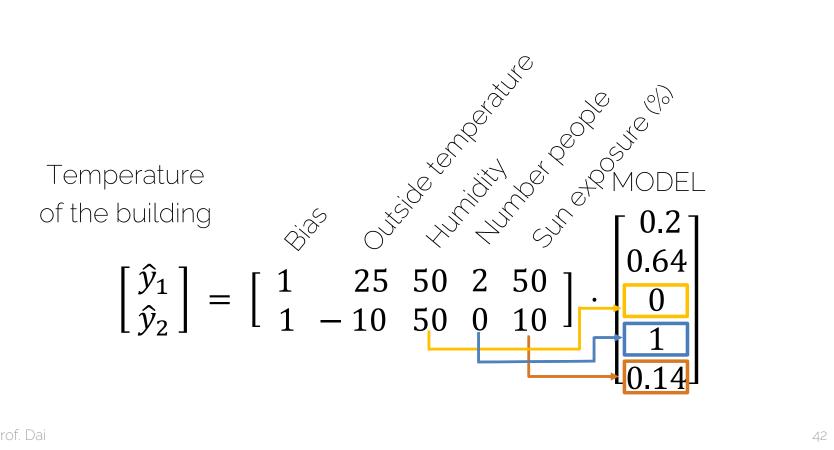
I2DI : Prof. D

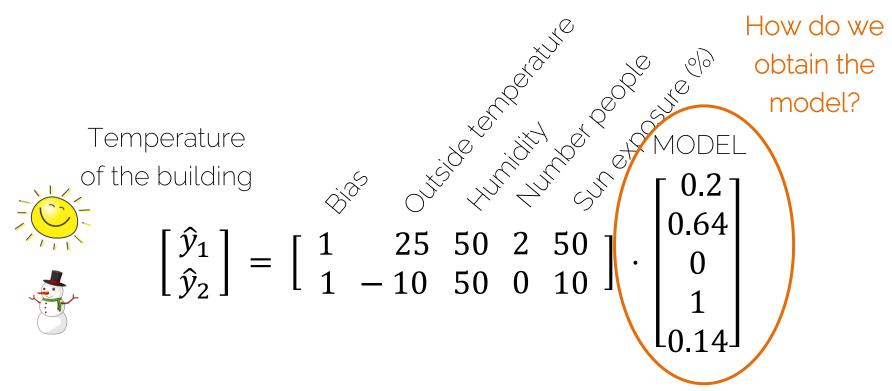


$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \theta_0 + \begin{bmatrix} x_{11} & \cdots & x_{1d} \\ x_{21} & \cdots & x_{2d} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{bmatrix} \cdot \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_d \end{bmatrix}$$

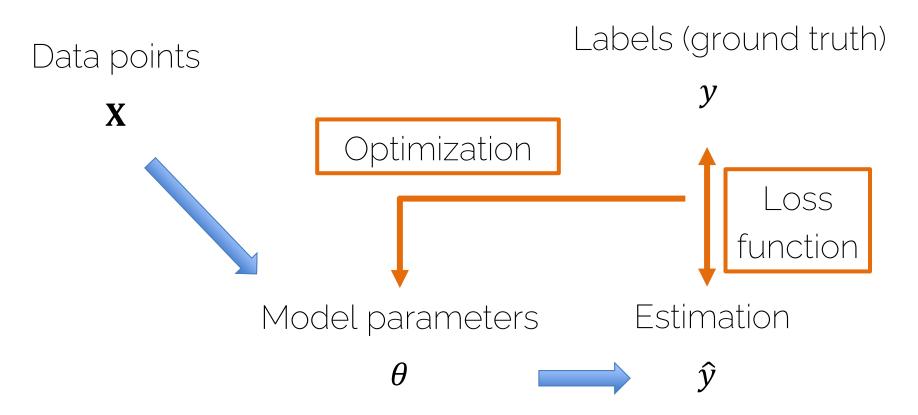
$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ 1 & x_{21} & \cdots & x_{2d} \\ \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nd} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \implies \hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$$







How to Obtain the Model?

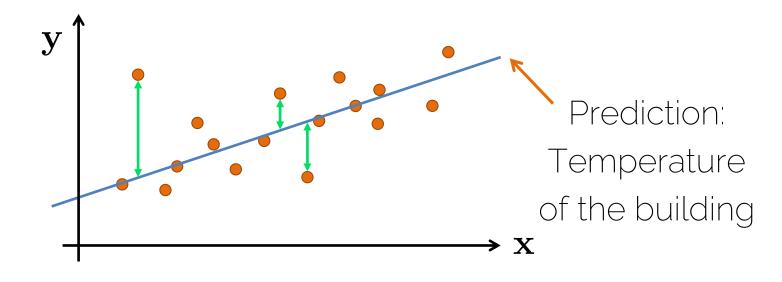


How to Obtain the Model?

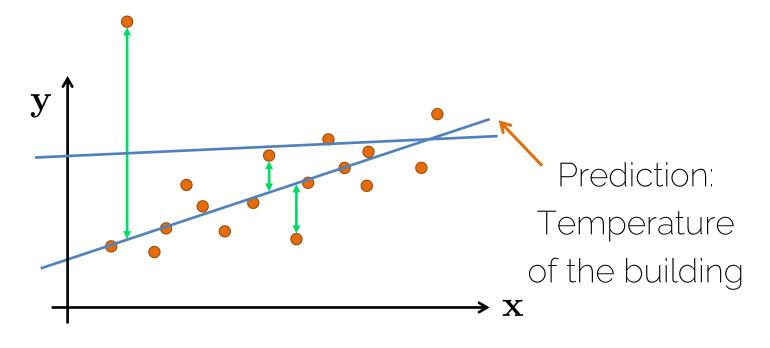
• Loss function: measures how good my estimation is (how good my model is) and tells the optimization method how to make it better.

• Optimization: changes the model in order to improve the loss function (i.e., to improve my estimation).

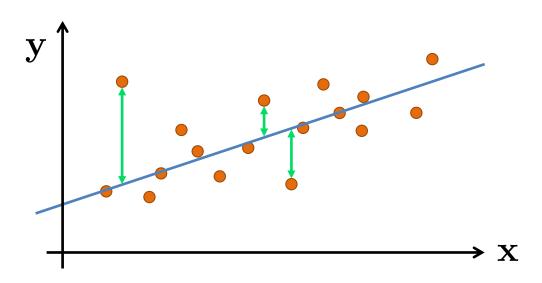
Linear Regression: Loss Function



Linear Regression: Loss Function



Linear Regression: Loss Function



Minimizing

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

Objective function

Energy

Cost function

 Linear least squares: an approach to fit a linear model to the data

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

• Convex problem, there exists a closed-form solution that is unique.

$$\min_{\theta} J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i \theta - y_i)^2$$



n training samples

The estimation comes from the linear model

$$\min_{\theta} J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i \theta - y_i)^2$$

$$\min_{\boldsymbol{\theta}} \ J(\boldsymbol{\theta}) = (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})^T (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})$$

$$n \text{ training samples,} \qquad n \text{ labels}$$

each input vector has

size d

Matrix notation

$$\min_{\theta} J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i \theta - y_i)^2$$

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})^T (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})$$

Matrix notation

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More on matrix notation in the next exercise session

$$\min_{\theta} J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i \theta - y_i)^2$$

$$\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})^T (\mathbf{X}\boldsymbol{\theta} - \boldsymbol{y})$$

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 0$$
Convex
Optimum

Optimization

$$\frac{\partial J(\theta)}{\partial \theta} = 2\mathbf{X}^T \mathbf{X} \boldsymbol{\theta} - 2\mathbf{X}^T \mathbf{y} = 0$$

 $\theta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$

Details in the exercise session!

We have found an analytical solution to a convex problem

Inputs: Outside temperature, number of people,

True output:
Temperature of
the building

Is this the best Estimate?

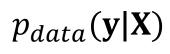
Least squares estimate

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



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Maximum Likelihood



True underlying distribution



 $p_{model}(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$ Parametric family of distributions

Controlled by parameter(s)

 A method of estimating the parameters of a statistical model given observations,

$$p_{model}(\mathbf{y}|\mathbf{X},oldsymbol{ heta})$$

Observations from $p_{data}(\mathbf{y}|\mathbf{X})$

• A method of estimating the parameters of a statistical model given observations, by finding the parameter values that maximize the likelihood of making the observations given the parameters.

$$\boldsymbol{\theta_{ML}} = \arg \max_{\boldsymbol{\theta}} \ p_{model}(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$$

 MLE assumes that the training samples are independent and generated by the same probability distribution

$$p_{model}(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \prod_{i=1}^{n} p_{model}(y_i|\mathbf{x}_i,\boldsymbol{\theta})$$

"i.i.d." assumption

$$\theta_{ML} = \arg \max_{\theta} \left[\prod_{i=1}^{n} p_{model}(y_i | \mathbf{x}_i, \theta) \right]$$

$$\theta_{ML} = \arg \max_{\theta} \left[\sum_{i=1}^{n} \log p_{model}(y_i | \mathbf{x}_i, \theta) \right]$$

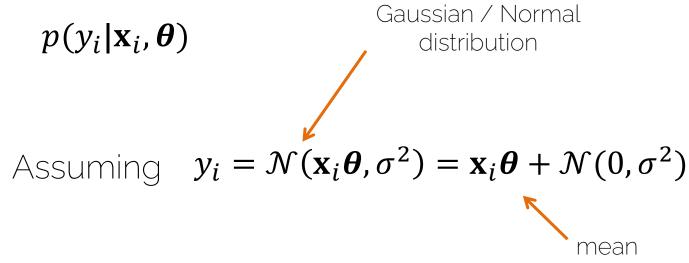
Logarithmic property $\log ab = \log a + \log b$

$$\boldsymbol{\theta_{ML}} = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{model}(y_i|\mathbf{x}_i,\boldsymbol{\theta})$$

What shape does our probability distribution have?

 $p(y_i|\mathbf{x}_i,\boldsymbol{\theta})$

What shape does our probability distribution have?



Gaussian:

$$p(y_i) = \frac{1}{\sqrt{(2\pi\sigma^2)}} e^{-\frac{1}{2\sigma^2}(y_i - \mu)^2}$$
 $y_i \sim \mathcal{N}(\mu, \sigma^2)$

$$p(y_i|\mathbf{x}_i,\boldsymbol{\theta}) = ?$$

Assuming
$$y_i = \mathcal{N}(\mathbf{x}_i \boldsymbol{\theta}, \sigma^2) = \mathbf{x}_i \boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$$
 mean Gaussian:
$$p(y_i) = \frac{1}{\sqrt{(2\pi\sigma^2)}} e^{-\frac{1}{2\sigma^2}(y_i - \mu)^2} \qquad y_i \sim \mathcal{N}(\mu, \sigma^2)$$

$$p(y_i|\mathbf{x}_i,\boldsymbol{\theta}) = (2\pi\sigma^2)^{-1/2}e^{-\frac{1}{2\sigma^2}(y_i-\mathbf{x}_i\boldsymbol{\theta})^2}$$
 Assuming $y_i = \mathcal{N}(\mathbf{x}_i\boldsymbol{\theta},\sigma^2) = \mathbf{x}_i\boldsymbol{\theta} + \mathcal{N}(0,\sigma^2)$ mean
$$p(y_i) = \frac{1}{\sqrt{(2\pi\sigma^2)}}e^{-\frac{1}{2\sigma^2}(y_i-\mu)^2}$$

$$y_i \sim \mathcal{N}(\mu,\sigma^2)$$

$$p(y_i|\mathbf{x}_i,\boldsymbol{\theta}) = (2\pi\sigma^2)^{-1/2}e^{-\frac{1}{2\sigma^2}(y_i-\mathbf{x}_i\boldsymbol{\theta})^2}$$

Original problem

Original optimization
$$\theta_{ML} = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{model}(y_i|\mathbf{x}_i,\boldsymbol{\theta})$$

$$\sum_{i=1}^{n} \log \left[(2\pi\sigma^2)^{-\frac{1}{2}} e^{-\frac{1}{2\sigma^2} (y_i - x_i \theta)^2} \right]$$
Canceling log and e

$$\sum_{i=1}^{n} -\frac{1}{2} \log (2\pi\sigma^2) + \sum_{i=1}^{n} \left(-\frac{1}{2\sigma^2}\right) (y_i - x_i\theta)^2$$

$$-\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (y - X\theta)^T (y - X\theta)$$

$$\theta_{ML} = \arg \max_{\theta} \left[\sum_{i=1}^{n} \log p_{model}(y_i | \mathbf{x}_i, \boldsymbol{\theta}) \right]$$
$$-\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \right]$$

Details in the exercise session!

$$\frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = 0$$

How can we find the estimate of theta?

$$\boldsymbol{\theta} = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \mathbf{y}$$

Linear Regression

 Maximum Likelihood Estimate (MLE) corresponds to the Least Squares Estimate (given the assumptions)

 Introduced the concepts of loss function and optimization to obtain the best model for regression

Image Classification

















Regression vs Classification

 Regression: predict a continuous output value (e.g., temperature of a room)

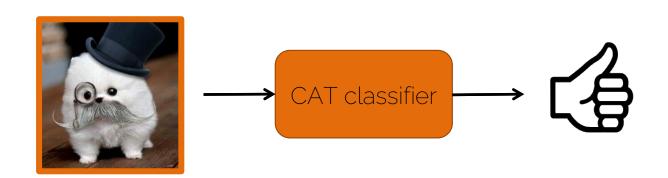
- Classification: predict a discrete value
 - Binary classification: output is either 0 or 1



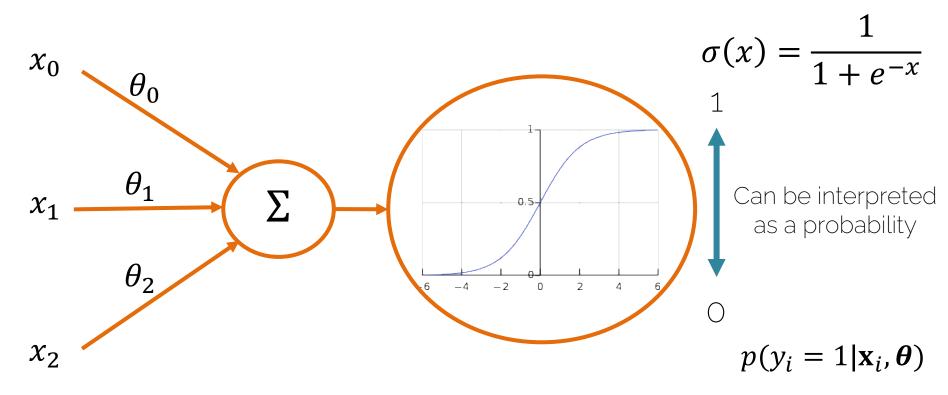
Multi-class classification; set of N classes



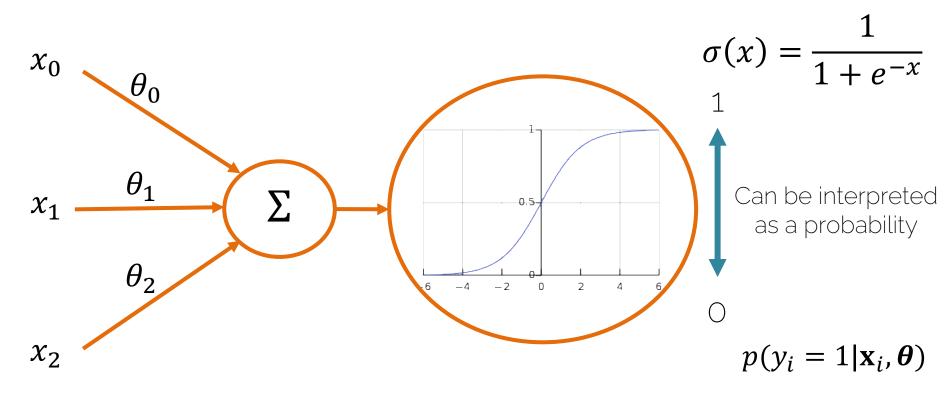
Logistic Regression



Sigmoid for Binary Predictions



Spoiler Alert: 1-Layer Neural Network



Logistic Regression

Probability of a binary output

$$\hat{\mathbf{y}} = p(\mathbf{y} = 1 | \mathbf{X}, \boldsymbol{\theta}) = \prod_{i=1}^n p(y_i = 1 | \mathbf{x}_i, \boldsymbol{\theta})$$

The prediction of our sigmoid $\hat{y}_i = \sigma(\mathbf{x}_i \boldsymbol{\theta})$

Logistic Regression

Probability of a binary output

$$\hat{\mathbf{y}} = p(\mathbf{y} = 1 | \mathbf{X}, \boldsymbol{\theta}) = \prod_{i=1}^{n} p(y_i = 1 | \mathbf{x}_i, \boldsymbol{\theta})$$

Bernoulli trial

$$p(z|\phi) = \phi^z (1-\phi)^{1-z} = \begin{cases} \phi & \text{, if } z=1\\ 1-\phi & \text{if } z=0 \end{cases}$$
The prediction of our sigmoid

Logistic Regression

Probability of a binary output

$$\hat{\mathbf{y}} = p(\mathbf{y} = 1 | \mathbf{X}, \boldsymbol{\theta}) = \prod_{i=1}^{n} p(y_i = 1 | \mathbf{x}_i, \boldsymbol{\theta})$$

$$\hat{\mathbf{y}} = \prod_{i=1}^{n} \hat{y}_i^{y_i} (1 - \hat{y}_i)^{(1 - y_i)}$$
Model for coins

Prediction of the True labels: 0 or 1

12DL: Prof. Dai Sigmoid: continuous

Probability of a binary output

$$p(y|X, \theta) = \hat{y} = \prod_{i=1}^{n} \hat{y}_i^{y_i} (1 - \hat{y}_i)^{(1-y_i)}$$

Maximum Likelihood Estimate

$$\theta_{ML} = \arg \max_{\theta} \log p(y|\mathbf{X}, \theta)$$

$$p(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \hat{\mathbf{y}} = \prod_{i=1}^{n} \hat{y}_i^{y_i} (1 - \hat{y}_i)^{(1-y_i)}$$

$$\sum_{i=1}^{n} \log \left(\hat{y}_i^{y_i} (1 - \hat{y}_i)^{(1-y_i)} \right)$$

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

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

$$y_i = 1 \longrightarrow \mathcal{L}(\hat{y}_i, 1) = \log \hat{y}_i$$

Maximize!
$$\boldsymbol{\theta}_{ML} = \arg \max_{\boldsymbol{\theta}} \log p(y|\mathbf{X}, \boldsymbol{\theta})$$

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

$$y_i = 1 \longrightarrow \mathcal{L}(\hat{y}_i, 1) = \log \hat{y}_i$$

We want $\log \hat{y}_i$ large; since logarithm is a monotonically increasing function, we also want large \hat{y}_i .

(1 is the largest value our model's estimate can take!)

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

$$y_i = 1 \longrightarrow \mathcal{L}(\hat{y}_i, 1) = \log \hat{y}_i$$
$$y_i = 0 \longrightarrow \mathcal{L}(\hat{y}_i, 0) = \log(1 - \hat{y}_i)$$

We want $\log(1-\hat{y}_i)$ large; so we want \hat{y}_i to be small

(0 is the smallest value our model's estimate can take!)

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

Referred to as *binary cross-entropy* loss (BCE)

 Related to the multi-class loss you will see in this course (also called softmax loss)

Logistic Regression: Optimization

Loss function

$$\mathcal{L}(\hat{y}_i, y_i) = y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

Cost function

$$C(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(\hat{y}_i, y_i)$$

Minimization

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

12DL: Prof. Dai

 $\hat{\mathbf{y}}_i = \sigma(\mathbf{x}_i \boldsymbol{\theta})$

Logistic Regression: Optimization

No closed-form solution

Make use of an iterative method → gradient descent

Gradient descent – later on!

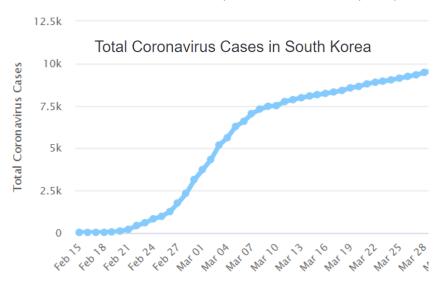
Why Machine Learning so Cool

- We can learn from experience
 - -> Intelligence, certain ability to infer the future!

- Even linear models are often pretty good for complex phenomena: e.g., weather:
 - Linear combination of day-time, day-year etc. is often pretty good

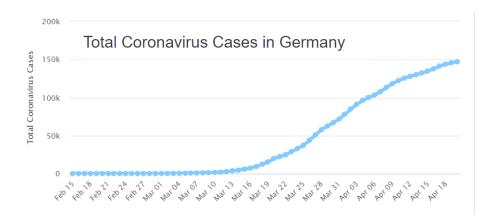
Many Examples of Logistic Regression

- Coronavirus models behave like logistic regressions
 - Exponential spread at beginning
 - Plateaus when certain portion of pop. is infected/immune



Many Examples of Logistic Regression

- Coronavirus models behave like logistic regressions
 - Exponential spread at beginning
 - Plateaus when certain portion of pop. is infected/immune



Think about good features:

- Total population
- Population density
- Implementation of Measures
- Reasonable government © ?
- Etc. (many more of course)

The Model Matters

• Each case requires different models; linear vs logistic

- Many models:
 - #coronavirus_infections cannot be > #total_population
 - Munich housing prizes seem exponential though
 - No hard upper bound -> prizes can always grow!

Next Lectures

Next exercise session: Math Recap II

- Next Lecture: Lecture 3:
 - Jumping towards our first Neural Networks and Computational Graphs

References for further Reading

- Cross validation:
 - https://medium.com/@zstern/k-fold-cross-validationexplained-5aebagoebb3
 - https://towardsdatascience.com/train-test-split-andcross-validation-in-python-80b61beca4b6
- General Machine Learning book:
 - Pattern Recognition and Machine Learning. C. Bishop.



See you next week ©