

Machine Learning Basics





































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Pose I2DL: Prof. Dai









Occlusions

Background clutter





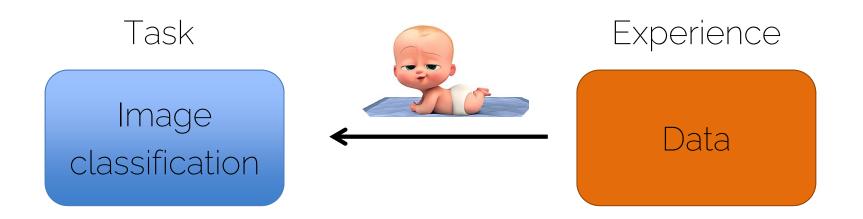
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Representation



• How can we learn to perform image classification?

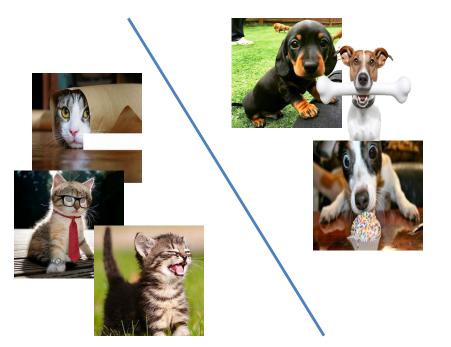


Unsupervised learning

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

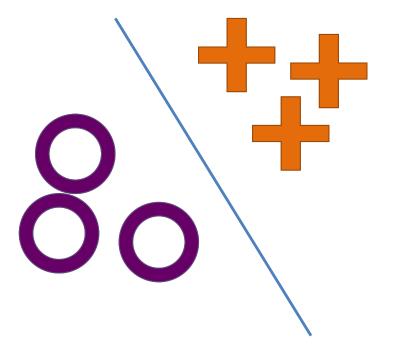
Supervised learning

Unsupervised learning



Supervised learning

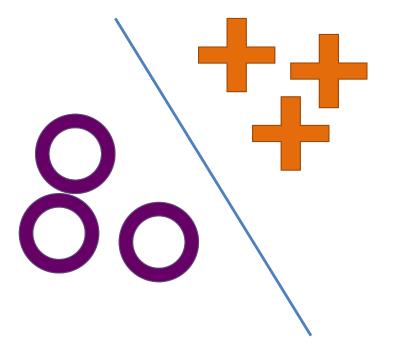
Unsupervised learning



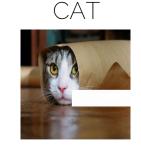
Supervised learning

• Labels or target classes

Unsupervised learning



Supervised learning











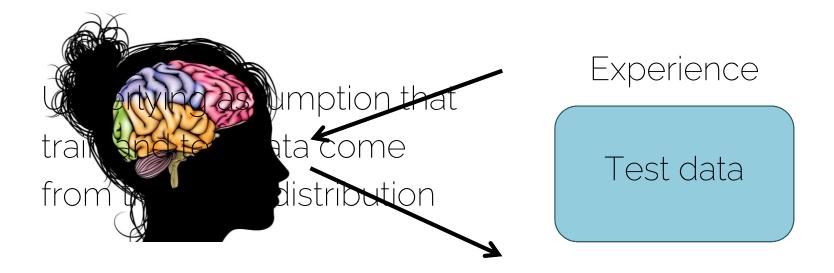
CAT



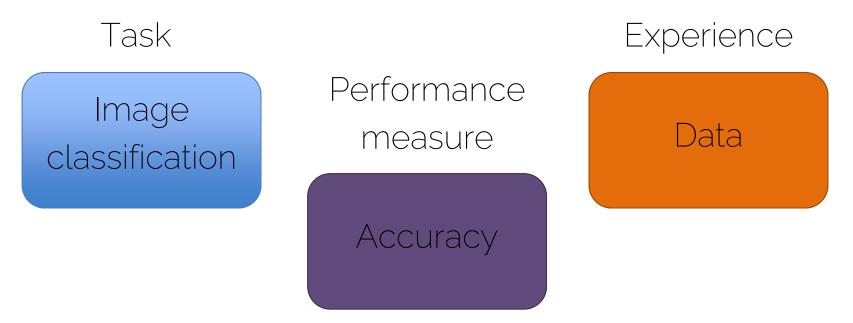


DOG

• How can we learn to perform image classification?



• How can we learn to perform image classification?



Unsupervised learning



Supervised learning



Reinforcement learning



Unsupervised learning



Supervised learning



Reinforcement learning



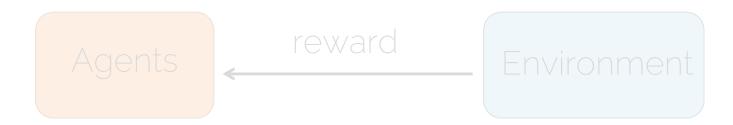
Unsupervised learning



Supervised learning



Reinforcement learning



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A Simple Classifier







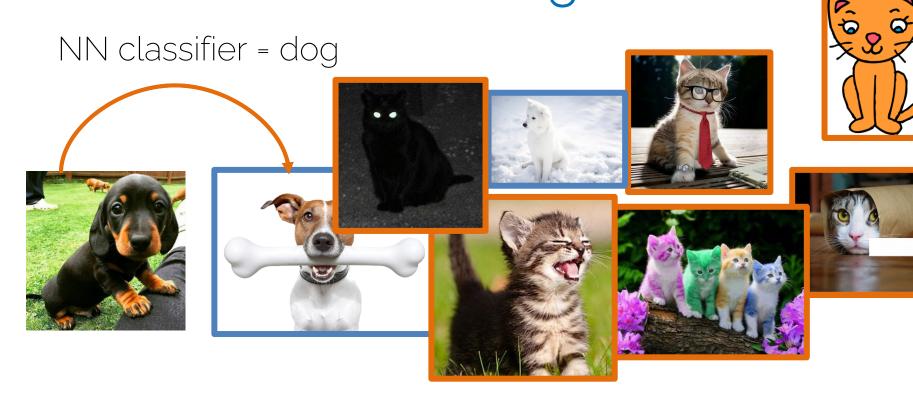








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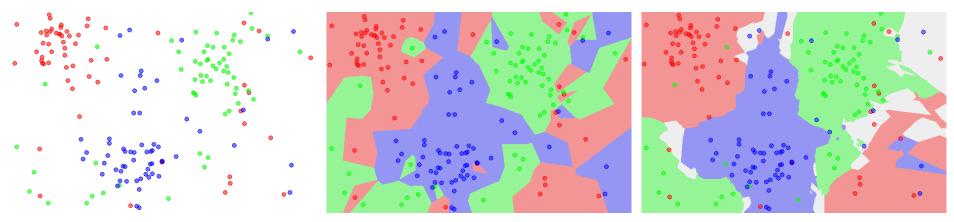
k-NN classifier = cat



The Data

NN Classifier

5NN Classifier



How does the NN classifier perform on training data?

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

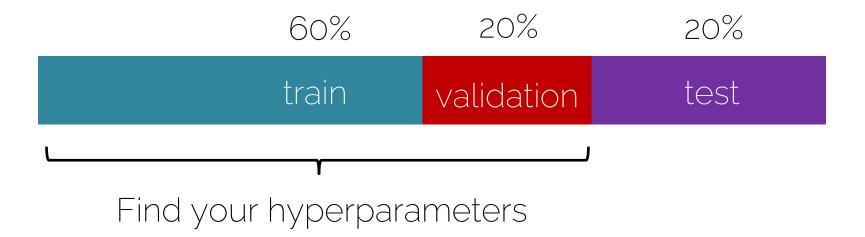
Source: https://commons.wikimedia.org/wiki/File:Data3classes.png

- Hyperparameters \leftarrow L1 distance : |x c|L2 distance : $||x - c||_2$ No. of Neighbors: k
- These parameters are problem dependent.

• How do we choose these hyperparameters?

Basic Recipe for Machine Learning

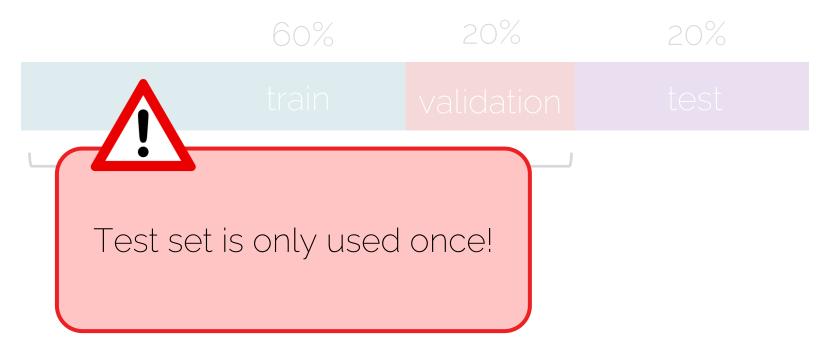
• Split your data



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

Basic Recipe for Machine Learning

• Split your data



Cross Validation

train validation

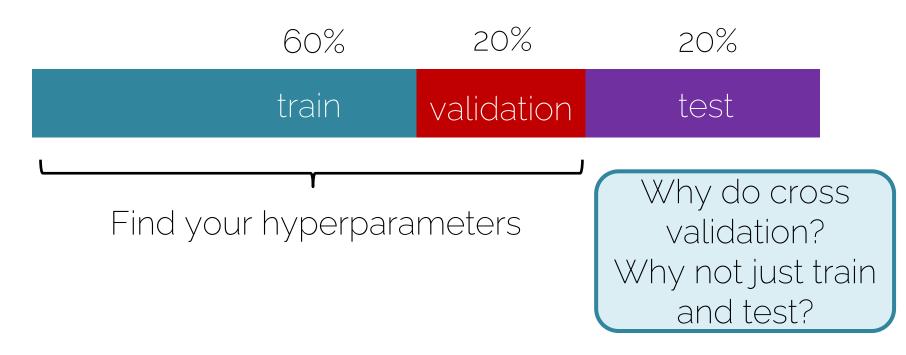
Run 2 Run 3 Run 4

Run 5

Run 1

Split the **training data** into N folds

Cross Validation



Cross Validation



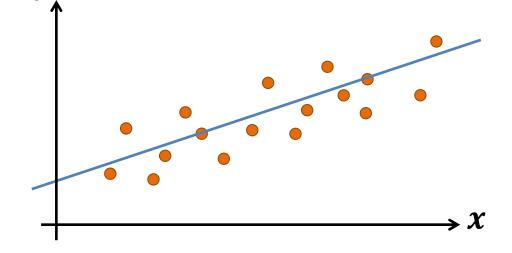
Linear Decision Boundaries

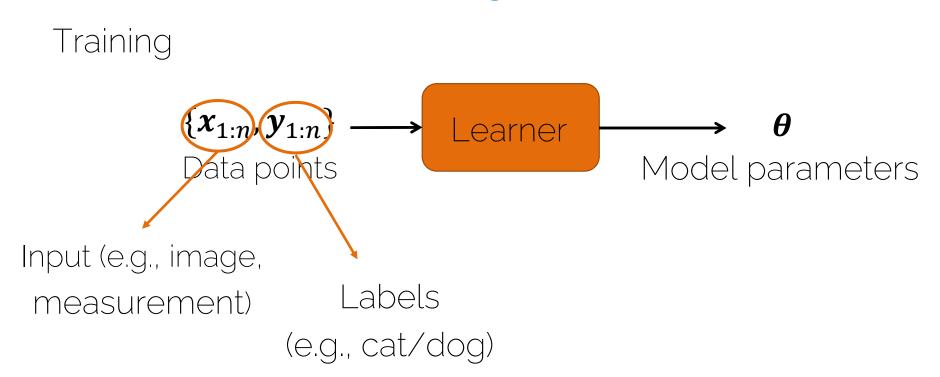
This lecture

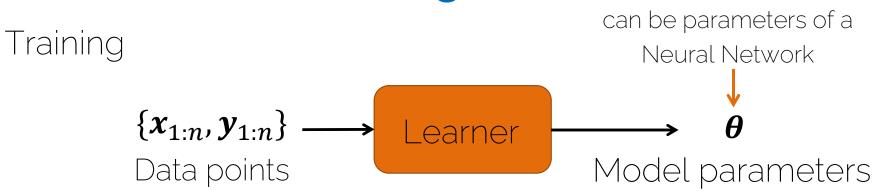
What are the pros and cons for using linear decision boundaries?



- Supervised learning
- Find a linear model that explains a target y given inputs x







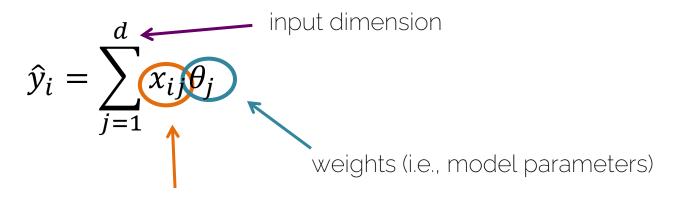


$$x_{n+1}, \theta \longrightarrow \text{Predictor} \longrightarrow \hat{y}_{n+1}$$

Estimation

Linear Prediction

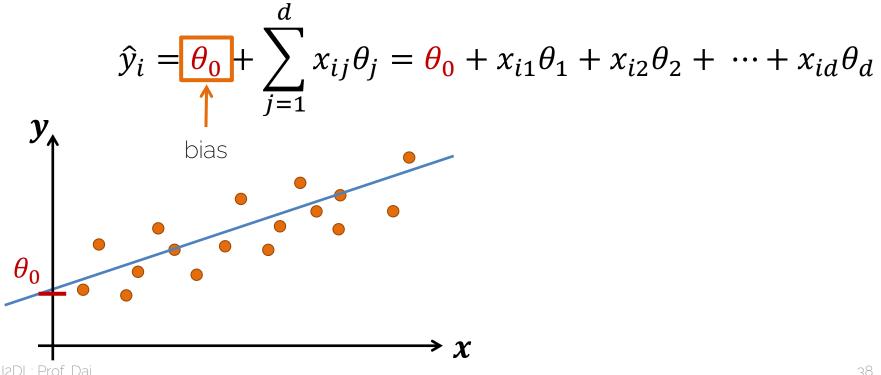
• A linear model is expressed in the form

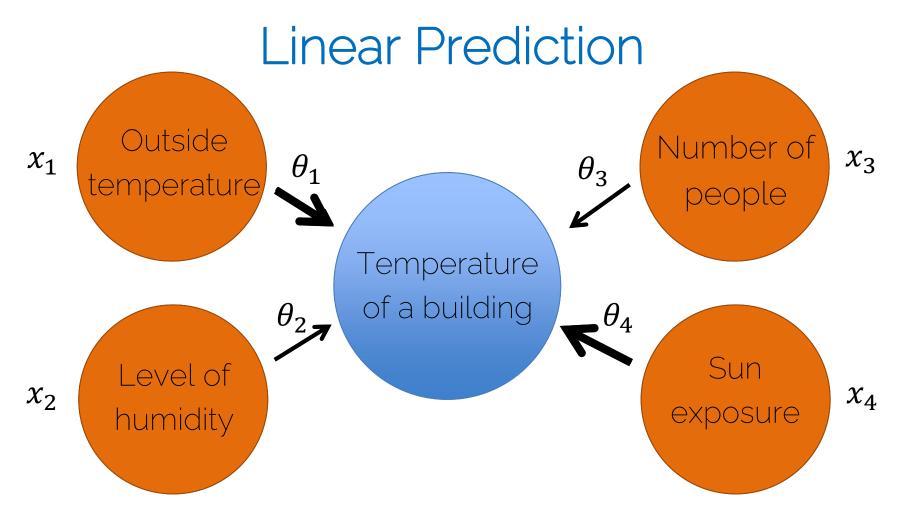


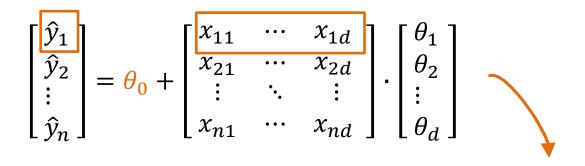
Input data, features

Linear Prediction

• A linear model is expressed in the form

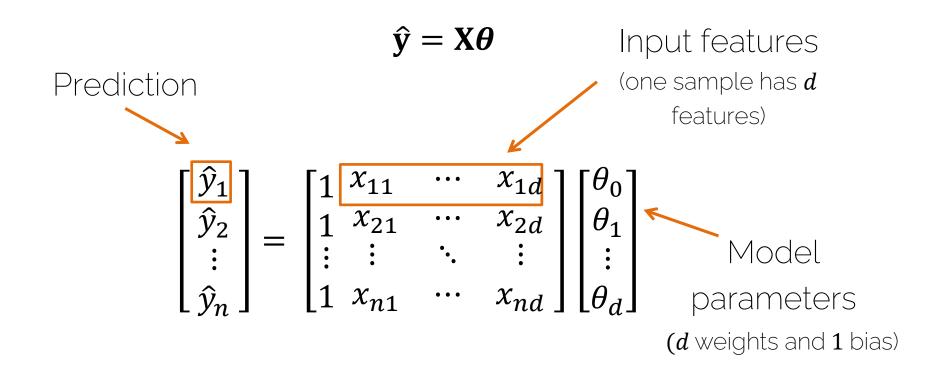


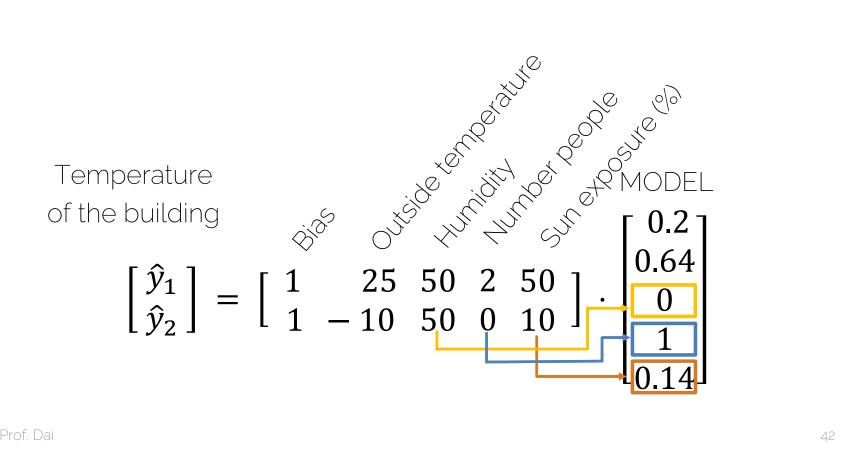


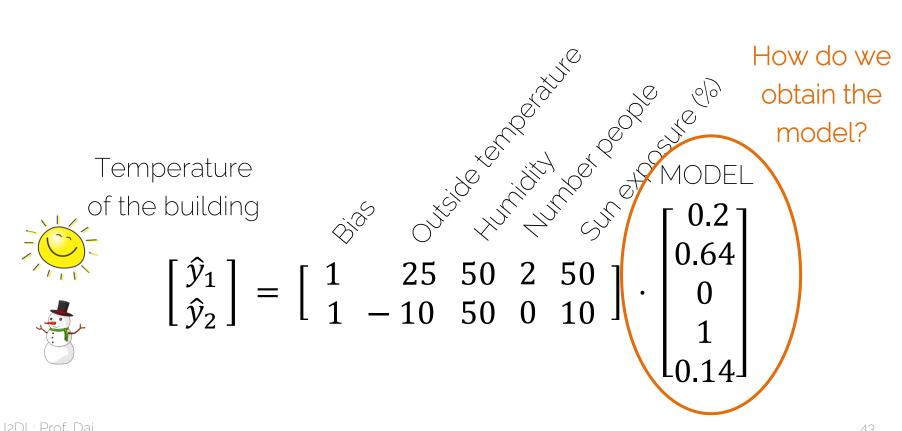


$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ 1 & x_{21} & \cdots & x_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{nd} \end{bmatrix} \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}$$

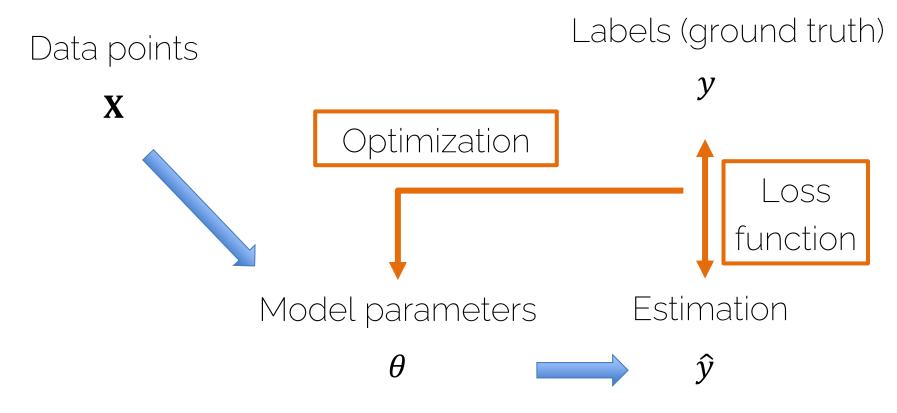
 $\Rightarrow \hat{\mathbf{y}} = \mathbf{X}\boldsymbol{\theta}$







How to Obtain the Model?

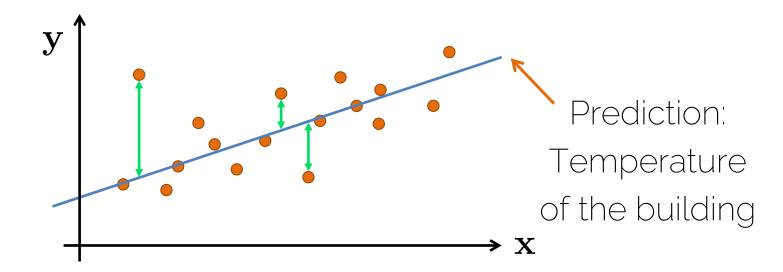


How to Obtain the Model?

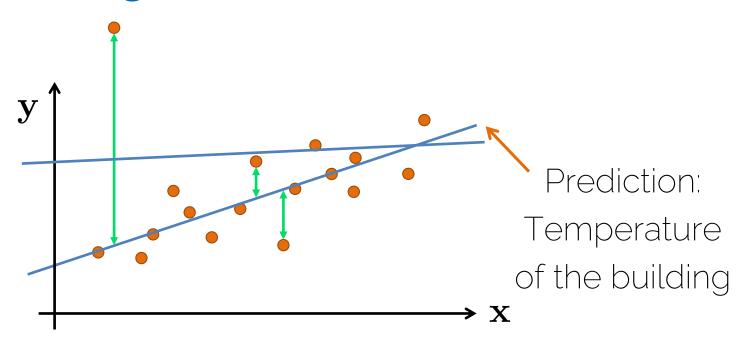
• Loss function: measures how good my estimation is (how good my model is) and tells the optimization method how to make it better.

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

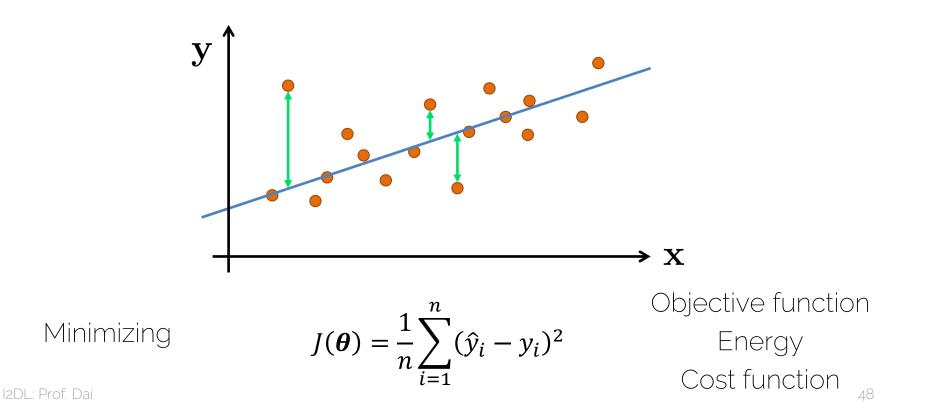
Linear Regression: Loss Function



Linear Regression: Loss Function



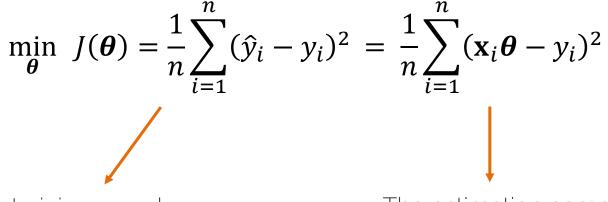
Linear Regression: Loss Function



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

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

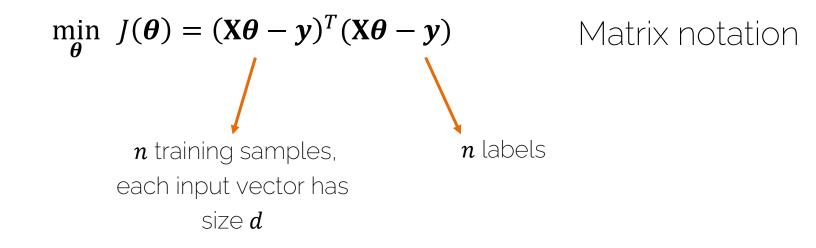
• Convex problem, there exists a closed-form solution that is unique.



n training samples

The estimation comes from the linear model

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



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

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

More on matrix notation in the next exercise session

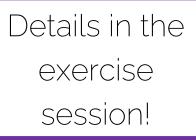
$$\min_{\theta} J(\theta) = \frac{1}{n} \sum_{i=1}^{n} (\hat{y}_i - y_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{x}_i \theta - y_i)^2$$

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

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

Optimum

Optimization



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

$$\theta = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$
nd
Ind
Inputs: Outside

We have found an analytical solution to a convex problem

Inputs: Outside temperature, number of people,

....

True output: Temperature of the building

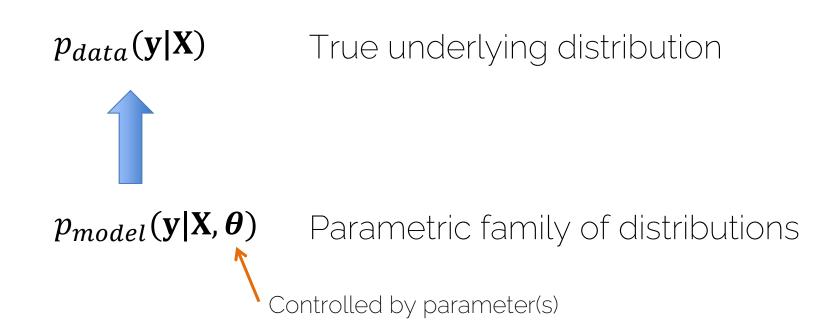
Is this the best Estimate?

• Least squares estimate

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



Maximum Likelihood



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

 $p_{model}(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$

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

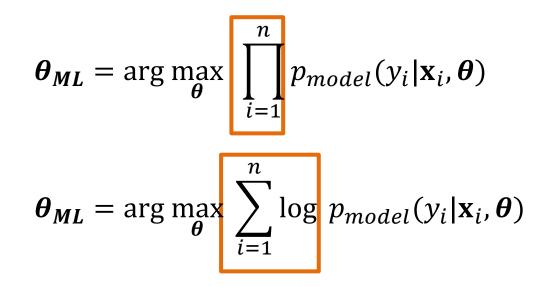
• A method of estimating the parameters of a statistical model given observations, by finding the parameter values that **maximize the likelihood** of making the observations given the parameters.

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

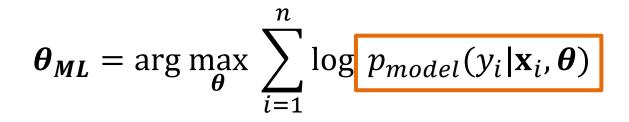
• MLE assumes that the training samples are independent and generated by the same probability distribution

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

"i.i.d." assumption



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

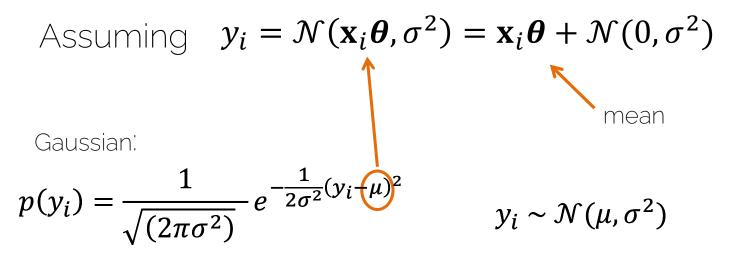


What shape does our probability distribution have?

 $p(y_i | \mathbf{x}_i, \boldsymbol{\theta})$ What shape does our probability distribution have?

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

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



Back to Linear Regression

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

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

Back to Linear Regression

$$p(y_i | \mathbf{x}_i, \boldsymbol{\theta}) = (2\pi\sigma^2)^{-1/2} e^{-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i \boldsymbol{\theta})^2}$$
Original
optimization $\boldsymbol{\theta}_{ML} = \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p_{model}(y_i | \mathbf{x}_i, \boldsymbol{\theta})$
problem

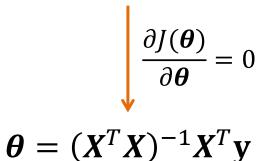
Back to Linear Regression

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

$$\sum_{i=1}^{n} -\frac{1}{2} \log (2\pi\sigma^2) + \sum_{i=1}^{n} \left(-\frac{1}{2\sigma^2} \right) (\mathbf{y}_i - \mathbf{x}_i \theta)^2$$
Matrix notation
$$-\frac{n}{2} \log(2\pi\sigma^2) - \frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta)$$

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

Details in the exercise session!



How can we find the estimate of theta?

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

















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Regression vs Classification

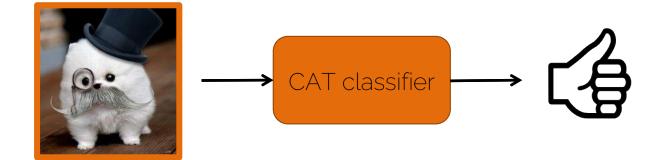
• Regression: predict a continuous output value (e.g., temperature of a room)

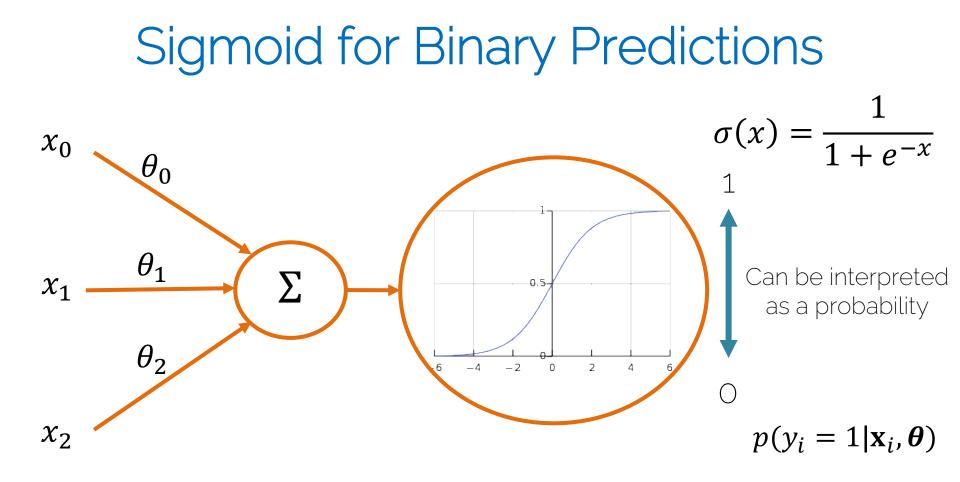
- Classification: predict a discrete value
 - Binary classification: output is either 0 or 1
 - Multi-class classification: set of N classes

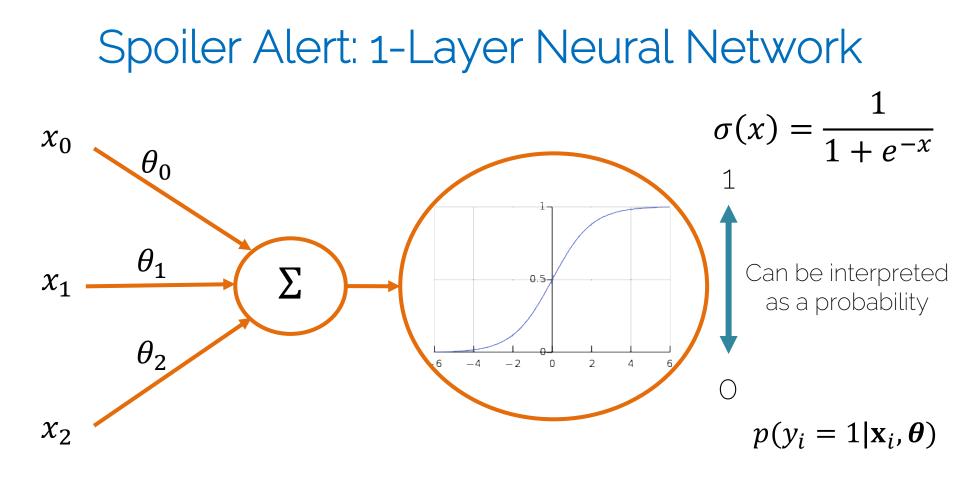




Logistic Regression







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 $\hat{y}_i = \sigma(\mathbf{x}_i \boldsymbol{\theta})$
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
Sigmoid: continuous
Model for

• Probability of a binary output

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

• Maximum Likelihood Estimate

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

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

$$\sum_{i=1}^{n} \log \left(\hat{y}_{i}^{y_{i}} (1 - \hat{y}_{i})^{(1-y_{i})} \right)$$
$$\sum_{i=1}^{n} y_{i} \log \hat{y}_{i} + (1 - y_{i}) \log(1 - \hat{y}_{i})$$

$$\mathcal{L}(\hat{y}_{i}, y_{i}) = y_{i} \log \hat{y}_{i} + (1 - y_{i}) \log(1 - \hat{y}_{i})$$

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

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

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$$\mathcal{L}(\hat{y}_{i}, y_{i}) = y_{i} \log \hat{y}_{i} + (1 - y_{i}) \log(1 - \hat{y}_{i})$$

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

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!)

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

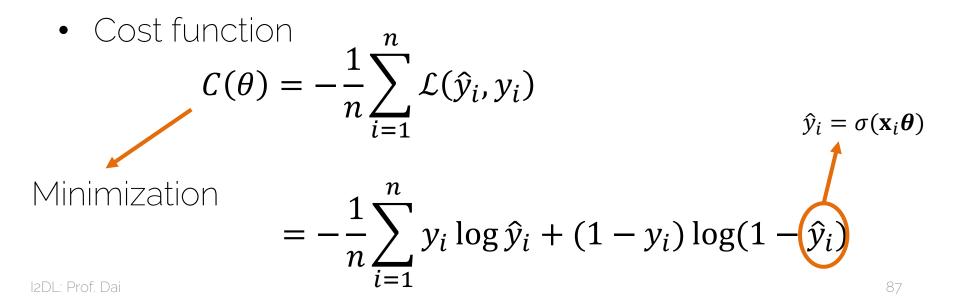
Referred to as *binary cross-entropy* loss (BCE)

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

Logistic Regression: Optimization

• Loss function

$$\mathcal{L}(\hat{y}_{i}, y_{i}) = y_{i} \log \hat{y}_{i} + (1 - y_{i}) \log(1 - \hat{y}_{i})$$



Logistic Regression: Optimization

• No closed-form solution

• Make use of an iterative method \rightarrow gradient descent

Gradient descent – later on!

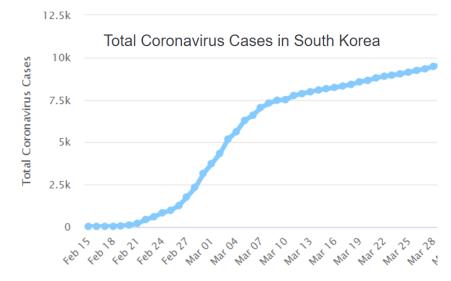
Why Machine Learning so Cool

- 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

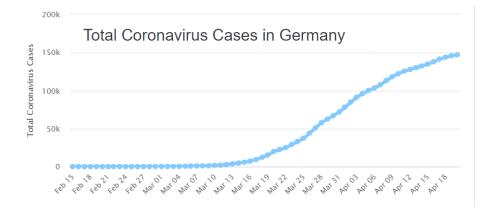
Many Examples of Logistic Regression

- 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:
 - <u>https://medium.com/@zstern/k-fold-cross-validation-</u>
 <u>explained-5aebag0ebb3</u>
 - <u>https://towardsdatascience.com/train-test-split-and-cross-validation-in-python-80b61beca4b6</u>
- General Machine Learning book:
 - Pattern Recognition and Machine Learning. C. Bishop.



See you next week 🕲