Plan

Today

- Wrap-up regularization (for now)
- MLE
  - Probability / likelihood
  - Maximum likelihood estimation
  - Probabilistic formulation of linear and logistic regression

Wrap up Neural Nets

Switch to regression slides

10-315
Introduction to ML

MLE and Probabilistic Formulation of Machine Learning

Instructor: Pat Virtue

Poll 1: Exercise

Implement a function in Python for the pdf of a Gaussian distribution.

Python numpy or math packages are fine, no scipy, etc.

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

def gaussian(x, mu, sigmaSq):

pdf

$f(x)$

$= p(x)$

$= p(x; \mu, \sigma)$

$= p(x \mid \mu, \sigma)$

Exercises

Calculate the probability of these event sequences happening

1) Coin

a. Fair: H, H, T, H $\frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{16}$

b. Biased, $\phi = \underline{3/4}$ heads: H, H, T, H $\frac{3}{4} \cdot \frac{3}{4} \cdot \frac{1}{4} \cdot \frac{3}{4} = \frac{27}{256}$

2) 4-sided die with sides: A, B, C, D

a. Fair: A, B, D, D, A $\frac{1}{4} \frac{1}{4} \frac{1}{4} \frac{1}{4} \frac{1}{4} = \frac{1}{1024}$

b. Weighted, $[\phi_A, \phi_B, \phi_C, \phi_D] = [1/10,\ 2/10,\ 3/10,\ 4/10]$
A, B, D, D, A

$\frac{1}{10} \cdot \frac{2}{10} \frac{4}{10} \frac{4}{10} \frac{1}{10} = \frac{32}{100000}$

Probability

Probability Vocab

Outcomes

Sample space

Events

Probability

Random variable

Discrete random variable

Continuous random variable

Probability mass function

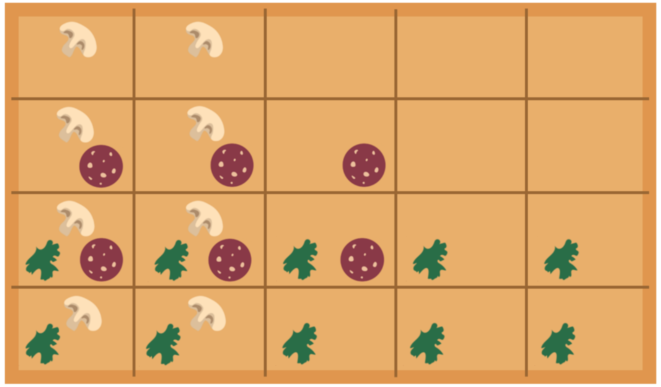
Probability density function

Parameters

Example

$S \in \{0, 1\}$

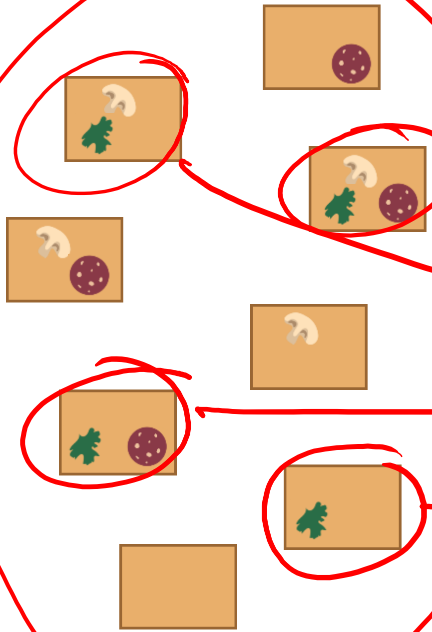
$S : \Omega \rightarrow \{0, 1\}$



Random variable for spinach or no spinach

Ω

events



Random variable

R

0

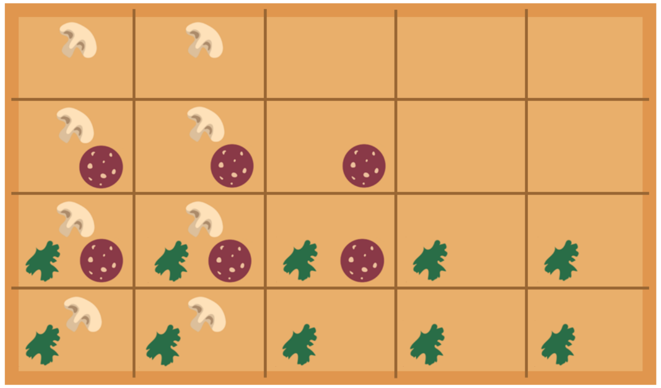
1

Distribution

Sample space → Values → Probabilities or Densities

Icons: CC, https://openclipart.org/detail/296791/pizza-slice

Example



true

Random variable for spinach or no spinach

$S: \Omega \to \{0,1\}$

Ω

outcomes

Random variable

$S(\omega) \to \{0,1\}$

Distribution

$\mathbb{R} \to [0,1]$ pmf

0

1

$\frac{1}{2}$

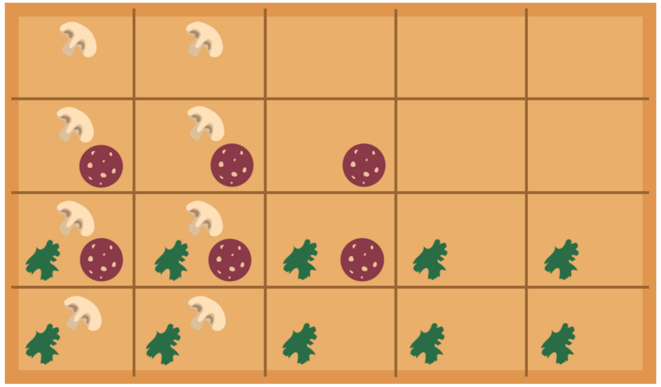
pmf

Sample space → Values → Probabilities or Densities

Icons: CC, https://openclipart.org/detail/296791/pizza-slice

Example

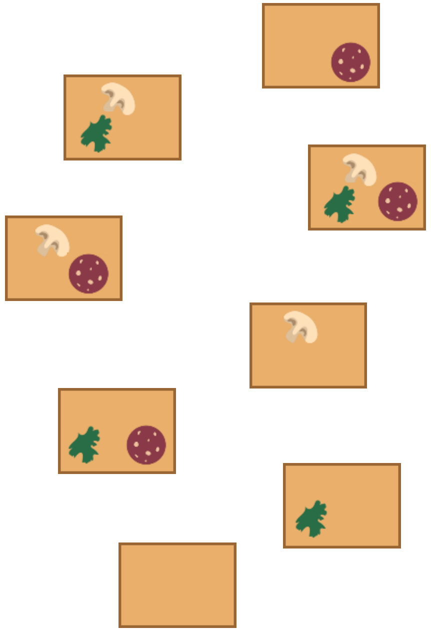
true



Random variable for topping type with three categories: none, non-meat, meat

Random variable

Distribution



1

2

3

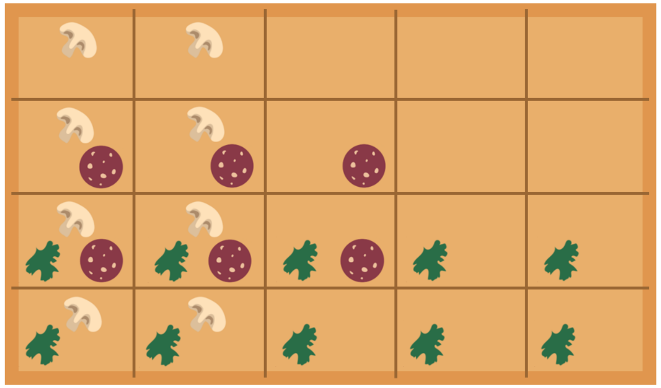
pmf

Sample space → Values → Probabilities or Densities

Icons: CC, https://openclipart.org/detail/296791/pizza-slice

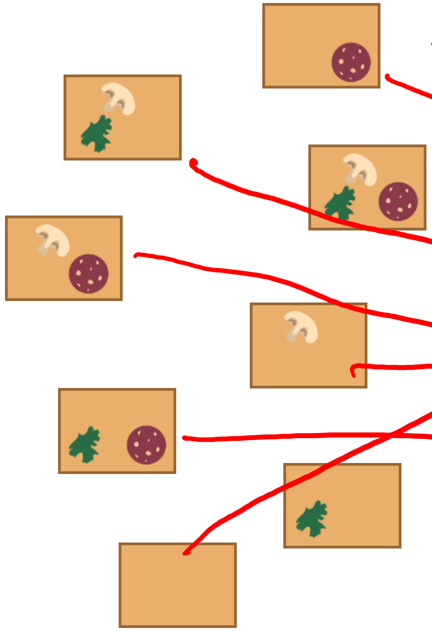
Example

true



Random variable for topping type with three categories: none, non-meat, meat

Random variable | Distribution



1 → 5/20

2 → 9/20

3 → 6/20

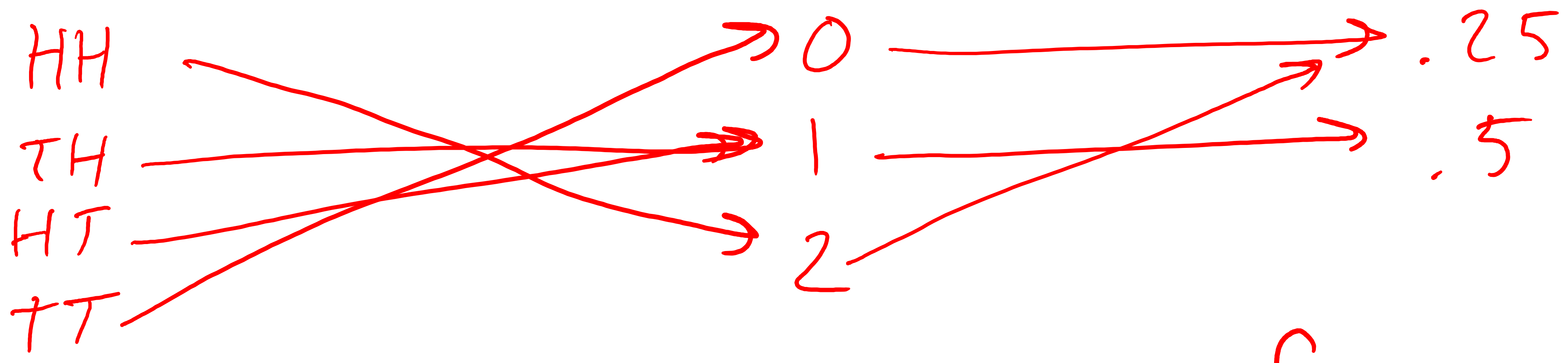
pmf

Sample space → Values → Probabilities or Densities

Example

Random variable for number of heads after two flips of a fair coin

Random variable | Distribution



pmf

Sample space → Values → Probabilities or Densities

Icons: CC, https://openclipart.org/detail/296791/pizza-slice

Example

Random variable for number of heads after two flips of a *biased* coin that lands heads 75%

Random variable | Distribution

HH → 2

TH → 1

HT → 1

TT → 0

$\frac{1}{4} \cdot \frac{1}{4}$

$\frac{1}{4} \cdot \frac{3}{4} + \frac{3}{4} \frac{1}{4}$

$\frac{3}{4} \frac{3}{4}$

Sample space → Values → Probabilities or Densities

Example

Random variable for cat in picture or not

Sample space → Values → Probabilities or Densities

Icons: CC, https://openclipart.org/detail/296791/pizza-slice

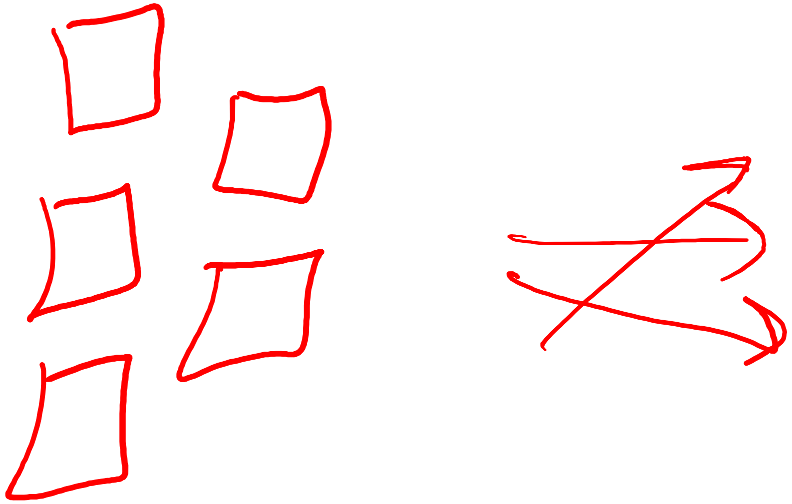
Example

Random variable for animal species in picture assuming one animal picture and available species: dog, cat, pig

$$\sum_{i=1}^{3} q_i = 1$$

Random variable

Distribution



1

2

3

q_1

q_2

$q_3 = (1 - q_1 - q_2)$

$\text{Categorical}(q_1, q_2, q_3)$

Sample space → Values → Probabilities or Densities

Example

Random variable for height of student

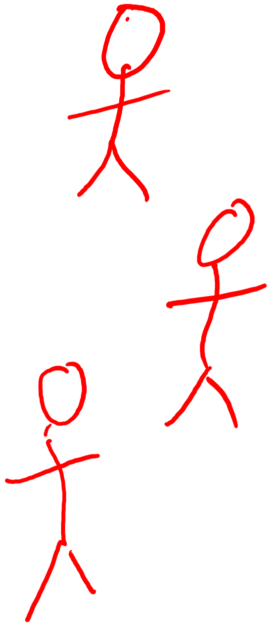
$H(\omega) \rightarrow \mathbb{R}$ Continuos $f(x) \rightarrow \mathbb{R}^+$

Random variable

Distribution

Gaussian

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



$\mathbb{R}$

$f(x; \mu, \sigma^2)$ parameters

pdf

Sample space → Values → Probabilities or Densities

Probability Vocab

Outcomes

Sample space

Events

Probability

Random variable

Discrete random variable

Continuous random variable

Probability mass function $p(x) = P(X = x)$

Probability density function $f(x)$ $\quad p(x)$

Parameters

$\Pr[\text{event}]$

$P(\text{event})$

$p(\text{value})$

$P(Y = 1)$

CDF

$F(x) = P(X \le x)$

Example Discrete Distributions

$\boxed{\text{Bern} \quad \text{Binom.} \quad \text{Categorial} \quad \text{Multinom}}$

Bernoulli

$P(Y=1) = \phi$

$Y \in \{0,1\} \quad P(Y=0) = 1-\phi$

Categorical

$$Y = \begin{bmatrix} Y_1 \\ \vdots \\ Y_K \end{bmatrix} \qquad Y_k \in \{0,1\} \qquad \begin{bmatrix} P(Y_1=1) = \phi_1 \\ P(Y_2=1) = \phi_2 \\ \vdots \qquad \vdots \\ P(Y_K=1) = \phi_K \end{bmatrix} \qquad 1 = \sum_{k=1}^{K} \phi_k$$

Binomial

Multinomial

Uniform

Example Continuous Distributions

Gaussian

$$p(y; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

Beta

Laplace

Probability Vocab

Marginal $p(x) = \sum_{y} p(x, y)$ Marginalizing

Joint $p(x, y)$ $p(x, y, z, w)$

Conditional $p(x \mid y)$ $p(x, w \mid z, y)$

Notation

Dataset

Parameters, generically θ

$p(\mathcal{D} \mid \theta), p(\mathcal{D}\,;\,\theta)$

Random variables

Capital

$P(Y = y)$

A

Z

Values

lower case

Random variable: function that maps events to values

Y is rand variable that maps the event of a coin toss being heads to value one and the event of a coin toss being tails to zero

$P(Y = 1 \mid \phi) = 3/4$, where $\phi = 3/4$

$P(Y = 1) = 3/4$

Sometimes even

$P(Y = heads) = 3/4$

Probability Toolbox

- Algebra
- Three axioms of probability
- Theorem of total probability
- Definition of conditional probability
- Product rule
- Bayes' theorem
- Chain rule
- Independence
- Conditional independence

Probability Tools Summary

Adding to the toolbox

1. Definition of conditional probability

$$P(A|B) = \frac{P(A,B)}{P(B)}$$

2. Chain Rule   Product rule

$$P(A,B) = P(A \mid B)P(B)$$

3. Bayes' theorem

$$P(B|A) = \frac{P(A \mid B)P(B)}{P(A)}$$

4. Chain Rule…

$$P(A_1, \ldots A_N) = P(A_1)\sum_{i=2}^{N} P(A_i \mid A_{i-1})$$

Likelihood

Likelihood

Likelihood: The probability (or density) of random variable Y taking on value y given the distribution parameters, $\boldsymbol{\theta}$.

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Grades

$$\mathcal{D} = \{y^{(1)} \quad y^{(2)} \quad y^{(3)}\}$$

$$= \{80 \quad 70 \quad 85\}$$

$$p(\mathcal{D} \mid \mu \; \sigma^2)$$

Gaussian PDF: $p(y \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$

Likelihood

$\phi = \frac{1}{3}$

Trick coin: comes up heads only 1/3 of the time

1 flip: H probability: $\frac{1}{3}$

2 flips: H,H probability: $\frac{1}{3} \cdot \frac{1}{3}$

3 flips: H,H,T probability: $\frac{1}{3} \cdot \frac{1}{3} \cdot \left(1 - \frac{1}{3}\right)$

$p(D \mid \phi)$

$p(HHT \mid \phi)$

But why can we just multiply these?

Likelihood and i.i.d

Likelihood: The probability (or density) of random variable Y taking on value y given the distribution parameters, $\boldsymbol{\theta}$.

i.i.d.: Independent and identically distributed

$$p(D \mid \theta)$$

$$p(Y_1 = y^{(1)}, Y_2 = y^{(2)}, Y_3 = y^{(3)} \mid \phi_1, \phi_2, \phi_3)$$

ident

$$p(Y = y^{(1)}, Y = y^{(2)}, Y = y^{(3)} \mid \phi)$$

indep.

$$p(Y = y^{(1)} \mid \phi)\, p(Y = y^{(2)} \mid \phi)\, p(Y = y^{(3)} \mid \phi)$$

$$\prod_{i=1}^{N} p(Y = y^{(i)} \mid \phi)$$

Bernoulli Likelihood

Bernoulli distribution:

$$Y \sim Bern(\phi) \qquad p(y \mid \phi) = \begin{cases} \phi, & y = 1 \\ 1 - \phi, & y = 0 \end{cases}$$

What is the likelihood for three i.i.d. samples, given parameter ϕ:

$$\mathcal{D} = \{y^{(1)} = 1, y^{(2)} = 1, y^{(3)} = 0\}$$

$$\prod_{i=1}^{N} p(Y = y^{(i)} \mid \phi)$$

$$= \phi \cdot \phi \cdot (1 - \phi)$$

$\mathbb{1}(y^{(i)} = 1)$

$\mathbb{1}(y^{(i)} = 0)$

$$\phi^1 (1-\phi)^0 \cdot \phi^1 (1-\phi)^0 \; \phi^0 (1-\phi)^1$$

MLE

Maximum likelihood estimation

From Probability to Statistics

$\phi \longrightarrow p$

$D \longrightarrow \phi \longrightarrow$ predict

Poll 2

Assume that exam scores are drawn independently from the same Gaussian (Normal) distribution.

Given three exam scores 75, 80, 90, which pair of parameters is a better fit (a higher likelihood)?

θ_A A) Mean 80, standard deviation 3

θ_B B) Mean 85, standard deviation 7

2 models

2 sets of params

$\operatorname{argmax}_\theta \boxed{\begin{matrix} p(D \mid \theta_A) \\ p(D \mid \theta_B) \end{matrix}} \rightarrow \hat{\theta}_{MLE}$

Use a calculator/computer.

Gaussian PDF: $p(y \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$

Likelihood

Trick coin

$Y_i = 1$ Heads

$$D = [1, 0, 1, 1]$$

All T	1/3 H	Fair	2/3 H	All H
$\phi^{(A)} = 0$	$\phi^{(B)} = 1/3$	$\phi^{(C)} = 1/2$	$\phi^{(D)} = 2/3$	$\phi^{(E)} = 1$
A	B	C	D	E

Likelihood

Trick coin

$Y = 1$ Heads

$$D = [1, 0, 1, 1]$$

All T	1/3 H	Fair	2/3 H	All H
$\phi^{(A)} = 0$	$\phi^{(B)} = 1/3$	$\phi^{(C)} = 1/2$	$\phi^{(D)} = 2/3$	$\phi^{(E)} = 1$

Estimating Parameters with Likelihood

We model the outcome of a single mysterious weighted-coin flip as a Bernoulli random variable:

$$Y \sim Bern(\phi)$$

$$p(y \mid \phi) = \begin{cases} \phi, & y = 1 \ \ (Heads) \\ 1 - \phi, & y = 0 \ \ (Tails) \end{cases}$$

Given the ordered sequence of coin flip outcomes:

$$[1, 0, 1, 1]$$

What is the estimate of parameter $\hat{\phi}$?

Estimating Parameters with Likelihood

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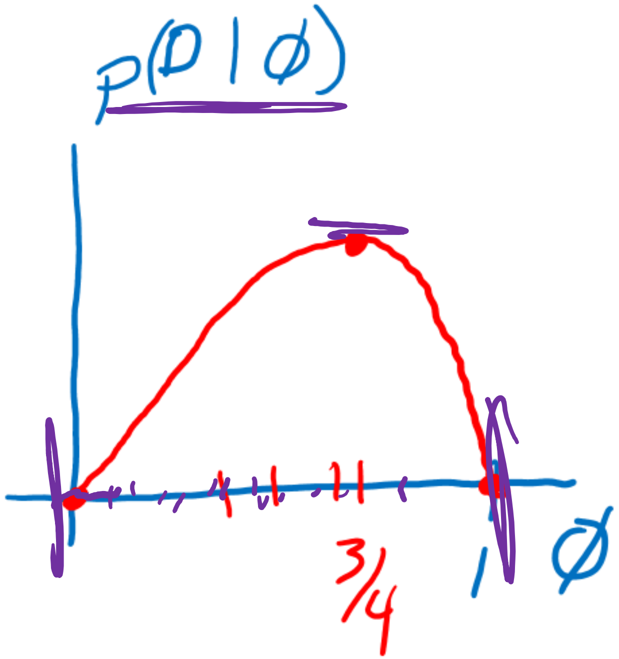


$$p(\,D \mid \phi\,) = \phi \cdot \phi \cdot (1 - \phi) \cdot \phi$$
$$= \phi^3 (1 - \phi)^1$$

$N_H = 300$ $\quad$ $N_T = 100$

Likelihood and Maximum Likelihood Estimation

Likelihood: The probability (or density) of random variable Y taking on value y given the distribution parameters, $\boldsymbol{\theta}$.

$$p(D \mid \theta)$$

Likelihood function: The value of likelihood as we change theta

(same as likelihood, but conceptually we are considering many different values of the parameters)

$$\mathcal{L}(\theta; D) = p(D \mid \theta)$$

Maximum Likelihood Estimation (MLE): Find the parameter value that maximizes the likelihood.

$$\arg\max_{\theta} \mathcal{L}(\theta)$$

MLE as Data Increases

Given the ordered sequence of coin flip outcomes:

$$[1, 0, 1, 1]$$

$$\mathrm{p}(\mathcal{D} \mid \phi) = \prod_{i}^{N} p\left(y^{(i)} \mid \phi\right) = \phi^{N_{y=1}}(1-\phi)^{N_{y=0}}$$

What happens as we flip more coins?

MLE for Gaussian

Gaussian distribution:

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

$$p(y \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

What is the log likelihood for three i.i.d. samples, given parameters μ, σ^2?

$$\mathcal{D} = \{y^{(1)} = 65, y^{(2)} = 95, y^{(3)} = 85\}$$

$$L(\mu, \sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(y^{(i)}-\mu\right)^2}{2\sigma^2}}$$

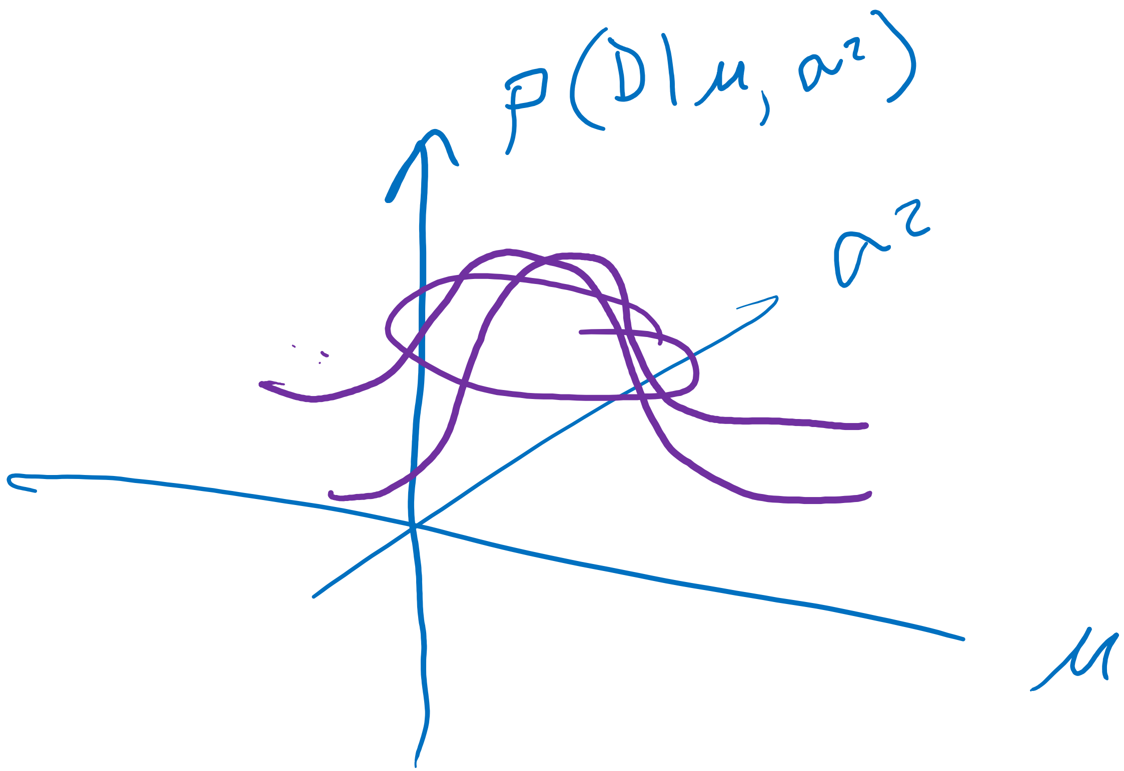
$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i}^{N} p\left(y^{(i)} \mid \boldsymbol{\theta}\right)$$

MLE for Gaussian

Assume that exam scores are drawn independently from the same Gaussian (Normal) distribution.

Given three exam scores 75, 80, 90, which pair of parameters is the best fit (the highest likelihood)?

$$p(\mathcal{D}|\mu, \sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(y^{(i)}-\mu\right)^2}{2\sigma^2}}$$



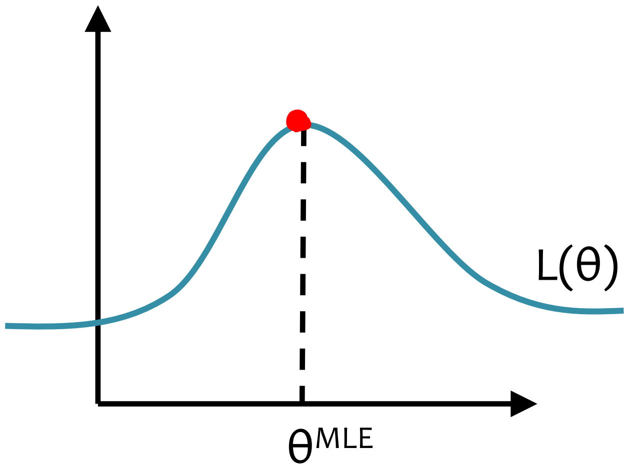
MLE

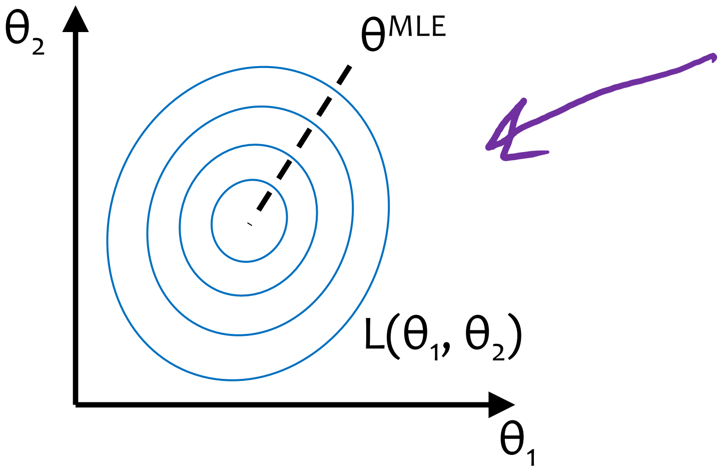
Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^{N}$

Principle of Maximum Likelihood Estimation:
Choose the parameters that maximize the likelihood of the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \prod_{i=1}^{N} p(\mathbf{x}^{(i)}|\boldsymbol{\theta})$$

Maximum Likelihood Estimate (MLE)





$\log xz = \log x + \log z$

Likelihood and Log Likelihood

Likelihood: The probability (or density) of random variable Y taking on value y given the distribution parameters, $\boldsymbol{\theta}$.

Likelihood function: The value of likelihood as we change theta

(same as likelihood, but conceptually we are considering many different values of the parameters)

$\log xz = \log x + \log z$

Likelihood and Log Likelihood

Likelihood: The probability (or density) of random variable Y taking on value y given the distribution parameters, $\boldsymbol{\theta}$.

$$p(D|\theta) = \prod p(y^{(i)}|\theta)$$

Likelihood function: The value of likelihood as we change theta

(same as likelihood, but conceptually we are considering many different values of the parameters)

likelihood $\mathcal{L}(\theta; D) = p(D|\theta) = \prod p(y^{(i)}|\theta)$

log likelihood $\ell(\theta; D) = \log p(D|\theta) = \sum \log p(y^{(i)}|\theta)$

Maximum Likelihood Estimation

MLE of parameter θ for i.i.d. dataset $\mathcal{D} = \{y^{(i)}\}_{i=1}^{N}$

$$\hat{\theta}_{MLE} = \underset{\theta}{\operatorname{argmax}}\, p(\mathcal{D} \mid \theta)$$

Recipe for Estimation

MLE

1. Formulate the likelihood, $p(\mathcal{D} \mid \theta)$
2. Set objective $J(\theta)$ equal to negative log of likelihood

   $$\mathrm{J}(\theta) = -\log p(\mathcal{D} \mid \theta)$$

3. Compute derivative of objective, $\partial J / \partial \theta$
4. Find $\hat{\theta}$, either
   a. Set derivate equal to zero and solve for θ
   b. Use (stochastic) gradient descent to step towards better θ

MLE for Gaussian

Gaussian distribution:

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

$$p(y \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\mu)^2}{2\sigma^2}}$$

What is the log likelihood for three i.i.d. samples, given parameters μ, σ^2?

$$\mathcal{D} = \{y^{(1)} = 65, y^{(2)} = 95, y^{(3)} = 85\}$$

$$L(\mu, \sigma^2) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\left(y^{(i)}-\mu\right)^2}{2\sigma^2}}$$

$$\ell(\mu, \sigma^2) = \sum_{i=1}^{N} -\log\sqrt{2\pi\sigma^2} - \frac{\left(y^{(i)} - \boxed{\mu}\right)^2}{2\sigma^2}$$

$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i}^{N} p\left(y^{(i)} \mid \boldsymbol{\theta} \right)$$

$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \sum_{i}^{N} \log p\left(y^{(i)} \mid \boldsymbol{\theta} \right)$$

Probabilistic Formulation for ML

MLE for Linear and Logistic Regression

Using Statistics for Machine Learning

likelihood $\longrightarrow p(D \mid \theta)$

$$\prod p(y^{(i)} \mid \theta)$$

---

conditional likelihood $\prod p(y^{(i)} \mid x, \theta)$

$$p(D \mid \theta)$$

Recipe for Estimation

MLE

1. Formulate the likelihood, $p(\mathcal{D} \mid \theta)$
2. Set objective $J(\theta)$ equal to negative log of likelihood

$$\mathrm{J}(\theta) = -\log p(\mathcal{D} \mid \theta)$$

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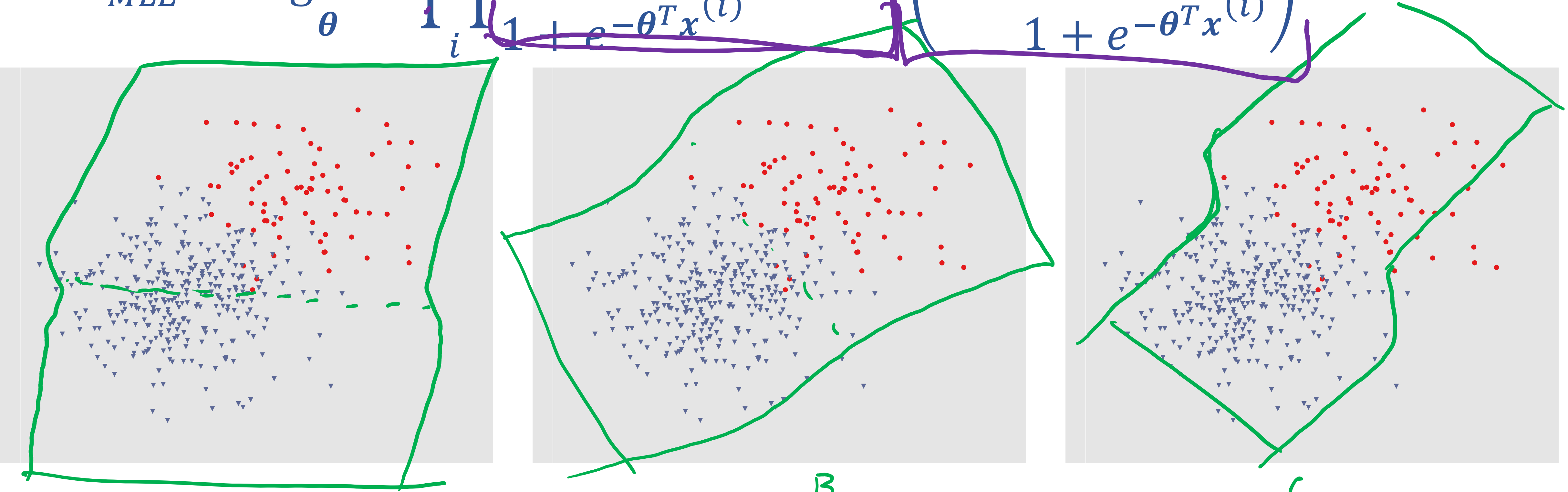
M(C)LE for Logistic Regression

$p(y \mid x; \theta)$

Learn to predict if a patient has cancer ($Y = 1$) or not ($Y = 0$) given the input of just one test results, X_A and X_B

$$\hat{\theta}_{MLE} = \underset{\theta}{\operatorname{argmax}} \prod_{i}^{N} \left(\frac{1}{1 + e^{-\boldsymbol{\theta}^T \boldsymbol{x}^{(i)}}}\right)^{\mathbb{I}(y^{(i)}=1)} \left(1 - \frac{1}{1 + e^{-\boldsymbol{\theta}^T \boldsymbol{x}^{(i)}}}\right)^{\mathbb{I}(y^{(i)}=0)}$$

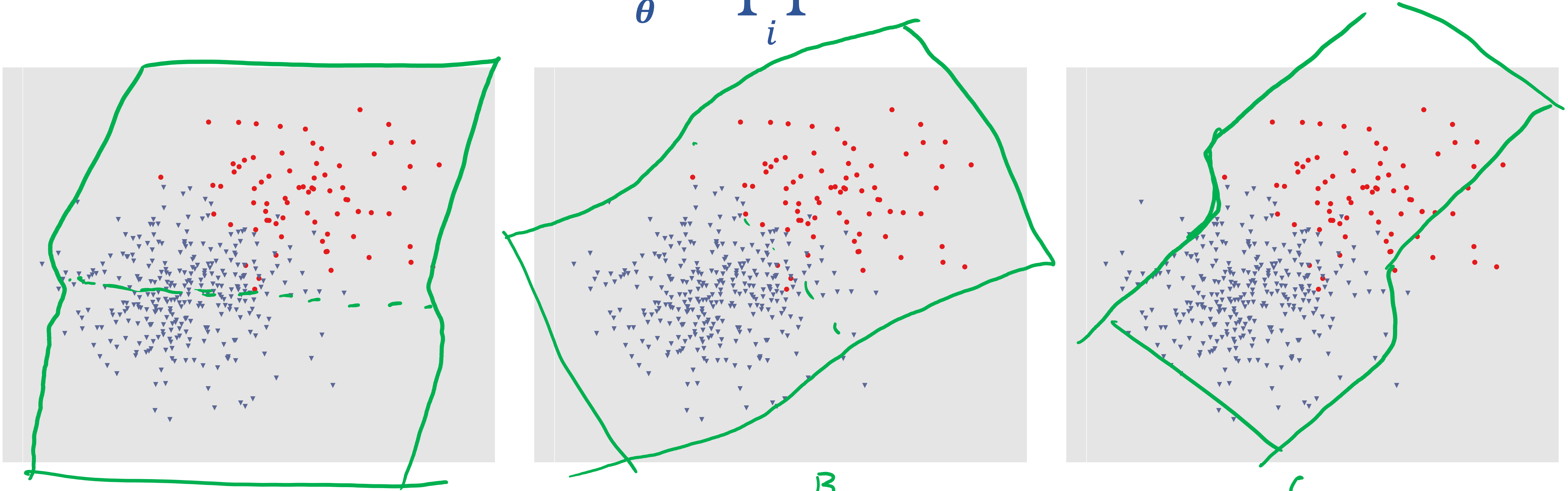


θ^A θ^B θ^C

M(C)LE for Logistic Regression

Learn to predict if a patient has cancer ($Y = 1$) or not ($Y = 0$) given the input of just one test results, X_A and X_B

$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i}^{N} p(\,y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}\,)$$



θ^A θ^B θ^C

M(C)LE for Multi-class Logistic Regression

Learn to predict if probability of output belonging to class k, Y_k , given input X, $P(Y_k = 1 \mid X, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K)$

$$\hat{\Theta}_{MLE} = \underset{\boldsymbol{\Theta}}{\operatorname{argmax}} \prod_{i}^{N} \prod_{k}^{K} \frac{e^{\boldsymbol{\theta}_k^T \boldsymbol{x}^{(i)}}}{\sum_{l=1}^{K} e^{\boldsymbol{\theta}_l^T \boldsymbol{x}^{(i)}}}^{\mathbb{I}\left(y_k^{(i)}=1\right)}$$

M(C)LE for Multi-class Logistic Regression

Sm!

Learn to predict if probability of output belonging to class k, Y_k, given input X, $P(Y_k = 1 \mid X, \boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_K)$

$$L(\Theta; \mathcal{D}) = \prod_i^N \prod_k^K \boxed{\frac{e^{\boldsymbol{\theta}_k^T \boldsymbol{x}^{(i)}}}{\sum_{l=1}^K e^{\boldsymbol{\theta}_l^T \boldsymbol{x}^{(i)}}}}^{\mathbb{I}\left(y_k^{(i)}=1\right)}$$

$$\ell(\Theta; \mathcal{D}) = \sum_i \log \prod_k \boxed{}^{\mathbb{I}(y_k^{(i)}=1)}$$

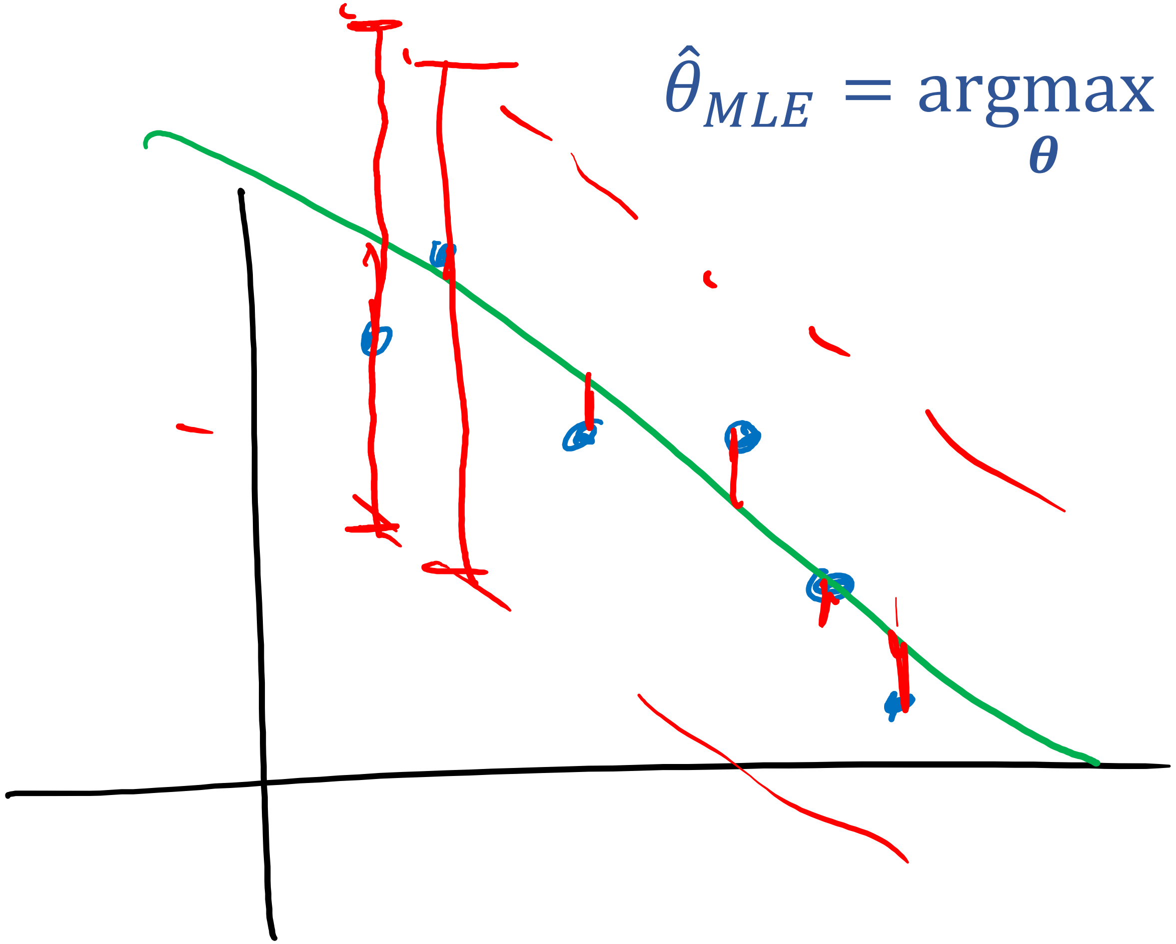
$$= \sum_i \sum_k \mathbb{I}(y_k^{(i)}=1) \log \boxed{}$$

$$y^{(i)} \log \hat{y}^{(i)}$$

M(C)LE for Linear Regression

Probabilistic interpretation of linear regression

$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i}^{N} p\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \boldsymbol{\theta} \right)$$



$\theta^T x + \epsilon$

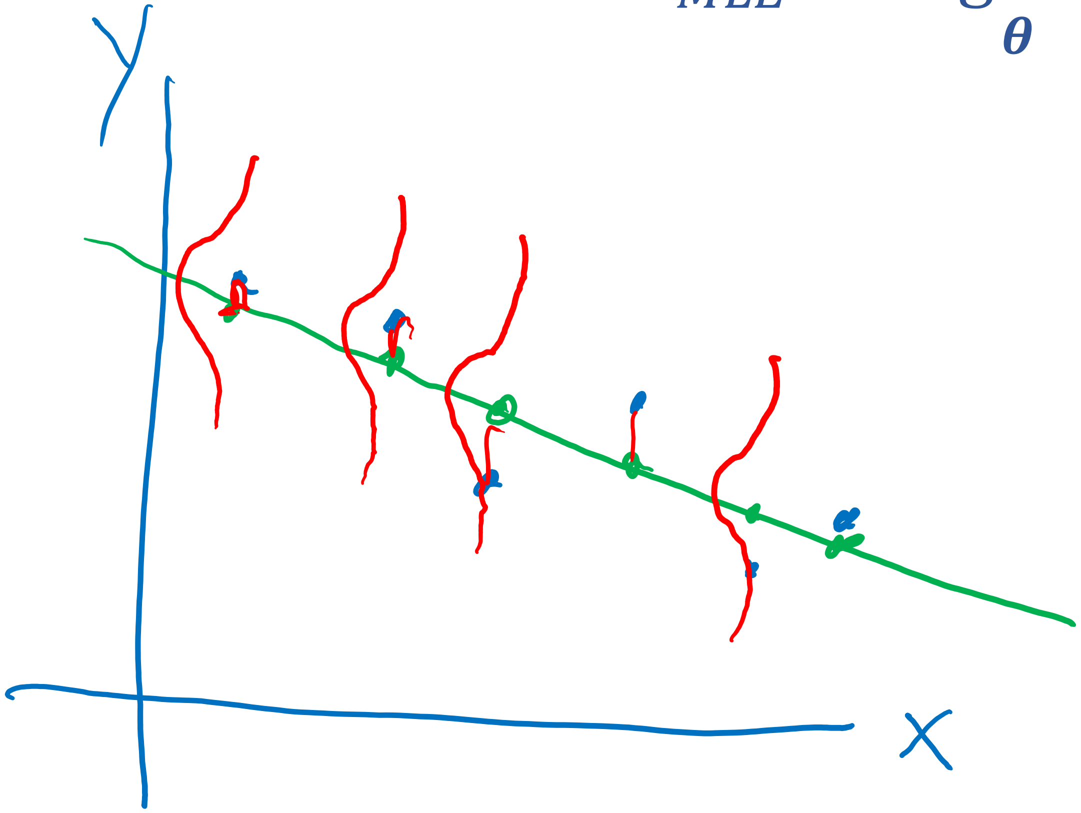
M(C)LE for Linear Regression

Probabilistic interpretation of linear regression

$$\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-\theta^T x)^2}{2\sigma^2}}$$

$$\hat{\theta}_{MLE} = \underset{\boldsymbol{\theta}}{\operatorname{argmax}} \prod_{i}^{N} p\left(y^{(i)} \mid \boldsymbol{x}^{(i)}, \boldsymbol{\theta} \right)$$

$\underline{\theta^T x}$



$$y = \underbrace{w^T x + b}_{} + \underline{\epsilon}$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$y \sim \underline{\mathcal{N}(\theta^T x, \sigma^2)}$$

$$\rightarrow p(y^{(i)} \mid x^{(i)}, w, b) =$$

M(C)LE for Linear Regression

Probabilistic interpretation of linear regression

$$L(\theta;\mathcal{D}) = \prod_{i}^{N} p\big(\, y^{(i)} \mid \boldsymbol{x}^{(i)}, \boldsymbol{\theta} \,\big)$$

$$\log \;\; - \;\; \frac{1}{2\sigma^2}\left(y - \theta^T x\right)^2$$