10-301/601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

MLE/MAP

+

Naïve Bayes

Matt Gormley
Lecture 16
Mar. 18, 2022

Reminders

- Homework 5: Neural Networks
  - Out: Sun, Feb 27
  - Due: Fri, Mar 18 at 11:59pm
- Homework 6: Learning Theory / Generative Models
  - Out: Fri, Mar. 18
  - Due: Fri, Mar. 25 at 11:59pm
  - IMPORTANT: only 2 grace/late days permitted
- Exam 2 (Thu, Mar 3rd)
- Exam 3 (Tue, May 3rd)

PROBABILISTIC LEARNING

Probabilistic Learning

Function Approximation

Previously, we assumed that our output was generated using a **deterministic target function:**

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$

$$y^{(i)} = c^*(\mathbf{x}^{(i)})$$

Our goal was to learn a hypothesis h(**x**) that best approximates c^*(**x**)

Probabilistic Learning

Today, we assume that our output is **sampled** from a conditional **probability distribution:**

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$

$$y^{(i)} \sim p^*(\cdot|\mathbf{x}^{(i)})$$

Our goal is to learn a probability distribution p(y|**x**) that best approximates p^*(y|**x**)

MAXIMUM LIKELIHOOD ESTIMATION (MLE)

Likelihood Function

One R.V.

- Given N **independent, identically distributed (iid)** samples $D = \{x^{(1)}, x^{(2)}, \ldots, x^{(N)}\}$ from a **random variable** X …

- The **likelihood** function is
  - Case 1: X is **discrete** with probability mass function (*pmf*) $p(x|\theta)$
    $L(\theta) = p(x^{(1)}|\theta)\, p(x^{(2)}|\theta) \ldots\, p(x^{(N)}|\theta)$
  - Case 2: X is **continuous** with probability density function (pdf) $f(x|\theta)$
    $L(\theta) = f(x^{(1)}|\theta)\, f(x^{(2)}|\theta) \ldots\, f(x^{(N)}|\theta)$

The **likelihood** tells us how likely one sample is relative to another

- The **log-likelihood** function is
  - Case 1: X is **discrete** with probability mass function (*pmf*) $p(x|\theta)$
    $\ell(\theta) = \log p(x^{(1)}|\theta) + \ldots + \log p(x^{(N)}|\theta)$
  - Case 2: X is **continuous** with probability density function (pdf) $f(x|\theta)$
    $\ell(\theta) = \log f(x^{(1)}|\theta) + \ldots + \log f(x^{(N)}|\theta)$

Likelihood Function

Two R.V.s

- Given N **iid** samples $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$ from a pair of **random variables** X, Y

- The **conditional likelihood** function:
  - Case 1: Y is **discrete** with *pmf* $p(y \mid x, \theta)$
    $$L(\theta) = p(y^{(1)} \mid x^{(1)}, \theta) \ldots p(y^{(N)} \mid x^{(N)}, \theta)$$
  - Case 2: Y is **continuous** with *pdf* $f(y \mid x, \theta)$
    $$L(\theta) = f(y^{(1)} \mid x^{(1)}, \theta) \ldots f(y^{(N)} \mid x^{(N)}, \theta)$$

- The **joint likelihood** function:
  - Case 1: X and Y are **discrete** with *pmf* $p(x,y|\theta)$
    $$L(\theta) = p(x^{(1)}, y^{(1)}|\theta) \ldots p(x^{(N)}, y^{(N)}|\theta)$$
  - Case 2: X and Y are **continuous** with *pdf* $f(x,y|\theta)$
    $$L(\theta) = f(x^{(1)}, y^{(1)}|\theta) \ldots f(x^{(N)}, y^{(N)}|\theta)$$

Likelihood Function

Two R.V.s

- Given N **iid** samples $D = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$ from a pair of **random variables** X, Y

- The **joint likelihood** function:
  - Case 1: X and Y are **discrete** with *pmf* $p(x,y|\theta)$
    $L(\theta) = p(x^{(1)}, y^{(1)}|\theta) \ldots p(x^{(N)}, y^{(N)}|\theta)$
  - Case 2: X and Y are **continuous** with *pdf* $f(x,y|\theta)$
    $L(\theta) = f(x^{(1)}, y^{(1)}|\theta) \ldots f(x^{(N)}, y^{(N)}|\theta)$
  - Case 3: Y is **discrete** with *pmf* $p(y|\beta)$ and
    X is **continuous** with *pdf* $f(x|y,\alpha)$
    $L(\alpha, \beta) = f(x^{(1)}| y^{(1)}, \alpha)\, p(y^{(1)}|\beta) \ldots f(x^{(N)}| y^{(N)}, \alpha)\, p(y^{(N)}|\beta)$
  - Case 4: Y is **continuous** with *pdf* $f(y|\beta)$ and
    X is **discrete** with *pmf* $p(x|y,\alpha)$
    $L(\alpha, \beta) = p(x^{(1)}| y^{(1)}, \alpha)\, f(y^{(1)}|\beta) \ldots p(x^{(N)}| y^{(N)}, \alpha)\, f(y^{(N)}|\beta)$

Mixed discrete/ continuous!

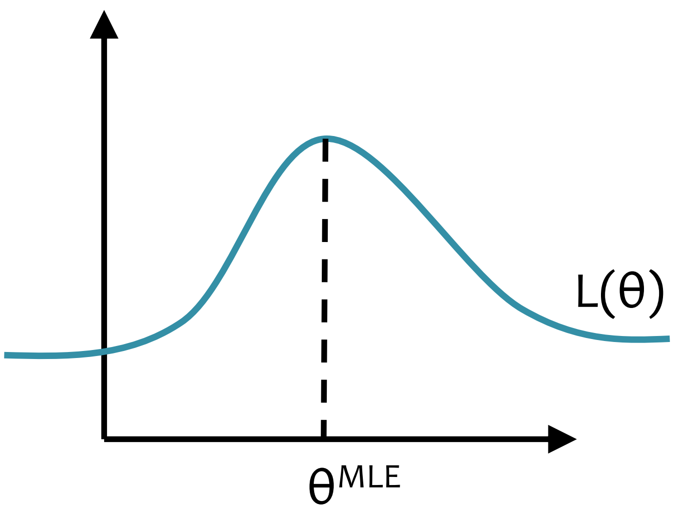
MLE

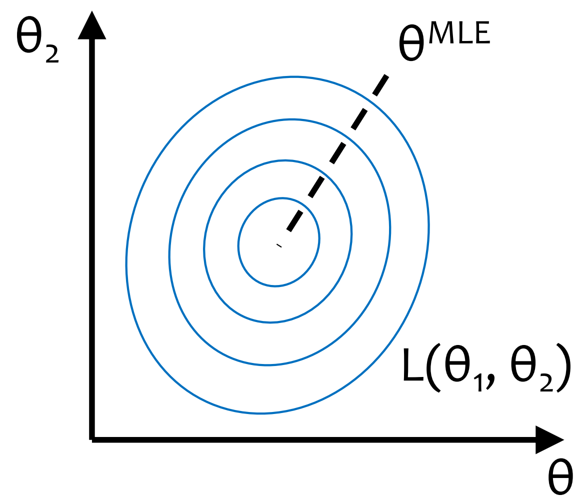
Suppose we have data $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$

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

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

Maximum Likelihood Estimate (MLE)





MLE

What does maximizing likelihood accomplish?

- There is only a finite amount of probability mass (i.e. sum-to-one constraint)
- MLE tries to allocate **as much** probability mass **as possible** to the things we have observed…

  … **at the expense** of the things we have **not** observed

Recipe for Closed-form MLE

1. Assume data was generated iid from some model, i.e., write the *generative story*

   $x^{(i)} \sim p(x|\boldsymbol{\theta})$

2. Write the log-likelihood

   $\ell(\boldsymbol{\theta}) = \log p(x^{(1)}|\boldsymbol{\theta}) + \ldots + \log p(x^{(N)}|\boldsymbol{\theta})$

3. Compute partial derivatives, i.e., the gradient

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_1 = \ldots$

   $\ldots$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_M = \ldots$

4. Set derivatives equal to zero and solve for $\boldsymbol{\theta}$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_m = 0$ for all $m \in \{1, \ldots, M\}$

   $\boldsymbol{\theta}^{MLE}$ = solution to system of M equations and M variables

5. Compute the second derivative and check that $\ell(\boldsymbol{\theta})$ is concave down at $\boldsymbol{\theta}^{MLE}$

What we earlier called “Closed Form Solution for Linear Regression”

EXAMPLE:
MLE FOR LINEAR REGRESSION

Linear Regression as Function Approximation

$\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^N$
where $\mathbf{x} \in \mathbb{R}^M$ and $y \in \mathbb{R}$

1. Assume $\mathcal{D}$ generated as:

$$\mathbf{x}^{(i)} \sim p^*(\cdot)$$
$$y^{(i)} = h^*(\mathbf{x}^{(i)})$$

2. Choose hypothesis space, $\mathcal{H}$:
all linear functions in M-dimensional space

$$\mathcal{H} = \{h_{\boldsymbol{\theta}} : h_{\boldsymbol{\theta}}(\mathbf{x}) = \boldsymbol{\theta}^T \mathbf{x}, \boldsymbol{\theta} \in \mathbb{R}^M\}$$

3. Choose an objective function:
mean squared error (MSE)

$$\begin{aligned} J(\boldsymbol{\theta}) &= \frac{1}{N} \sum_{i=1}^N e_i^2 \\ &= \frac{1}{N} \sum_{i=1}^N \left(y^{(i)} - h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)})\right)^2 \\ &= \frac{1}{N} \sum_{i=1}^N \left(y^{(i)} - \boldsymbol{\theta}^T \mathbf{x}^{(i)}\right)^2 \end{aligned}$$

4. Solve the unconstrained optimization problem via favorite method:
   - *gradient descent*
   - *closed form*
   - *stochastic gradient descent*
   - $\ldots$

$$\hat{\boldsymbol{\theta}} = \operatorname*{argmin}_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$

5. Test time: given a new $\mathbf{x}$, make prediction $\hat{y}$

$$\hat{y} = h_{\hat{\boldsymbol{\theta}}}(\mathbf{x}) = \hat{\boldsymbol{\theta}}^T \mathbf{x}$$

Linear Regression: Closed Form

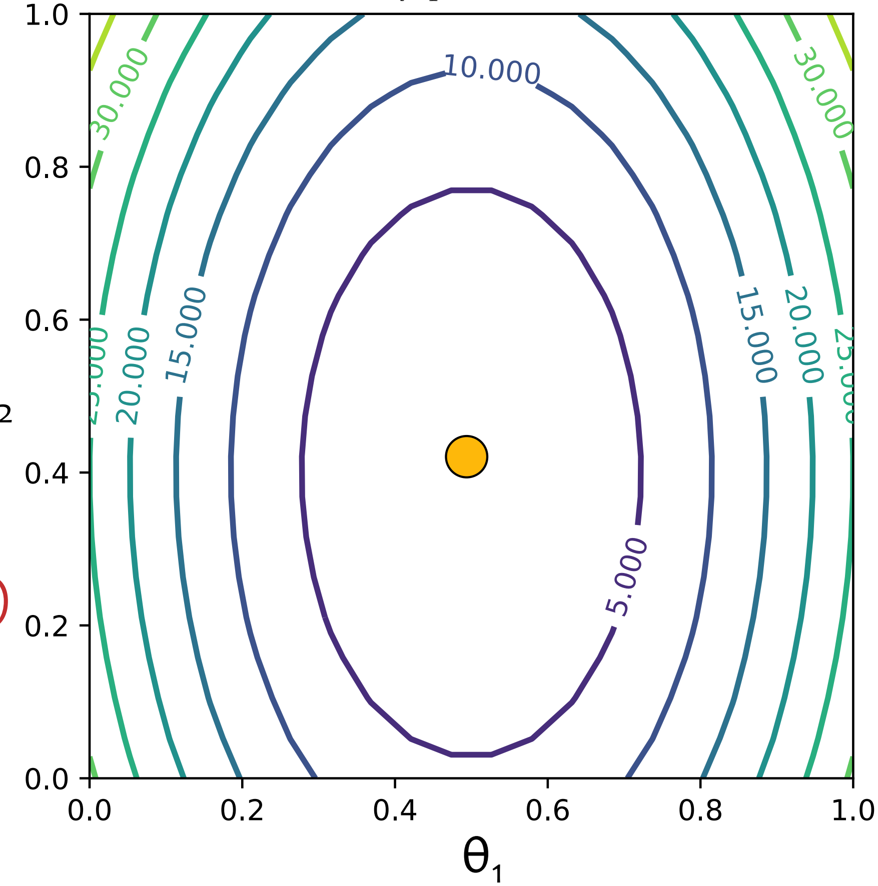
Optimization Method #2: Closed Form

1. Evaluate

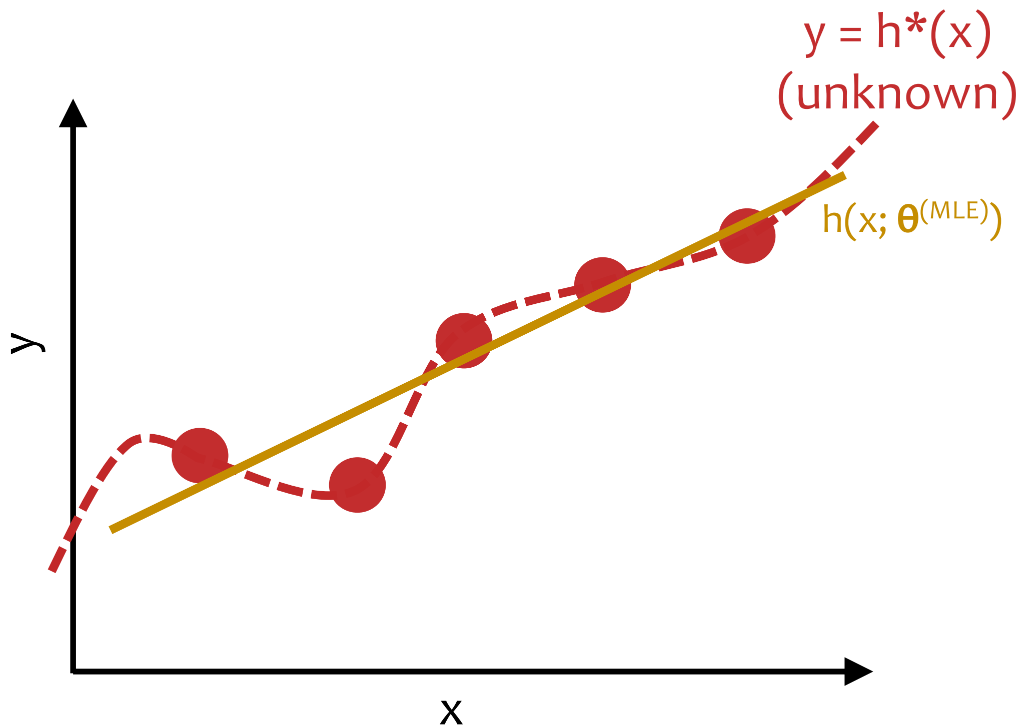
$$\boldsymbol{\theta}^{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

2. Return $\boldsymbol{\theta}^{\text{MLE}}$

$$J(\boldsymbol{\theta}) = J(\theta_1, \theta_2) = \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)} - \boldsymbol{\theta}^T\mathbf{x}^{(i)}\right)^2$$



t	θ_1	θ_2	$J(\theta_1, \theta_2)$
MLE	0.59	0.43	0.2



MLE for Linear Regression

You'll work through the view of linear regression as a probabilistic model in the homework!

MLE EXAMPLES

MLE of Exponential Distribution

Goal:

- pdf of Exponential(λ): $f(x) = \lambda e^{-\lambda x}$
- Suppose $X_i \sim$ Exponential(λ) for $1 \leq i \leq N$.
- Find MLE for data $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$

Steps:

- First write down log-likelihood of sample.
- Compute first derivative, set to zero, solve for λ.
- Compute second derivative and check that it is concave down at λ^{MLE}.

MLE of Exponential Distribution

- pdf of Exponential(λ): $f(x) = \lambda e^{-\lambda x}$
- Suppose $X_i \sim$ Exponential(λ) for $1 \leq i \leq N$.
- Find MLE for data $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$

- First write down log-likelihood of sample.

$$\ell(\lambda) = \sum_{i=1}^{N} \log f(x^{(i)}) \tag{1}$$

$$= \sum_{i=1}^{N} \log(\lambda \exp(-\lambda x^{(i)})) \tag{2}$$

$$= \sum_{i=1}^{N} \log(\lambda) + -\lambda x^{(i)} \tag{3}$$

$$= N \log(\lambda) - \lambda \sum_{i=1}^{N} x^{(i)} \tag{4}$$

MLE of Exponential Distribution

- pdf of Exponential(λ): $f(x) = \lambda e^{-\lambda x}$
- Suppose $X_i \sim$ Exponential(λ) for $1 \leq i \leq N$.
- Find MLE for data $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$

- Compute first derivative, set to zero, solve for λ.

$$\frac{d\ell(\lambda)}{d\lambda} = \frac{d}{d\lambda} N \log(\lambda) - \lambda \sum_{i=1}^{N} x^{(i)} \qquad (1)$$

$$= \frac{N}{\lambda} - \sum_{i=1}^{N} x^{(i)} = 0 \qquad (2)$$

$$\boxed{\Rightarrow \lambda^{\text{MLE}} = \frac{N}{\sum_{i=1}^{N} x^{(i)}}} \qquad (3)$$

MLE of Bernoulli

In-Class Exercise

Show that the MLE of parameter ϕ for N samples drawn from Bernoulli(ϕ) is:

$$\phi_{MLE} = \frac{\text{Number of } x_i = 1}{N}$$

Steps to answer:

1. Write log-likelihood of sample
2. Compute derivative w.r.t. ϕ
3. Set derivative to zero and solve for ϕ

MLE of Bernoulli

Question:

Assume we have N iid samples $x^{(1)}, x^{(2)}, \ldots, x^{(N)}$ drawn from a Bernoulli(ϕ).

Step 1: What is the **log-likelihood** of the data $\ell(\phi)$?

Assume $N_1 = \#\ of\ (x^{(i)} = 1)$

$N_0 = \#\ of\ (x^{(i)} = 0)$

Answer:

A. $l(\phi) = N_1 \log(\phi) + N_0 (1 - \log(\phi))$

B. $l(\phi) = N_1 \log(\phi) + N_0 \log(1-\phi)$

C. $l(\phi) = \log(\phi)^{N_1} + (1 - \log(\phi))^{N_0}$

D. $l(\phi) = \log(\phi)^{N_1} + \log(1-\phi)^{N_0}$

E. $l(\phi) = N_0 \log(\phi) + N_1 (1 - \log(\phi))$

F. $l(\phi) = N_0 \log(\phi) + N_1 \log(1-\phi)$

G. $l(\phi) = \log(\phi)^{N_0} + (1 - \log(\phi))^{N_1}$

H. $l(\phi) = \log(\phi)^{N_0} + \log(1-\phi)^{N_1}$

I. $l(\phi) = N_0 + N_1$

MLE of Bernoulli

Question:

Assume we have N iid samples $x^{(1)}, x^{(2)}, \ldots, x^{(N)}$ drawn from a Bernoulli(ϕ).

Step 2: What is the **derivative** of the log-likelihood $\partial\ell(\boldsymbol{\theta})/\partial\theta$?

Assume $N_1 = \#\ of\ (x^{(i)} = 1)$
$N_0 = \#\ of\ (x^{(i)} = 0)$

Answer:

A. $\partial\ell(\boldsymbol{\theta})/\partial\theta = \phi^{N_1} - (1 - \phi)^{N_0}$

B. $\partial\ell(\boldsymbol{\theta})/\partial\theta = \phi / N_1 - (1 - \phi) / N_0$

C. $\partial\ell(\boldsymbol{\theta})/\partial\theta = N_1 / \phi - N_0 / (1 - \phi)$

D. $\partial\ell(\boldsymbol{\theta})/\partial\theta = \log(\phi) / N_1 - \log(1 - \phi) / N_0$

E. $\partial\ell(\boldsymbol{\theta})/\partial\theta = N_1 / \log(\phi) - N_0 / \log(1 - \phi)$

F. $\partial\ell(\boldsymbol{\theta})/\partial\theta = 0$

MLE of Bernoulli

Whiteboard

- Example: MLE of Bernoulli

MAP ESTIMATION

MLE vs. MAP

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.

$$\boldsymbol{\theta}^{\text{MLE}} = \text{argmax}_{\boldsymbol{\theta}}\, p(\mathcal{D}|\boldsymbol{\theta}) = \text{argmax}_{\boldsymbol{\theta}} \prod_{i=1}^{N} p\left(\mathbf{x}^{(i)}|\boldsymbol{\theta}\right)$$

Maximum Likelihood Estimate (MLE)

Principle of Maximum *a posteriori* (MAP) Estimation:
Choose the parameters that maximize the posterior of the parameters given the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \text{argmax}_{\boldsymbol{\theta}}\, p(\boldsymbol{\theta}|\mathcal{D}) = \text{argmax}_{\boldsymbol{\theta}}\, f(\boldsymbol{\theta}) \prod_{i=1}^{N} p\left(\mathbf{x}^{(i)}|\boldsymbol{\theta}\right)$$

Maximum *a posteriori* (MAP) estimate

MLE vs. MAP

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

Principle of Maxi

Choose the paran hood of the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \text{argma} \quad \boldsymbol{\theta})$$

Important!

Usually the parameters are **continuous,** so the prior is a probability **density** function

Maximum Likelihood Estimate (MLE)

Principle of Maximum *a posteriori* (MAP) Es mation:

Choose the parameters that maximize the sterior of the parameters given the data.

$$\boldsymbol{\theta}^{\text{MLE}} = \text{argmax}_{\boldsymbol{\theta}}\, p(\boldsymbol{\theta}|\mathcal{D}) = \text{argmax}_{\boldsymbol{\theta}}\, \overbrace{f(\boldsymbol{\theta})}^{\text{Prior}} \prod_{i=1}^{N} p\left(\mathbf{x}^{(i)}|\boldsymbol{\theta}\right)$$

Maximum *a posteriori* (MAP) estimate

Learning from Data (Bayesian)

Whiteboard

– *maximum a posteriori* (MAP) estimation

Recipe for Closed-form MLE

1. Assume data was generated iid from some model, i.e., write the *generative story*

   $x^{(i)} \sim p(x|\boldsymbol{\theta})$
2. Write the log-likelihood

   $\ell(\boldsymbol{\theta}) = \log p(x^{(1)}|\boldsymbol{\theta}) + \ldots + \log p(x^{(N)}|\boldsymbol{\theta})$
3. Compute partial derivatives, i.e., the gradient

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_1 = \ldots$

   $\ldots$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_M = \ldots$
4. Set derivatives equal to zero and solve for $\boldsymbol{\theta}$

   $\partial\ell(\boldsymbol{\theta})/\partial\theta_m = 0$ for all $m \in \{1, \ldots, M\}$

   $\boldsymbol{\theta}^{MLE}$ = solution to system of M equations and M variables
5. Compute the second derivative and check that $\ell(\boldsymbol{\theta})$ is concave down at $\boldsymbol{\theta}^{MLE}$

Recipe for Closed-form MAP

1. Assume data was generated iid from some model, i.e., write the *generative story*

   $\boldsymbol{\theta} \sim p(\boldsymbol{\theta})$ and then for all i: $x^{(i)} \sim p(x|\boldsymbol{\theta})$

2. Write the log posterior

   $\ell_{MAP}(\boldsymbol{\theta}) = \log p(\boldsymbol{\theta}) + \log p(x^{(1)}|\boldsymbol{\theta}) + \ldots + \log p(x^{(N)}|\boldsymbol{\theta})$

3. Compute partial derivatives, i.e., the gradient

   $\partial \ell_{MAP}(\boldsymbol{\theta})/\partial \theta_1 = \ldots$

   $\ldots$

   $\partial \ell_{MAP}(\boldsymbol{\theta})/\partial \theta_M = \ldots$

4. Set derivatives to equal zero and solve for $\boldsymbol{\theta}$

   $\partial \ell_{MAP}(\boldsymbol{\theta})/\partial \theta_m = 0$ for all $m \in \{1, \ldots, M\}$

   $\boldsymbol{\theta}^{MAP}$ = solution to system of M equations and M variables

5. Compute the second derivative and check that $\ell(\boldsymbol{\theta})$ is concave down at $\boldsymbol{\theta}^{MAP}$

MAP of Beta-Bernoulli Model

Whiteboard

- Example: MAP of Beta-Bernoulli Model

Takeaways

- One view of what ML is trying to accomplish is **function approximation**
- The principle of **maximum likelihood estimation** provides an alternate view of learning

- **Synthetic data** can help **debug** ML algorithms
- Probability distributions can be used to **model** real data that occurs in the world
  (don't worry we'll make our distributions more interesting soon!)

Learning Objectives

MLE / MAP

You should be able to…

1. Recall probability basics, including but not limited to: discrete and continuous random variables, probability mass functions, probability density functions, events vs. random variables, expectation and variance, joint probability distributions, marginal probabilities, conditional probabilities, independence, conditional independence
2. Describe common probability distributions such as the Beta, Dirichlet, Multinomial, Categorical, Gaussian, Exponential, etc.
3. State the principle of maximum likelihood estimation and explain what it tries to accomplish
4. State the principle of maximum a posteriori estimation and explain why we use it
5. Derive the MLE or MAP parameters of a simple model in closed form

NAÏVE BAYES

Naïve Bayes

- Why are we talking about Naïve Bayes?
  - It's **just another decision function** that fits into our "big picture" recipe from last time
  - But it's our first **example of a Bayesian Network** and provides a *clearer* picture of **probabilistic learning**
  - Just like the other Bayes Nets we'll see, it **admits a closed form solution** for MLE and MAP
  - So learning is **extremely efficient** (just counting)

Fake News Detector

Today's Goal: To define a generative model of emails of two different classes (e.g. real vs. fake news)

The Economist

Soybean Prices Surge as South American Outlook Deteriorates

Drought is pushing prices up, with shortfalls in production expected to boost demand for U.S. beans

Agricultural research firm Farm Futures last month forecast that planted soybean acreage in the U.S. may exceed corn for only the second time in history.
PHOTO: RORY DOYLE/BLOOMBERG NEWS

By *Kirk Maltais*
Feb. 12, 2022 7:00 am ET

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Listen to article (2 minutes)

U.S. soybean prices have surged in recent months amid shrinking forecasts for South American crops.

Prices for soybeans—the base ingredient in many food products, poultry and livestock feed and renewable fuel, among other things—are edging back toward highs reached last year, which hadn't previously been seen in a decade.

The Onion

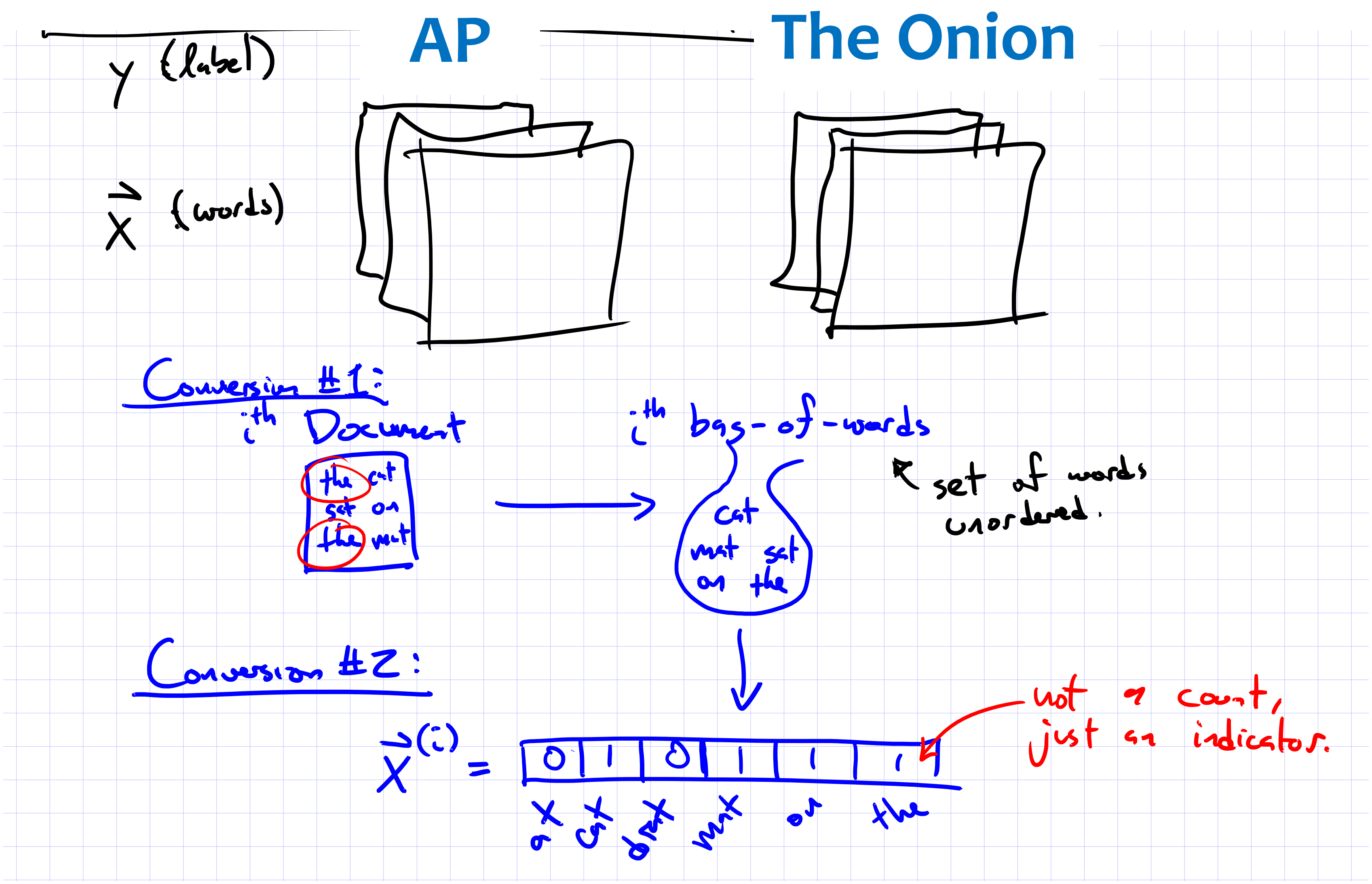
NEWS IN BRIEF

Watchdog Warns Nearly Every Food Brand In U.S. Owned By Handful Of Companies, Which In Turn Are Controlled By Newman's Own

Today 9:25AM | Alerts

WASHINGTON—Calling for a full-scale Federal Trade Commission investigation into the sauce and salad dressing brand, the American Antitrust Institute issued a report Thursday warning that nearly every food brand in the United States was owned by a handful of companies, which in turn were controlled by Newman's Own. "Kellogg's, General Mills, PepsiCo, Kraft Heinz—all of these companies are just Newman's Own by another name," said Diana L.

Fake News Detector



We can pretend the natural process generating these vectors is stochastic…

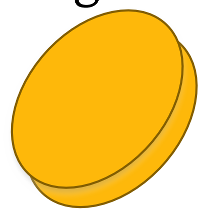
Naive Bayes: Model

Whiteboard

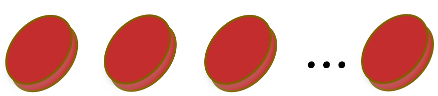
- Generating synthetic "labeled documents"
- Definition of model
- Naive Bayes assumption
- Counting # of parameters with / without NB assumption

Model 1: Bernoulli Naïve Bayes

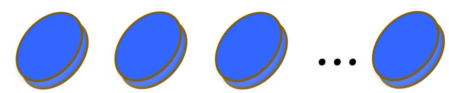
Flip weighted coin



If HEADS, flip
each red coin



If TAILS, flip
each blue coin



y	x_1	x_2	x_3	…	x_M
0	1	0	1	…	1
1	0	1	0	…	1
1	1	1	1	…	1
0	0	0	1	…	1
0	1	0	1	…	0
1	1	0	1	…	0

We can **generate** data in this fashion. Though in practice we never would since our data is **given**.

Instead, this provides an explanation of **how** the data was generated (albeit a terrible one).

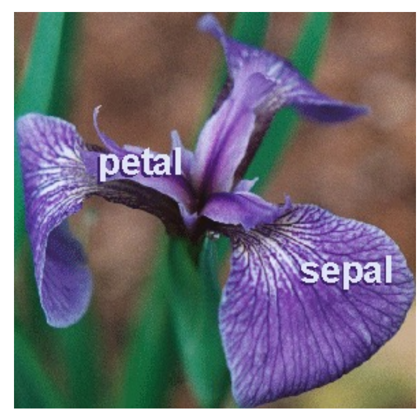
Each red coin corresponds to an x_m

What's wrong with the Naïve Bayes Assumption?

The features might not be independent!!

- Example 1:
  – If a document contains the word "Donald", it's extremely likely to contain the word "Trump"
  – These are not independent!

- Example 2:
  – If the petal width is very high, the petal length is also likely to be very high



Naïve Bayes: Learning from Data

Whiteboard

- Data likelihood
- MLE for Naive Bayes
- Example: MLE for Naïve Bayes with Two Features
- MAP for Naive Bayes

Recipe for Closed-form MLE

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5. Compute the second derivative and check that $\ell(\boldsymbol{\theta})$ is concave down at $\boldsymbol{\theta}^{MLE}$