PAC Learning

MLE/MAP
### Q&A

#### Q: Why did the experiments in HW4 take so long?

**A:** Sorry! When I heard, 5k epochs only takes 40 minutes that sounded short to me. But I’ve been in the ML biz for too long...

#### Q: What is “bias”?

**A:** That depends. The word “bias” shows up all over machine learning! Watch out...

1. The additive term in a linear model (i.e. $b$ in $w^Tx + b$)
2. Inductive bias is the principle by which a learning algorithm generalizes to unseen examples
3. Bias of a model in a societal sense may refer to racial, socio-economic, gender biases that exist in the predictions of your model
4. The difference between the expected predictions of your model and the ground truth (as in “bias-variance tradeoff”)

Reminders

• Homework 5: Neural Networks
  – Out: Sun, Feb 27
  – Due: Fri, Mar 18 at 11:59pm

• Peer Tutoring
SAMPLE COMPLEXITY RESULTS
Sample Complexity Results

**Definition 0.1.** The *sample complexity* of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

**Four Cases we care about...**

| Finite $|\mathcal{H}|$ | Realizable | Agnostic |
|------------------------|------------|----------|
| **Thm. 1** $N \geq \frac{1}{\epsilon} \left[ \log(|\mathcal{H}|) + \log\left(\frac{1}{\delta}\right) \right]$ labeled examples are sufficient so that with probability $(1 - \delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$. | | |

Infinite $|\mathcal{H}|$
Background: Contrapositive

• **Definition:** The *contrapositive* of the statement $A \Rightarrow B$ is the statement $\neg B \Rightarrow \neg A$ and the two are logically equivalent (i.e. they share all the same truth values in a truth table!)

• **Proof by contrapositive:**
  If you want to prove $A \Rightarrow B$, instead prove $\neg B \Rightarrow \neg A$ and then conclude that $A \Rightarrow B$

• **Caution:** sometimes negating a statement is easier said than done, just be careful!
Probably Approximately Correct (PAC) Learning

Whiteboard:

– Proof of Theorem 1
Sample Complexity Results

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| Infinite $|\mathcal{H}|$ | |
|-------------------------| |
| Thm. 2  $N \geq \frac{1}{2\epsilon^2} \left[ \log(|\mathcal{H}|) + \log\left(\frac{2}{\delta}\right) \right]$ labeled examples are sufficient so that with probability $(1 - \delta)$ for all $h \in \mathcal{H}$ we have that $|R(h) - \hat{R}(h)| \leq \epsilon$. |
1. Bound is **inversely linear in epsilon** (e.g. halving the error requires double the examples)
2. Bound is **only logarithmic in |H|** (e.g. quadrupling the hypothesis space only requires double the examples)

---

**Realizable**

**Infinite |H|**

**Thm. 1** \( N \geq \frac{1}{\epsilon} \left[ \log(|\mathcal{H}|) + \log(\frac{1}{\delta}) \right] \) labeled examples are sufficient so that with probability \((1 - \delta)\) all \( h \in \mathcal{H} \) with \( \hat{R}(h) = 0 \) have \( R(h) \leq \epsilon \).

**Finite |H|**

**Agnostic**

**Infinite |H|**

**Thm. 2** \( N \geq \frac{1}{2\epsilon^2} \left[ \log(|\mathcal{H}|) + \log(\frac{2}{\delta}) \right] \) labeled examples are sufficient so that with probability \((1 - \delta)\) for all \( h \in \mathcal{H} \) we have that \( |R(h) - \hat{R}(h)| \leq \epsilon \).
Sample Complexity Results

**Definition 0.1.** The **sample complexity** of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

**Four Cases we care about…**

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### Sample Complexity Results

**Definition 0.1.** The *sample complexity* of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

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| Infinite $|\mathcal{H}|$ | **Thm. 3** $N = O\left(\frac{1}{\epsilon^2} \left[ \text{VC}(\mathcal{H}) \log\left(\frac{1}{\epsilon}\right) + \log\left(\frac{1}{\delta}\right) \right] \right)$ labeled examples are sufficient so that with probability $(1 - \delta)$ all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have $R(h) \leq \epsilon$. | **Thm. 4** $N = O\left(\frac{1}{\epsilon^2} \left[ \text{VC}(\mathcal{H}) + \log\left(\frac{1}{\delta}\right) \right] \right)$ labeled examples are sufficient so that with probability $(1 - \delta)$ for all $h \in \mathcal{H}$ we have that $|R(h) - \hat{R}(h)| \leq \epsilon$. |
VC-DIMENSION
Finite vs. Infinite $|H|$  

**Finite $|H|$**  
- *Example:* $H = \text{the set of all decision trees of depth } D \text{ over binary feature vectors of length } M$

  ![Decision Tree Diagram]

  - *Example:* $H = \text{the set of all conjunctions over binary feature vectors of length } M$

**Infinite $|H|$**  
- *Example:* $H = \text{the set of all linear decision boundaries in } M \text{ dimensions}$

- *Example:* $H = \text{the set of all neural networks with 1-hidden layer with length } M \text{ inputs}$

![Linear Boundaries Diagram]
IMPORTANT NOTE

In our discussion of PAC Learning, we are only concerned with the problem of **binary classification**
Labelings & Shattering

**Def:** A hypothesis $h$ applied to some dataset $S$ generates a **labeling** of $S$.

**Def:** Let $\mathcal{H}[S]$ be the set of all (distinct) labelings of $S$ generated by hypotheses $h \in \mathcal{H}$. $\mathcal{H}$ **shatters** $S$ if $|\mathcal{H}[S]| = 2^{|S|}$

Equivalently, the hypotheses in $\mathcal{H}$ can generate every possible labeling of $S$. 
Labelings & Shattering

Whiteboard:

– Shattering example: binary classification
**VC-dimension**

*Def:* The **VC-dimension** (or Vaporik-Chervonenkis dimension) of $\mathcal{H}$ is the cardinality of the largest set $S$ such that $\mathcal{H}$ can shatter $S$.

**Special Case:** If $\mathcal{H}$ can shatter arbitrarily large finite sets, then the VC-dimension of $\mathcal{H}$ is infinity.

**Notation:** We write $\text{VC}(\mathcal{H}) = d$ to say the VC-Dimension of a hypothesis space $\mathcal{H}$ is $d$. 
**VC-dimension Proof**

*Proof Technique:* To prove that $\text{VC}(\mathcal{H}) = d$, there are two steps:

1. show that there exists a set of $d$ points that can be shattered by $\mathcal{H}$
   \[ \Rightarrow \text{VC}(\mathcal{H}) \geq d \]

2. show that there does NOT exist a set of $d + 1$ points that can be shattered by $\mathcal{H}$
   \[ \Rightarrow \text{VC}(\mathcal{H}) < d + 1 \]
VC-dimension

Whiteboard:

– VC-dimension Example: linear separators
– Proof sketch of VC-dimension for linear separators in 2D
∃ vs. ∀

VC-dimension

- Proving **VC-dimension** requires us to show that **there exists (∃)** a dataset of size $d$ that can be shattered and that **there does not exist (∀)** a dataset of size $d+1$ that can be shattered.

Shattering

- Proving that a particular dataset can be **shattered** requires us to show that **for all (∀)** labelings of the dataset, our hypothesis class contains a hypothesis that can correctly classify it.
VC-dimension Examples

- **Definition:** If $\text{VC}(H) = d$, then there exists ($\exists$) a dataset of size $d$ that can be shattered and that there does not exist ($\not\exists$) a dataset of size $d+1$ that can be shattered.

**Question:**
What is the VC-dimension of $H = \text{1D positive rays}$. That is for a threshold $w$, everything to the right of $w$ is labeled as +1, everything else is labeled -1.

**Answer:**
VC-dimension Examples

- **Definition**: If $\text{VC}(H) = d$, then there exists ($\exists$) a dataset of size $d$ that can be shattered and that there does not exist ($\nexists$) a dataset of size $d+1$ that can be shattered

**Question:**
What is the VC-dimension of $H = 1D$ positive intervals. That is for an interval $(w_1, w_2)$, everything inside the interval is labeled as $+1$, everything else is labeled $-1$.

**Answer:**
Sample Complexity Results

**Definition 0.1.** The sample complexity of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

**Four Cases we care about...**

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SLT-STYLE COROLLARIES
SLT-style Corollaries

**Thm. 1** \( N \geq \frac{1}{\epsilon} \left[ \log(|\mathcal{H}|) + \log\left(\frac{1}{\delta}\right) \right] \) labeled examples are sufficient so that with probability \((1 - \delta)\) all \( h \in \mathcal{H} \) with \( \hat{R}(h) = 0 \) have \( R(h) \leq \epsilon \).

**Corollary 1 (Realizable, Finite \(|\mathcal{H}|\)).** For some \( \delta > 0 \), with probability at least \((1 - \delta)\), for any \( h \) in \( \mathcal{H} \) consistent with the training data (i.e. \( \hat{R}(h) = 0 \)),

\[
R(h) \leq \frac{1}{N} \left[ \ln(|\mathcal{H}|) + \ln \left( \frac{1}{\delta} \right) \right]
\]

We can obtain similar corollaries for each of the theorems...
**SLT-style Corollaries**

**Corollary 1 (Realizable, Finite $|\mathcal{H}|$).** For some $\delta > 0$, with probability at least $(1 - \delta)$, for any $h$ in $\mathcal{H}$ consistent with the training data (i.e. $\hat{R}(h) = 0$),

$$R(h) \leq \frac{1}{N} \left[ \ln(|\mathcal{H}|) + \ln \left( \frac{1}{\delta} \right) \right]$$

**Corollary 2 (Agnostic, Finite $|\mathcal{H}|$).** For some $\delta > 0$, with probability at least $(1 - \delta)$, for all hypotheses $h$ in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + \sqrt{\frac{1}{2N} \left[ \ln(|\mathcal{H}|) + \ln \left( \frac{2}{\delta} \right) \right]}$$
Corollary 3 (Realizable, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1 - \delta)$, for any hypothesis $h$ in $\mathcal{H}$ consistent with the data (i.e. with $\hat{R}(h) = 0$),

$$R(h) \leq O \left( \frac{1}{N} \left[ \text{VC}(\mathcal{H}) \ln \left( \frac{N}{\text{VC}(\mathcal{H})} \right) + \ln \left( \frac{1}{\delta} \right) \right] \right)$$  (1)

Corollary 4 (Agnostic, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1 - \delta)$, for all hypotheses $h$ in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + O \left( \sqrt{\frac{1}{N} \left[ \text{VC}(\mathcal{H}) + \ln \left( \frac{1}{\delta} \right) \right]} \right)$$  (2)
Corollary 3 (Realizable, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1 - \delta)$, for any hypothesis $h$ in $\mathcal{H}$ consistent with the data (i.e. with $\hat{R}(h) = 0$),

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$$R(h) \leq \hat{R}(h) + O \left( \sqrt{\frac{1}{N} \left[ \text{VC}(\mathcal{H}) + \ln \left( \frac{1}{\delta} \right) \right]} \right) \quad (2)$$

Should these corollaries inform how we do model selection?
Q: Is Corollary 4 useful? A: Yes!

Key Point: we want to tradeoff between low training error and keeping $H$ simple (low VC-Dim)
Questions For Today

1. Given a classifier with zero training error, what can we say about generalization error? (Sample Complexity, Realizable Case)

2. Given a classifier with low training error, what can we say about generalization error? (Sample Complexity, Agnostic Case)

3. Is there a theoretical justification for regularization to avoid overfitting? (Structural Risk Minimization)
Learning Theory Objectives

You should be able to...

• Identify the properties of a learning setting and assumptions required to ensure low generalization error
• Distinguish true error, train error, test error
• Define PAC and explain what it means to be approximately correct and what occurs with high probability
• Apply sample complexity bounds to real-world learning examples
• Distinguish between a large sample and a finite sample analysis
• Theoretically motivate regularization
PROBABILITY
## Random Variables: Definitions

<table>
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<tr>
<th>Discrete Random Variable</th>
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<th>Random variable whose values come from a countable set (e.g. the natural numbers or {True, False})</th>
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<tr>
<td>Probability mass function (pmf)</td>
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<td>Function giving the probability that discrete r.v. $X$ takes value $x$.</td>
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$$p(x) := P(X = x)$$
# Random Variables: Definitions

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<th>Continuous Random Variable</th>
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<th>Random variable whose values come from an interval or collection of intervals (e.g. the real numbers or the range $(3, 5)$)</th>
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<td>Probability density function (pdf)</td>
<td>$f(x)$</td>
<td>Function the returns a nonnegative real indicating the relative likelihood that a continuous r.v. $X$ takes value $x$</td>
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- For any continuous random variable: $P(X = x) = 0$
- Non-zero probabilities are only available to intervals:

$$
P(a \leq X \leq b) = \int_{a}^{b} f(x) \, dx$$
Random Variables: Definitions

Cumulative distribution function

$F(x)$

Function that returns the probability that a random variable $X$ is less than or equal to $x$:

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

- For **discrete** random variables:

  $F(x) = P(X \leq x) = \sum_{x' < x} P(X = x') = \sum_{x' < x} p(x')$

- For **continuous** random variables:

  $F(x) = P(X \leq x) = \int_{-\infty}^{x} f(x') \, dx'$
Notational Shortcuts

A convenient shorthand:

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

⇒ For all values of \(a\) and \(b\):

\[ P(A = a|B = b) = \frac{P(A = a, B = b)}{P(B = b)} \]
Notational Shortcuts

But then how do we tell $P(E)$ apart from $P(X)$?

Instead of writing:

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

We should write:

\[ P_{A|B}(A|B) = \frac{P_{A,B}(A, B)}{P_B(B)} \]

...but only probability theory textbooks go to such lengths.
COMMON PROBABILITY DISTRIBUTIONS
Common Probability Distributions

• For Discrete Random Variables:
  – Bernoulli
  – Binomial
  – Multinomial
  – Categorical
  – Poisson

• For Continuous Random Variables:
  – Exponential
  – Gamma
  – Beta
  – Dirichlet
  – Laplace
  – Gaussian (1D)
  – Multivariate Gaussian
Common Probability Distributions

Beta Distribution

probability density function:

\[ f(\phi|\alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1 - x)^{\beta-1} \]
Common Probability Distributions

Dirichlet Distribution

The probability density function:

\[ f(\phi | \alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1 - x)^{\beta-1} \]
Common Probability Distributions

Dirichlet Distribution

Probability density function:

\[ p(\phi | \alpha) = \frac{1}{B(\alpha)} \prod_{k=1}^{K} \phi_k^{\alpha_k - 1} \]

where \( B(\alpha) = \frac{\prod_{k=1}^{K} \Gamma(\alpha_k)}{\Gamma(\sum_{k=1}^{K} \alpha_k)} \)
EXPECTATION AND VARIANCE
The **expected value** of $X$ is $E[X]$. Also called the mean.

- **Discrete random variables:**
  
  Suppose $X$ can take any value in the set $\mathcal{X}$.
  
  $$E[X] = \sum_{x \in \mathcal{X}} xp(x)$$

- **Continuous random variables:**
  
  $$E[X] = \int_{-\infty}^{+\infty} xf(x)dx$$
The variance of $X$ is $Var(X)$.

$$Var(X) = E[(X - E[X])^2]$$

- **Discrete random variables:**
  $$Var(X) = \sum_{x \in \mathcal{X}} (x - \mu)^2 p(x)$$

- **Continuous random variables:**
  $$Var(X) = \int_{-\infty}^{+\infty} (x - \mu)^2 f(x) \, dx$$

$\mu = E[X]$
Joint probability
Marginal probability
Conditional probability

MULTIPLE RANDOM VARIABLES
Joint Probability

- Key concept: two or more random variables may interact. Thus, the probability of one taking on a certain value depends on which value(s) the others are taking.

- We call this a joint ensemble and write

\[ p(x, y) = \text{prob}(X = x \text{ and } Y = y) \]
Marginal Probabilities

- We can "sum out" part of a joint distribution to get the marginal distribution of a subset of variables:

\[ p(x) = \sum_y p(x, y) \]

- This is like adding slices of the table together.

- Another equivalent definition: \( p(x) = \sum_y p(x|y)p(y) \).

Slide from Sam Roweis (MLSS, 2005)
Conditional Probability

- If we know that some event has occurred, it changes our belief about the probability of other events.
- This is like taking a ”slice” through the joint table.

\[ p(x|y) = \frac{p(x, y)}{p(y)} \]
Independence and Conditional Independence

- Two variables are independent iff their joint factors:

\[ p(x, y) = p(x)p(y) \]

- Two variables are conditionally independent given a third one if for all values of the conditioning variable, the resulting slice factors:

\[ p(x, y|z) = p(x|z)p(y|z) \quad \forall z \]
MAXIMUM LIKELIHOOD ESTIMATION (MLE)
Likelihood Function

• 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) \( p(x|\theta) \)
    
    \[
    L(\theta) = p(x^{(1)}|\theta) \cdot p(x^{(2)}|\theta) \cdots p(x^{(N)}|\theta)
    \]
  
  – **Case 2**: \( X \) is **continuous** with probability density function (pdf) \( f(x|\theta) \)
    
    \[
    L(\theta) = f(x^{(1)}|\theta) \cdot f(x^{(2)}|\theta) \cdots f(x^{(N)}|\theta)
    \]

• 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) \( f(x|\theta) \)
    
    \[
    \ell(\theta) = \log f(x^{(1)}|\theta) + \ldots + \log f(x^{(N)}|\theta)
    \]

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

- 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 $p(y | x, \theta)$
    \[
    L(\theta) = p(y^{(1)} | x^{(1)}, \theta) \ldots p(y^{(N)} | x^{(N)}, \theta)
    \]
  - **Case 2**: $Y$ is continuous with pdf $f(y | x, \theta)$
    \[
    L(\theta) = f(y^{(1)} | x^{(1)}, \theta) \ldots f(y^{(N)} | x^{(N)}, \theta)
    \]

- 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

- 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 $p(x|y,\alpha)$
    \[
    L(\alpha, \beta) = p(x^{(1)}| y^{(1)}, \alpha) f(y^{(1)}|\beta) \ldots p(x^{(N)}| y^{(N)}, \alpha) f(y^{(N)}|\beta)
    \]
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.

$$\theta^{MLE} = \arg \max_{\theta} \prod_{i=1}^{N} p(x^{(i)}|\theta)$$

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 \textbf{as much} probability mass \textbf{as possible} to the things we have observed...

... \textbf{at the expense} of the things we have \textbf{not} observed
Recipe for Closed-form MLE

1. Assume data was generated iid from some model, i.e., write the generative story
   \[ x^{(i)} \sim p(x|\theta) \]

2. Write the log-likelihood
   \[ \ell(\theta) = \log p(x^{(1)}|\theta) + \ldots + \log p(x^{(N)}|\theta) \]

3. Compute partial derivatives, i.e., the gradient
   \[ \frac{\partial \ell(\theta)}{\partial \theta_1} = \ldots \]
   \[ \ldots \]
   \[ \frac{\partial \ell(\theta)}{\partial \theta_M} = \ldots \]

4. Set derivatives equal to zero and solve for \( \theta \)
   \[ \frac{\partial \ell(\theta)}{\partial \theta_m} = 0 \text{ for all } m \in \{1, \ldots, M\} \]
   \( \theta^{MLE} = \text{solution to system of } M \text{ equations and } M \text{ variables} \)

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

Whiteboard

– Example: MLE of Exponential Distribution
In-Class Exercise
Show that the MLE of parameter $\phi$ for $N$ samples drawn from $\text{Bernoulli}(\phi)$ 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. $\phi$
3. Set derivative to zero and solve for $\phi$
MLE

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

What is the log-likelihood of the data $l(\phi)$?

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

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. $l(\phi) = \text{the most likely answer}$
MLE

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

What is the **derivative** of the log-likelihood \( \partial \ell(\theta)/\partial \theta \)?

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

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

Answer:
A. \( \partial \ell(\theta)/\partial \theta = \phi^{N_1} - (1 - \phi)^{N_0} \)
B. \( \partial \ell(\theta)/\partial \theta = \phi / N_1 - (1 - \phi) / N_0 \)
C. \( \partial \ell(\theta)/\partial \theta = N_1 / \phi - N_0 / (1 - \phi) \)
D. \( \partial \ell(\theta)/\partial \theta = \log(\phi) / N_1 - \log(1 - \phi) / N_0 \)
E. \( \partial \ell(\theta)/\partial \theta = N_1 / \log(\phi) - N_0 / \log(1 - \phi) \)
F. \( \partial \ell(\theta)/\partial \theta = \) the derivative of the most likely answer
Learning from Data (Frequentist)

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.

$$\theta^{\text{MLE}} = \arg\max_{\theta} p(\mathcal{D}|\theta) = \arg\max_{\theta} \prod_{i=1}^N p(x^{(i)}|\theta)$$

Maximum Likelihood Estimate (MLE)

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

$$\theta^{\text{MAP}} = \arg\max_{\theta} p(\theta|\mathcal{D}) = \arg\max_{\theta} f(\theta) \prod_{i=1}^N p(x^{(i)}|\theta)$$

Maximum a posteriori (MAP) estimate
MLE vs. MAP

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

**Principle of Maximum Likelihood Estimation (MLE):**
Choose the parameters that maximize the likelihood of the data.

\[
\theta^{\text{MLE}} = \arg\max_{\theta} p(D|\theta)
\]

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

\[
\theta^{\text{MAP}} = \arg\max_{\theta} p(\theta|D) = \arg\max_{\theta} f(\theta) \prod_{i=1}^{N} p(x^{(i)}|\theta)
\]

Important!
Usually the parameters are **continuous**, so the prior is a probability **density** function.
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
   \[ x^{(i)} \sim p(x|\theta) \]

2. Write the log-likelihood
   \[ \ell(\theta) = \log p(x^{(1)}|\theta) + \ldots + \log p(x^{(N)}|\theta) \]

3. Compute partial derivatives, i.e., the gradient
   \[ \frac{\partial \ell(\theta)}{\partial \theta_1} = \ldots \]
   \[ \ldots \]
   \[ \frac{\partial \ell(\theta)}{\partial \theta_M} = \ldots \]

4. Set derivatives equal to zero and solve for \( \theta \)
   \[ \frac{\partial \ell(\theta)}{\partial \theta_m} = 0 \text{ for all } m \in \{1, \ldots, M\} \]
   \[ \theta^{\text{MLE}} = \text{solution to system of } M \text{ equations and } M \text{ variables} \]

5. Compute the second derivative and check that \( \ell(\theta) \) is concave down at \( \theta^{\text{MLE}} \)
Recipe for Closed-form MAP

1. Assume data was generated iid from some model, i.e., write the generative story
   \[ \theta \sim p(\theta) \] and then for all \( i \): \( x^{(i)} \sim p(x|\theta) \)

2. Write the log posterior
   \[ \ell_{\text{MAP}}(\theta) = \log p(\theta) + \log p(x^{(1)}|\theta) + \ldots + \log p(x^{(N)}|\theta) \]

3. Compute partial derivatives, i.e., the gradient
   \[ \frac{\partial \ell_{\text{MAP}}(\theta)}{\partial \theta_1} = \ldots \]
   \[ \frac{\partial \ell_{\text{MAP}}(\theta)}{\partial \theta_M} = \ldots \]

4. Set derivatives to equal zero and solve for \( \theta \)
   \[ \frac{\partial \ell_{\text{MAP}}(\theta)}{\partial \theta_m} = 0 \text{ for all } m \in \{1, \ldots, M\} \]
   \[ \theta_{\text{MAP}} = \text{solution to system of } M \text{ equations and } M \text{ variables} \]

5. Compute the second derivative and check that \( \ell(\theta) \) is concave down at \( \theta_{\text{MAP}} \)
Learning from Data (Bayesian)

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