# UVA CS 4774: Machine Learning

# Lecture 10: Maximum Likelihood Estimation (MLE)

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## Machine Learning in a Nutshell



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### **Probability Review**

- The big picture
- Events and Event spaces
- Random variables
- Joint probability, Marginalization, conditioning, chain rule, Bayes Rule, law of total probability, etc.
- Structural properties, e.g., Independence, conditional independence
- Maximum Likelihood Estimation

### Sample space and Events

- O : Sample Space,
  - set of all outcomes
  - If you toss a coin twice O = {HH,HT,TH,TT}
- Event: a subset of O
  - First toss is head = {HH,HT}
- S: event space, a set of events:
  - Contains the empty event and O

### From Events to Random Variable

- Concise way of specifying attributes of outcomes
- Modeling students (Grade and Intelligence):
  - O = all possible students (sample space)
  - What are events (subset of sample space)
    - Grade\_A = all students with grade A
    - HardWorking\_Yes = ... who works hard
  - Very cumbersome
  - Need "functions" that maps from O to an attribute space T.
  - P(H = YES) = P({student ε O : H(student) = YES})

If hard to directly estimate from data, most likely we can estimate

P(x, Y)

- 1. Joint probability
  - Use Chain Rule
- •2. Marginal probability
  - Use the total law of probability
- 3. Conditional probability
  - Use the Bayes Rule

p (Y(X)

P(X)

# If hard to directly estimate from data, most likely we can estimate

- 1. Joint probability
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- 2. Marginal probability
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$$\varphi(A, B) = \varphi(B) \varphi(A|B)$$

P(B) = P(B, A) + P(B, ~A) $H''_{P(B, A \cup ~A)} //$ 

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

### Simplify Notation: To Calculate Conditional Probability

• Bayes Rule  
$$P(x | y) = \frac{P(x)P(y | x)}{P(y)}$$

• You can condition on more variables

$$P(x \mid y, z) = \frac{P(x \mid z)P(y \mid x, z)}{P(y \mid z)}$$

### One Example: Joint

Assume we have a dark box with 3 red balls and 1 blue ball. That is, we have the set {r,r,r,b}. What is the probability of drawing 2 red balls in the first 2 tries?

 $P(B_1 = r, B_2 = r) =$ 

### **One Example: Joint**

Assume we have a dark box with 3 red balls and 1 blue ball. That is, we have the set {r,r,r,b}. What is the probability of drawing 2 red balls in the first 2 tries?

$$P(B_{1}=r,B_{2}=r) = P(B_{1}-r) P(B_{2}-r | B_{1}=r)$$

$$P(B_{1}-r) = \frac{3}{4}$$

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$$P(B_{1}-r) = \frac{1}{4}$$

$$P(B_{1}-r) = \frac{1}{4}$$

Adapt from Prof. Nando de Freitas's review slides

1

### One Example: Joint

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$$P(B_1 = r, B_2 = r) = P(B_1 = r) P(B_2 = r | B_1 = r)$$

$$= \frac{3}{4} \times \frac{2}{3} = \frac{1}{2}$$

Adapt from Prof. Nando de Freitas's review slides

5

### **One Example: Marginal**

What is the probability that the 2<sup>nd</sup> ball drawn from the set {r,r,r,b} will be red?

Using marginalization,  $P(B_2 = r) = P(B_2 = r, B_1 = r) + P(B_2 = r, B_1 = b)$ 

### **One Example: Marginal**

What is the probability that the 2<sup>nd</sup> ball drawn from the set {r,r,r,b} will be red?

Using marginalization,  $P(B_2 = r) = P(B_2 = r \land B_1 = r)$ +  $P(B_2 = r \land B_1 = b)$ =  $P(B_1 = r)P(B_2 = r \mid B_1 = r) + P(B_1 = b)P(B_2 = r \mid B_1 = b)$ =  $\frac{3}{4} \times \frac{2}{3} + \frac{1}{4} \times 1$ 

One Example: Conditional  

$$P(B_{1} = Y | B_{2} = Y)$$

$$= \underbrace{P(B_{2} = Y | B_{1} = Y) P(B_{1} = Y) P(B_{1} = Y) P(B_{1} = Y) P(B_{2} = Y)}_{P(B_{2} = Y | B_{1} = Y) P(B_{1} = Y)} P(B_{1} = Y)$$

$$= \underbrace{P(B_{2} = Y | B_{1} = Y) P(B_{1} = Y)}_{P(B_{2} = Y, B_{1} = Y) + P(B_{2} = Y, B_{1} = b)}$$

# One Example

Assume we have a dark box with 3 red balls and 1 blue ball. That is, we have the set {r,r,r,b}. What is the probability of drawing 2 red balls in the first 2 tries?

$$P(B_{1} = r, B_{2} = r) = \frac{P(B_{1} = r) P(B_{2} = r | B_{1} = r)}{\frac{3}{4} r \frac{2}{3}}$$

$$P(B_{2} = r) = P(B_{1} = r, B_{2} = r) + P(B_{1} = b, B_{2} = r)$$

$$P(B_{1} = r | B_{2} = r) = \frac{P(B_{1} = r, B_{2} = r)}{P(B_{2} = r)}$$

### Today : MLE

- The big picture
- Events and Event spaces
- Random variables
- Joint probability, Marginalization, conditioning, chain rule, Bayes Rule, law of total probability, etc.
- Structural properties, e.g., Independence, conditional independence
- Maximum Likelihood Estimation

### Roadmap

#### Basic MLE

- □ MLE for Discrete RV
- □ MLE for Continuous RV (Gaussian)
- □ MLE connects to Normal Equation of LR
- □ More about Mean and Variance

# Maximum Likelihood Estimation Z: {H,T}->{Z1,Z2...,Zn}

A general Statement

P(Z): {7, 1-p] Consider a sample set  $T=(Z_1...Z_n)$  which is drawn from a probability distribution P(Z|\theta) where \theta are parameters.

If the Zs are independent with probability density function  $P(Z_i|\theta)$ , the joint probability of the whole set is

$$\boldsymbol{\theta} = \operatorname{Org}(Z_1, \dots, Z_n | \boldsymbol{\theta}) = \prod_{i=1}^n P(Z_i | \boldsymbol{\theta})$$

this may be maximised with respect to \theta to give the maximum likelihood estimates.

HHTT.H

 $\checkmark$  assume a particular model with unknown parameters,  $\theta$ 

✓ assume a particular model with unknown parameters, θ
 ✓ we can then define the probability of observing a given event conditional on a particular set of parameters. P(Z<sub>i</sub>|θ)

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- ✓ we can then define the probability of observing a given event conditional on a particular set of parameters.  $P(Z_i | \theta)$
- $\checkmark$  We have observed a set of outcomes in the real world.

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- $\checkmark$  we can then define the probability of observing a given event conditional on a particular set of parameters.  $P(Z_i|\theta)$
- ✓ We have observed a set of outcomes in the real world.
   ✓ It is then possible to choose a set of parameters which are most likely to have produced the observed results.

 $\checkmark$  assume a particular model with unknown parameters,  $\varTheta$ 

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- ✓ We have observed a set of outcomes in the real world.
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$$\hat{\theta} = \operatorname{argmax}_{\theta} P(Z_1 \dots Z_n | \theta) = \prod_{i \neq 1} P(2_i | \theta)$$

This is maximum likelihood.

In most cases it is both consistent and efficient.

$$\Theta = \operatorname{Minix}_{\Theta} \log(L(\theta)) = \sum_{i=1}^{n} \log(P(Z_i | \theta))$$

It is often convenient to work with the Log of the likelihood function.

- $\checkmark$  assume a particular model with unknown parameters,  $\varTheta$
- ✓ we can then define the probability of observing a given event conditional on a particular set of parameters.  $P(Z_i | \theta)$
- ✓ We have observed a set of outcomes in the real world.
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This is maximum likelihood.

In most cases this scorer is both consistent and efficient.

$$log(L(\theta)) = \sum_{i=1}^{n} log(P(Z_i | \theta))$$
 Log-Likelihood

It is often convenient to work with the Log of the likelihood function.

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### Roadmap

Basic MLE

 $\hfill\square$  MLE for Discrete RV

□ MLE for Continuous RV (Gaussian)

 $\hfill\square$  MLE connects to Normal Equation of LR

□ More about Mean and Variance

## Review: Bernoulli Distribution e.g. Coin Flips

Bernolli(P)

- You flip a coin
  - Z: {Who is Up: Head or Tail} is a discrete Random Variable

qH,T

- Head with probability p
- Binary random variable
- Bernoulli trial with success probability p

### Review: Bernoulli Distribution e.g. Coin Flips

- You flip *n* coins
  - Head with probability p (UNKNOWN, Need to estimate from data)
  - Number of heads X out of n trial
  - Each Trial following Bernoulli distribution with parameters p

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} P(Z_1 \dots Z_n | \theta)$$

### **Review:** Defining Likelihood for basic Bernoulli

Given: 
$$\{z_1, z_2, \dots, z_n\}$$
  
 $\{H, H, T, \dots H\}_n$   
 $\{H, H, T, \dots H\}_n$   
 $\{H, H, T, \dots H\}_n$   
 $\{I, I, 0, \dots, I\}_n$   
 $\{i, j, 0, \dots, I\}_n$   
 $\{z_i \mid \underline{\Theta}\} = p^{Z_i}(I-p)^{I-Z_i}$   
 $\{F(Z_i \mid \underline{\Theta}) = p^{Z_i}(I-p)$ 

### Deriving the Maximum Likelihood Estimate for Bernoulli

$$\log(L(p)) = \log\left[\prod_{i=1}^{n} p^{z_i} (1-p)^{1-z_i}\right]$$

$$= \sum_{i=1}^{n} (z_i \log p + (1 - z_i) \log(1 - p))$$

 $= \log p \sum_{i=1}^{n} z_i + \log (1-p) \sum_{i=1}^{n} (1-z_i)$ 

$$= x \log p + (n - x) \log (1 - p)$$

Observed data  $\rightarrow$  x heads-up from n trials

### Deriving the Maximum Likelihood Estimate for Bernoulli

#### maximize

$$\int L(p) = p^{x} (1-p)^{n-x}$$

$$\int \log(L(p)) = \log\left[p^{x}(1-p)^{n-x}\right]$$

Minimize the negative log-likelihood  

$$-l(p) = -\log \left[ p^{x} (1-p)^{n-x} \right]$$



### Deriving the Maximum Likelihood Estimate for Bernoulli

$$l(p) = \operatorname{argmin}_{p} \left\{ -x \log(p) - (n-x) \log(1-p) \right\}$$

$$\frac{dl(p)}{dp} = -\frac{x}{p} - \frac{-(n-x)}{1-p} \succeq 0$$

$$0 = -x + pn$$

$$0 = -\frac{x}{p} + \frac{n-x}{1-p}$$

$$0 = \frac{-x(1-p) + p(n-x)}{p(1-p)}$$

$$0 = -x + px + pn - px$$

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Minimize the negative log-likelihood

→ MLE parameter estimation

$$\hat{p} = \frac{x}{n}$$

i.e. Relative frequency of a binary event

# EXTRA

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### **Discrete** Random Variables

- Random variables (RVs) which may take on only a countable number of distinct values
  - E.g. Z as the total number of heads you get if you flip 100 coins
- Z is a RV with arity k if it can take on exactly one value out of a set size k
  - E.g. the possible values that Z can take on are 0, 1, 2,..., 100

### e.g. Coin Flips cont.

- You flip a coin
  - Z: {Who is Up: Head or Tail} is a discrete RV
  - Head with probability p
  - Binary random variable
  - Bernoulli trial with success probability p
- You flip *a* coin for *k* times
  - How many heads would you expect
  - Number of heads Z is also a discrete random variable
  - Binomial distribution with parameters k and p



### Roadmap - All the rest are EXTRA

#### Basic MLE

- □ MLE for Discrete RV
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### Review: Continuous Random Variables

- Probability density function (pdf) instead of probability mass function (pmf)
  - For discrete RV: Probability mass function (pmf):  $P(X = x_i)$
- A pdf (prob. Density func.) is any function f(x) that describes the probability density in terms of the input variable x.

### Review: Probability of Continuous RV

• Properties of pdf

$$f(x) \ge 0, \forall x$$

$$\int_{-\infty}^{+\infty} f(x) = 1 \qquad \longrightarrow \qquad \sum_{i=1}^{k} P(x = x_i) = 1$$

• Actual probability can be obtained by taking the integral of pdf

• E.g. the probability of X being between 5 and 6 is

$$P(5 \le X \le 6) = \int_{5}^{6} f(x) dx$$

#### Review: Mean and Variance of RV

- Mean (Expectation):
  - Discrete RVs:

$$\mu = E(\mathbf{X})$$
$$E(\mathbf{X}) = \sum_{v_i} v_i P(\mathbf{X} = v_i)$$
$$E(g(\mathbf{X})) = \sum_{v_i} g(v_i) P(\mathbf{X} = v_i)$$

• Continuous RVs:

$$E(X) = \int_{-\infty}^{+\infty} xf(x) dx$$
$$E(g(X)) = \int_{-\infty}^{+\infty} g(x)f(x) dx$$

 $-\infty$ 

Adapt From Carols' prob tutorial

### Review: Mean and Variance of RV

- •Variance:  $Var(X) = E((X \mu)^2)$   $\mathcal{O}_X = \sqrt{\sqrt{X}}$ 
  - Discrete RVs:

$$V(\mathbf{X}) = \sum_{v_i} (v_i - \mu)^2 \mathbf{P}(\mathbf{X} = v_i)$$

• Continuous RVs:

Adapt From Carols' prob tutorial

# Single-Variate Gaussian Distribution



Courtesy: http://research.microsoft.com/~cmbishop/PRML/index.htm

# **Bi-Variate Gaussian Distribution**



• The covariance matrix captures linear dependencies among the variables

Courtesy: http://research.microsoft.com/~cmbishop/PRML/index.htm

# Multivariate Normal (Gaussian) PDFs

The only widely used continuous joint PDF is the multivariate normal (or Gaussian):



• The covariance matrix captures linear dependencies among the variables

Example: the Bivariate Normal distribution

$$f(x_1, x_2) = \frac{1}{(2\pi) |\Sigma|^{1/2}} e^{-\frac{1}{2} (\vec{x} - \vec{\mu})^T \Sigma^{-1} (\vec{x} - \vec{\mu})}$$



# Surface Plots of the bivariate Normal distribution



### Contour Plots of the bivariate Normal distribution



Scatter Plots of data from the bivariate Normal distribution



#### Trivariate Normal distribution



### How to Estimate 1D Gaussian: MLE



• In the 1D Gaussian case, we simply set the mean and the variance to the sample mean and the sample variance:





How to Estimate p-D Gaussian: MLE  $\{1, 2, ..., \}$  $< X_1, X_2, \cdots, X_p > \sim N(\vec{\mu}, \Sigma)$ Sam NIP Jarl

### Today

#### Basic MLE

□ MLE for Discrete RV

□ MLE for Continuous RV (Gaussian)

 $\hfill\square$  MLE connects to Normal Equation of LR

More about Mean and Variance

# **DETOUR:** Probabilistic Interpretation of Linear Regression



• Let us assume that the target variable and the inputs are related by the equation:

$$y_i = \boldsymbol{\theta}^T \mathbf{x}_i + \boldsymbol{\varepsilon}_i$$

where  $\boldsymbol{\varepsilon}$  is an error term of unmodeled effects or random noise

# **DETOUR:** Probabilistic Interpretation of Linear Regression



where  $\varepsilon$  is an error term of unmodeled effects or random noise  $\frac{2}{2}$ 

• Now assume that  $\varepsilon$  follows a Gaussian N(0, $\sigma$ ), then we have:

$$p(y_i | x_i; \theta) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{(y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$
  
RV  $y | x_i; \theta \sim N(\theta^T x, \theta)$ 

# **DETOUR:** Probabilistic Interpretation of Linear Regression



• By IID (independent and identically distributed) assumption, we have data likelihood

$$L(\theta) = \prod_{i=1}^{n} p(y_i | x_i; \theta) = \left(\frac{1}{\sqrt{2\pi\sigma}}\right)^n \exp\left(-\frac{\sum_{i=1}^{n} (y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

$$l(\theta) = \log(L(\theta)) = n \log \frac{1}{\sqrt{2\pi\sigma}} - \frac{1}{\sigma^2} \frac{1}{2} \sum_{i=1}^n (y_i - \theta^T \mathbf{x}_i)^2$$

$$L(\theta) = \prod_{i=1}^{n} p(y_i | x_i; \theta) = \left(\frac{1}{\sqrt{2\pi\sigma}}\right)^n \exp\left(-\frac{\sum_{i=1}^{n} (y_i - \theta^T \mathbf{x}_i)^2}{2\sigma^2}\right)$$

We can learn \theta by maximizing the probability / likelihood of generating the observed samples:

 $\left(\vec{x}_1, \mathcal{Y}_1\right) \wedge \left(\vec{x}_2, \mathcal{Y}_2\right) \wedge \cdots \quad \left(\vec{x}_N, \mathcal{Y}_N\right)$  $\frac{N}{TT} p(Y_i, \vec{x}_i) = \frac{N}{TT} p(Y_i, \vec{x}_i)$ =  $argmax \frac{N}{11} p(Y_i | X_{i_i}, \theta)$ 

Thus under independence Gaussian residual assumption, residual square error is equivalent to MLE of  $\theta$  !

$$y|_{X;\Theta} \sim N(\Theta^{T}X, G)$$
  
 $Two Un known$   
 $panmeters: {\Theta, of}$ 

$$l(\theta) = \log(L(\theta)) = n \log \frac{1}{\sqrt{2\pi\sigma}} - \frac{1}{\sigma^2} \frac{1}{2} \sum_{i=1}^n (y_i - \theta^T \mathbf{x}_i)^2$$

$$argmax \ l(\theta) \Rightarrow$$

$$argmin \ \mathcal{J}(\theta)$$

$$1 n$$

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

 $y_i \sim N(exp(wx_i), 1)$ 

- (b) (6 points) (no explanation required) Suppose you decide to do a maximum likelihood estimation of w. You do the math and figure out that you need w to satisfy one of the following equations. Which one?
  - A.  $\Sigma_i x_i exp(wx_i) = \Sigma_i x_i y_i exp(wx_i)$ B.  $\Sigma_i x_i exp(2wx_i) = \Sigma_i x_i y_i exp(wx_i)$ C.  $\Sigma_i x_i^2 exp(wx_i) = \Sigma_i x_i y_i exp(wx_i)$ D.  $\Sigma_i x_i^2 exp(wx_i) = \Sigma_i x_i y_i exp(wx_i/2)$ E.  $\Sigma_i exp(wx_i) = \Sigma_i y_i exp(wx_i)$

Answer: B (this is an extra credit question.)

 $\left( 0 \right)$ (0) $\frac{\partial(L(\theta))}{\partial \theta} = 0 \implies (B)$ 

 $M_{i} \sim N(exp(wxi), l)$ 

### Today

#### Basic MLE

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Extra: about Mean and Variance

### Mean and Variance

• Correlation:

$$\rho(X,Y) = Cov(X,Y) / \sigma_x \sigma_y$$
$$-1 \le \rho(X,Y) \le 1$$

### Properties

• Mean 
$$E(X+Y) = E(X) + E(Y)$$
  
 $E(aX) = aE(X)$ 

• If X and Y are independent,

$$E(\mathbf{X}\mathbf{Y}) = E(\mathbf{X}) \cdot E(\mathbf{Y})$$

• Variance 
$$V(aX+b) = a^2 V(X)$$

If X and Y are independent,

V(X+Y) = V(X) + V(Y)

### Some more properties

• The conditional expectation of Y given X when the value of X = x is:

$$E(Y | X = x) = \int y^* p(y | x) dy$$

• The Law of Total Expectation or Law of Iterated Expectation:

$$E(Y) = E[E(Y|X)] = \int E(Y|X=x)p_X(x)dx$$

### Some more properties

• The law of Total Variance:

$$Var(Y) = Var[E(Y | X)] + E[Var(Y | X)]$$



Prof. Andrew Moore's review tutorial
 Prof. Nando de Freitas's review slides
 Prof. Carlos Guestrin recitation slides