photo: Chessex Borealis[™] Aquerple Polyhedral

BBN406 Fundamentals of Machine Learning

Lecture 7: Probability Review (cont'd.) Maximum Likelihood Estimation (MLE)



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Administrative

- Project proposal due November 15
- A half page description
 - problem to be investigated,
 - why it is interesting,
 - what data you will use,
 - related work.

Deadlines in the sylpus are closer than they appear

P. ...

Today

- Probabilities
 - Dependence, Independence, Conditional Independence
- Parameter estimation
 - Maximum Likelihood Estimation (MLE)
 - Maximum a Posteriori (MAP)

Last time... Sample space

Def: A **sample space** Ω is the set of all possible outcomes of a (conceptual or physical) random experiment. (Ω can be finite or infinite.)

Examples:

- Ω may be the set of all possible outcomes of a dice roll (1,2,3,4,5,6)
- Pages of a book opened randomly. (1-157)
- Real numbers for temperature, location, time, etc

Last time... Events

We will ask the question: What is the probability of a particular event?

Def: Event A is a **subset** of the sample space Ω

Examples:

What is the probability of

- the book is open at an odd number
- rolling a dice the number <4
- a random person's height X : a<X<b

Last time... Probability

Def: *Probability P(A), the probability that event* (*subset) A happens*, is a function that maps the event A onto the interval [0, 1]. *P(A)* is also called the **probability measure** of A.



What is the probability that the number on the dice is 2 or 4?

P(A) is the volume of the area.

Last time... Kolmogorov Axioms

(i) Nonnegativity: $P(A) \ge 0$ for each A event.

(ii) $P(\Omega) = 1$.

(iii) σ -additivity: For disjoint sets (events) A_i , we have

 $P(\bigcup_{i=1}^{\infty}A_i) = \sum_{i=1}^{\infty}P(A_i)$

Consequences:

$$P(\emptyset) = 0.$$

$$P(A \cup B) = P(A) + P(B) - P(A \cap B).$$

$$P(A^c) = 1 - P(A).$$

Last time... Venn Diagram



Last time... Random Variables

Def: Real valued **random variable** is a function of the outcome of a randomized experiment $X: \Omega \to \mathbb{R}$

$$P(a < X < b) \doteq P(\omega : a < X(\omega) < b)$$
$$P(X = a) \doteq P(\omega : X(\omega) = a)$$

Examples:

- Discrete random variable examples (Ω is discrete):
- $X(\omega) = True if a randomly drawn person (\omega) from our class (\Omega) is female$
- $X(\omega) =$ The hometown $X(\omega)$ of a randomly drawn person (ω) from our class (Ω)

Bernoulli distribution: Ber(p)

 $\Omega = \{\text{head, tail}\} X(\text{head}) = 1, X(\text{tail}) = 0.$



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Binomial distribution: Bin(n,p)

Suppose a coin with head prob. *p* is tossed *n* times. What is the probability of getting *k* heads and *n*-*k* tails?

- $\Omega = \{ \text{ possible } n \text{ long head/tail series} \}, |\Omega| = 2^n$
- $K(\omega) =$ number of heads in $\omega = (\omega_1, \dots, \omega_n) \in \{\text{head, tail}\}^n = \Omega$

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$$P(K=k) = P(\omega : K(\omega) = k) = \sum_{\omega : K(\omega) = k} p^k (1-p)^{n-k} = \binom{n}{k} p^k (1-p)^{n-k}$$

Last time... Conditional Probability

P(X|Y) = Fraction of worlds in which X event is true given Y event is true.

$$P(X|Y) = \frac{P(X,Y)}{P(Y)}$$

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Independence

Independent random variables: P(X,Y) = P(X)P(Y)P(X|Y) = P(X)

Y and X don't contain information about each other. Observing Y doesn't help predicting X. Observing X doesn't help predicting Y.

Examples:

Independent: Winning on roulette this week and next week. Dependent: Russian roulette

Dependent / Independent



Conditionally Independent

Conditionally independent:

P(X, Y|Z) = P(X|Z)P(Y|Z)Knowing Z makes X and Y independent

Examples:

Dependent: shoe size of children and reading skills Conditionally independent: shoe size of children and reading skills given age

Stork deliver babies: Highly statistically significant correlation exists between stork populations and

Conditionally Independent

 London taxi drivers: A survey has pointed out a positive and significant correlation between the number of accidents and wearing coats. They concluded that coats could hinder movements of drivers and be the cause of accidents. A new law was prepared to prohibit drivers from wearing coats when driving.

Finally, another study pointed out that people wear coats when it rains...

Correlation *≠* Causation

Number people who drowned by falling into a swimming-pool correlates with Number of films Nicolas Cage appeared in



Correlation: 0.666004

Conditional Independence

Formally: X is conditionally independent of Y given Z

$$P(X, Y|Z) = P(X|Z)P(Y|Z)$$

P(Accidents, Coats | Rain) = P(Accidents | Rain)P(Coats | Rain)

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Equivalent to: $(\forall x, y, z)P(X = x | Y = y, Z = z) = P(X = x | Z = z)$

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$$P(X, Y|Z) = P(X|Z)P(Y|Z)$$

P(Accidents, Coats | Rain) = P(Accidents | Rain)P(Coats | Rain)

$$(\forall x, y, z) P(X = x | Y = y, Z = z) = P(X = x | Z = z)$$

P(Thunder|Rain, Lightning) = P(Thunder|Lightning)

Note: does NOT mean Thunder is independent of Rain **But** given Lightning knowing Rain doesn't give more info about Thunder

Equivalent to:

Parameter estimation: MLE, MAP



I have a coin, if I flip it, what's the probability that it will fall with the head up?

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Let us flip it a few times to estimate the probability:

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The estimated probability is: 3/5 "Frequency of heads"



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Questions:(1) Why frequency of heads???(2) How good is this estimation???(3) Why is this a machine learning problem???

We are going to answer these questions

Question (1)

Why frequency of heads???

- Frequency of heads is exactly the maximum likelihood estimator for this problem
- MLE has nice properties (interpretation, statistical guarantees, simple)



$P(Heads) = \theta, P(Tails) = 1 - \theta$



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Flips are i.i.d.:



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- Independent events
 - Identically distributed according to Bernoulli distribution



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$$\widehat{ heta}_{MLE} = rg\max_{ heta} P(D| heta)$$

MLE: Choose θ that maximizes the probability of observed data

$$\widehat{\theta}_{MLE} = \arg \max_{\theta} P(D|\theta)$$
$$= \arg \max_{\theta} \prod_{i=1}^{n} P(X_i|\theta)$$

independent draws

$$\begin{split} \widehat{\theta}_{MLE} &= \arg \max_{\theta} P(D|\theta) \\ &= \arg \max_{\theta} \prod_{i=1}^{n} P(X_i|\theta) & \text{independent draws} \\ &= \arg \max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta) & \text{identically} \\ &\text{distributed} \end{split}$$

$$\begin{aligned} \widehat{\theta}_{MLE} &= \arg \max_{\theta} P(D|\theta) \\ &= \arg \max_{\theta} \prod_{i=1}^{n} P(X_i|\theta) & \text{independent draws} \\ &= \arg \max_{\theta} \prod_{i:X_i=H} \theta \prod_{i:X_i=T} (1-\theta) & \text{identically} \\ &= \arg \max_{\theta} \theta^{\alpha_H} (1-\theta)^{\alpha_T} \end{aligned}$$

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$$\begin{aligned} \widehat{\theta}_{MLE} &= \arg \max_{\theta} P(D|\theta) \\ &= \arg \max_{\theta} \theta^{\alpha_H} (1 - \theta)^{\alpha_T} \\ &= \arg \max_{\theta} \theta^{\alpha_H} (1 - \theta)^{\alpha_T} \\ &\int J(\theta|\theta) \end{aligned}$$

MLE: Choose θ that maximizes the probability of observed data

$$\begin{aligned} \widehat{\theta}_{MLE} &= \arg \max_{\theta} P(D|\theta) \\ &= \arg \max_{\theta} \theta^{\alpha_H} (\underbrace{1 - \theta}_{\theta})^{\alpha_T} \\ &= \arg \max_{\theta} \theta^{\alpha_H} (\underbrace{1 - \theta}_{\theta})^{\alpha_T} \\ &J(\boldsymbol{\theta}) \end{aligned}$$

. . .

$$\frac{\partial J(\theta)}{\partial \theta} = \alpha_H \theta^{\alpha_H - 1} (1 - \theta)^{\alpha_T} - \alpha_T \theta^{\alpha_H} (1 - \theta)^{\alpha_T - 1} \Big|_{\theta = \hat{\theta}_{\text{MLE}}} = 0$$

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$$\alpha_H (1 - \theta)^{\alpha_H} (1 - \theta)^{\alpha_T} - \alpha_T \theta^{\alpha_H} (1 - \theta)^{\alpha_T - 1} \Big|_{\theta = \hat{\theta}_{\text{MLE}}} = 0$$

Question (2)

How good is this MLE estimation???

$$\widehat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$$

How many flips do I need?

I flipped the coins 5 times: 3 heads, 2 tails

$$\widehat{ heta}_{MLE} = rac{3}{5}$$

What if I flipped 30 heads and 20 tails? $\widehat{\theta}_{MLE} = \frac{30}{50}$

slide by Barnabás Póczos & Alex Smola

Which estimator should we trust more? The more the merrier???

Let θ^* be the true parameter.

For
$$n = \alpha_H + \alpha_T$$
, and $\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$
For any $\epsilon > 0$:

Hoeffding's inequality:

$$P(|\hat{\theta} - \theta^*| \ge \epsilon) \le 2e^{-2n\epsilon^2}$$

Probably Approximate Correct (PAC) Learning

I want to know the coin parameter θ , within $\varepsilon = 0.1$ error with probability at least $1-\delta = 0.95$.

How many flips do I need? $P(|\hat{\theta} - \theta^*| \ge \epsilon) \le 2e^{-2n\epsilon^2}$

Sample complexity:

$$n \ge \frac{\ln(2/\delta)}{2\epsilon^2}$$

Question (3)

Why is this a machine learning problem???

- improve their performance (accuracy of the predicted prob.)
- at some task (predicting the probability of heads)
- with experience (the more coins we flip the better we are)

What about continuous features?







MLE for Gaussian mean and variance

Choose $\theta = (\mu, \sigma^2)$ that maximizes the probability of observed data

$$\hat{\theta}_{MLE} = \arg \max_{\theta} P(D \mid \theta)$$

$$= \arg \max_{\theta} \prod_{i=1}^{n} P(X_i \mid \theta) \quad \text{Independent draws}$$

$$= \arg \max_{\theta} \prod_{i=1}^{n} \frac{1}{2\sigma^2} e^{-(X_i - \mu)^2/2\sigma^2} \quad \text{Identically} \quad \text{distributed}$$

$$= \arg \max_{\theta = (\mu, \sigma^2)} \frac{1}{2\sigma^2} e^{-\sum_{i=1}^{n} (X_i - \mu)^2/2\sigma^2} \quad \int_{J(\theta)} J(\theta)$$

slide by Barnabás Póczos & Alex Smola

MLE for Gaussian mean and variance

$$\widehat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^{n} x_i$$

$$\widehat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i - \widehat{\mu})^2$$

Note: MLE for the variance of a Gaussian is **biased** [Expected result of estimation is not the true parameter!]

Jnbiased variance estimator:
$$\widehat{\sigma}_{unbiased}^2 = rac{1}{n-1} \sum_{i=1}^n (x_i - \widehat{\mu})^2$$

Next Class:

MAP estimation Naïve Bayes Classifier