Introduction to Machine Learning

Statistical Machine Learning

Varun Chandola

Computer Science & Engineering
State University of New York at Buffalo
Buffalo, NY, USA
chandola@buffalo.edu

University at Buffalo
Department of Computer Science and Engineering
School of Engeering and Applied Sciences

Outline

Statistical Machine Learning

Functional Methods

- $y = f(\mathbf{x})$
- Learn $f()$ using training data
- $y^* = f(\mathbf{x}^*)$ for a test data instance

Statistical Machine Learning

Functional Methods

- $y = f(\mathbf{x})$
- Learn $f()$ using training data
- $y^* = f(\mathbf{x}^*)$ for a test data instance

Statistical/Probabilistic Methods

- Calculate the *conditional probability* of the target to be y, given that the input is $\mathbf{x}$
- Assume that $y|\mathbf{x}$ is *random variable* generated from a *probability distribution*
- Learn parameters of the distribution using training data

What is Probability? [2, 1]

- Probability that a coin will land heads is 50%[1]
- **What does this mean?**

[1]Dr. Persi Diaconis showed that a coin is 51% likely to land facing the same way up as it is started.


FREQUENTISTS
BAYESIANS

Frequentist Interpretation

- Number of times an event will be observed in *n trials*

Frequentist Interpretation

- Number of times an event will be observed in *n trials*
- What if the event can only occur once?
  - *My winning the next month's powerball.*
  - *Polar ice caps melting by year 2020.*

Bayesian Interpretation

- **Uncertainty** of the event
- Use for making decisions
    - Should I put in an offer for a sports car?

What is a Random Variable (X)?

- Can take any value from $\mathcal{X}$
- **Discrete Random Variable** - $\mathcal{X}$ is finite/countably finite
  - Categorical??
- **Continuous Random Variable** - $\mathcal{X}$ is infinite
- $P(X = x)$ or $P(x)$ is the probability of X taking value x
  - an **event**
- What is a distribution?

Examples

1. Coin toss ($\mathcal{X} = \{heads, tails\}$)
2. Six sided dice ($\mathcal{X} = \{1, 2, 3, 4, 5, 6\}$)

Notation, Notation, Notation

- X - random variable ($\mathbf{X}$ if multivariate)
- x - a specific value taken by the random variable (($\mathbf{x}$ if multivariate))
- $P(X = x)$ or $P(x)$ is the probability of the event $X = x$
- $p(x)$ is either the **probability mass function** (discrete) or **probability density function** (continuous) for the random variable X at x
  - Probability mass (or density) at x

Basic Rules - Quick Review

- For two events A and B:
  - $P(A \vee B) = P(A) + P(B) - P(A \wedge B)$
  - **Joint Probability**
    - $P(A, B) = P(A \wedge B) = P(A|B)P(B)$
    - Also known as the *product rule*
  - **Conditional Probability**
    - $P(A|B) = \frac{P(A,B)}{P(B)}$

Chain Rule of Probability

- Given D random variables, $\{X_1, X_2, \ldots, X_D\}$

$$P(X_1, X_2, \ldots, X_D) = P(X_1)P(X_2|X_1)P(X_3|X_1, X_2)\ldots P(X_D|X_1, X_2, \ldots, X_D)$$

Marginal Distribution

- Given $P(A, B)$ what is $P(A)$?
  - Sum $P(A, B)$ over all values for B

$$P(A) = \sum_b P(A, B) = \sum_b P(A|B = b)P(B = b)$$

  - **Sum rule**

Bayes Rule or Bayes Theorem

- Computing $P(X = x|Y = y)$:

Bayes Theorem

$$
\begin{aligned}
P(X = x|Y = y) &= \frac{P(X = x, Y = y)}{P(Y = y)} \\
&= \frac{P(X = x)P(Y = y|X = x)}{\sum_{x'} P(X = x')P(Y = y|X = x')}
\end{aligned}
$$

Example

- Medical Diagnosis
- Random event 1: A *test* is positive or negative (X)
- Random event 2: A person has cancer (Y) – yes or no
- What we know:
  1. Test has accuracy of 80%
  2. Number of times the test is positive when the person has cancer

$$P(X = 1|Y = 1) = 0.8$$

  3. Prior probability of having cancer is 0.4%

$$P(Y = 1) = 0.004$$

Question?

If I test positive, does it mean that I have 80% rate of cancer?

Base Rate Fallacy

- Ignored the prior information
- What we need is:
$$P(Y = 1|X = 1) =?$$
- More information:
  - False positive (alarm) rate for the test
  - $P(X = 1|Y = 0) = 0.1$

$$P(Y = 1|X = 1) \quad = \quad \frac{P(X = 1|Y = 1)P(Y = 1)}{P(X = 1|Y = 1)P(Y = 1) + P(X = 1|Y = 0)P(Y = 0)}$$

Classification Using Bayes Rule

- Given input example **x**, find the true class

$$P(Y = c|\mathbf{X} = \mathbf{x})$$

- Y is the random variable denoting the true class
- Assuming the **class-conditional** probability is known

$$P(\mathbf{X} = \mathbf{x}|Y = c)$$

- Applying Bayes Rule

$$P(Y = c|\mathbf{X} = \mathbf{x}) = \frac{P(Y = c)P(\mathbf{X} = \mathbf{x}|Y = c)}{\sum_c P(Y = c'))P(\mathbf{X} = \mathbf{x}|Y = c')}$$

Independence

- One random variable does not depend on another
- $A \perp B \iff P(A,B) = P(A)P(B)$
- Joint written as a product of marginals
- **Conditional Independence**

$$A \perp B|C \iff P(A,B|C) = P(A|C)P(B|C)$$

Continuous Random Variables

- X is continuous
- Can take any value
- How does one define probability?
  - $\sum_x P(X = x) = 1$

Continuous Random Variables

- X is continuous
- Can take any value
- How does one define probability?
  - $\sum_x P(X = x) = 1$
- Probability that X lies in an interval $[a, b]$?
  - $P(a < X \leq b) = P(x \leq b) - P(x \leq a)$
  - $F(q) = P(x \leq q)$ is the **cumulative distribution function**
  - $P(a < X \leq b) = F(b) - F(a)$

Probability Density

Probability Density Function

$$p(x) = \frac{\partial}{\partial x} F(x)$$

$$P(a < X \leq b) = \int_a^b p(x)dx$$

- Can $p(x)$ be greater than 1?

Expectation

- Expected value of a random variable

$$\mathbb{E}[X]$$

- What is most likely to happen in terms of X?
- For discrete variables

$$\mathbb{E}[X] \triangleq \sum_{x \in \mathcal{X}} xP(X = x)$$

- For continuous variables

$$\mathbb{E}[X] \triangleq \int_{\mathcal{X}} xp(x)dx$$

- **Mean** of X (μ)

Expectation of Functions of Random Variable

- Let $g(X)$ be a function of X
- If X is discrete:

$$\mathbb{E}[g(X)] \triangleq \sum_{x \in \mathcal{X}} g(x)P(X = x)$$

- If X is continuous:

$$\mathbb{E}[g(X)] \triangleq \int_{\mathcal{X}} g(x)p(x)dx$$

Properties

- $\mathbb{E}[c] = c$, c - constant
- If $X \leq Y$, then $\mathbb{E}[X] \leq \mathbb{E}[Y]$
- $\mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y]$
- $\mathbb{E}[aX] = a\mathbb{E}[X]$
- $var[X] = \mathbb{E}[(X - \mu)^2] = \mathbb{E}[X^2] - \mu^2$
- $Cov[X, Y] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$
- Jensen's inequality: If $\varphi(X)$ is convex,

$$\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)]$$

What is a Probability Distribution?

Discrete

- Binomial, *Bernoulli*
- Multinomial, *Multinoulli*
- Poisson
- Empirical

Continuous

- Gaussian (Normal)
- Degenerate pdf
- Laplace
- Gamma
- Beta
- Pareto

Binomial Distribution

- X = Number of heads observed in n coin tosses
- Parameters: n, θ
- $X \sim Bin(n, \theta)$
- Probability mass function (*pmf*)

$$Bin(k|n,\theta) \triangleq \binom{n}{k}\theta^k(1-\theta)^{n-k}$$

Bernoulli Distribution

- Binomial distribution with $n = 1$
- Only one parameter ($\boldsymbol{\theta}$)

Multinomial Distribution

- Simulates a K sided die
- Random variable $\mathbf{x} = (x_1, x_2, \ldots, x_K)$
- Parameters: n, θ
- $\theta \leftarrow \Re^K$
- θ_j - probability that j^{th} side shows up

$$Mu(\mathbf{x}|n, \boldsymbol{\theta}) \triangleq \binom{n}{x_1, x_2, \ldots, x_K} \prod_{j=1}^{K} \theta_j^{x_j}$$

Multinoulli Distribution

- Multinomial distribution with $n = 1$
- $\mathbf{x}$ is a vector of 0s and 1s with only one bit set to 1
- Only one parameter (θ)

Gaussian (Normal) Distribution

$$\mathcal{N}(x|\mu,\sigma^2) \triangleq \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

- Parameters:
  1. $\mu = \mathbb{E}[X]$
  2. $\sigma^2 = var[X] = \mathbb{E}[(X-\mu)^2]$
- $X \sim \mathcal{N}(\mu,\sigma^2) \Leftrightarrow p(X = x) = \mathcal{N}(\mu,\sigma^2)$
- $X \sim \mathcal{N}(0,1) \Leftarrow X$ is a **standard normal random variable**
- **Cumulative distribution function**:

$$\Phi(x;\mu,\sigma^2) \triangleq \int_{-\infty}^{x} \mathcal{N}(z|\mu,\sigma^2)dz$$

Joint Probability Distributions

- Multiple *related* random variables
- $p(x_1, x_2, \ldots, x_D)$ for $D > 1$ variables $(X_1, X_2, \ldots, X_D)$
- Discrete random variables?
- Continuous random variables?
- What do we measure?

Covariance

- How does X vary with respect to Y
- For linear relationship:

$$cov[X, Y] \triangleq \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y]$$

Covariance and Correlation

- **x** is a *d*-dimensional random vector

$$cov[\mathbf{X}] \triangleq \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top]$$

$$= \begin{pmatrix} var[X_1] & cov[X_1, X_2] & \cdots & cov[X_1, X_d] \\ cov[X_2, X_1] & var[X_2] & \cdots & cov[X_2, X_d] \\ \vdots & \vdots & \ddots & \vdots \\ cov[X_d, X_1] & cov[X_d, X_2] & \cdots & var[X_d] \end{pmatrix}$$

- Covariances can be between 0 and ∞
- Normalized covariance $\Rightarrow$ **Correlation**

Correlation

- *Pearson* Correlation Coefficient

$$corr[X, Y] \triangleq \frac{cov[X, Y]}{\sqrt{var[X]var[Y]}}$$

- What is $corr[X, X]$?
- $-1 \leq corr[X, Y] \leq 1$
- When is $corr[X, Y] = 1$?

Correlation

- *Pearson* Correlation Coefficient

$$corr[X, Y] \triangleq \frac{cov[X, Y]}{\sqrt{var[X]var[Y]}}$$

- What is $corr[X, X]$?
- $-1 \leq corr[X, Y] \leq 1$
- When is $corr[X, Y] = 1$?
  - $Y = aX + b$

Multivariate Gaussian Distribution

- Most widely used joint probability distribution

$$\mathcal{N}(\mathbf{X}|\mu,\mathbf{\Sigma}) \triangleq \frac{1}{(2\pi)^{D/2}|\mathbf{\Sigma}|^{1/2}} exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^\top\mathbf{\Sigma}^{\mathbf{-1}}(\mathbf{x}-\mu)\right]$$

References

E. Jaynes and G. Bretthorst.
Probability Theory: The Logic of Science.
Cambridge University Press Cambridge:, 2003.

L. Wasserman.
All of Statistics: A Concise Course in Statistical Inference (Springer Texts in Statistics).
Springer, Oct. 2004.