

EE 046202 - Technion - Unsupervised Learning & Data Analysis

Tal Daniel

Tutorial 00 - Probability, Optimization and Inequalities Refresher



Agenda

- Probability Basics
 - Bayes Rule
 - <u>Expectation & Variance</u>-&-Variance)
- Vectors of Random Variables
- Lagrange Multipliers
 - Maximum Entropy Exercise
- <u>Useful Inequalities</u>
- Recommended Videos
- Credits

```
In [1]: # imports for the tutorial
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from matplotlib import cm
from mpl_toolkits.mplot3d import Axes3D
from scipy.stats import multivariate_normal
%matplotlib notebook
```



Probability Basics

Term	Usually denoted by	Definition	Example
Experiment		any procedure that can be infinitely repeated and has a well-defined set of possible outcomes	toss a coin twice
Sample	ω	A single outcome of an experiment	A single outcome. For example: HH
Sample Space	Ω	The set of all possible outcomes	The set of all possible outcomes, for example: {HH, HT, TH, TT} $$
Event	A	a subset of possible outcomes	$ A = \{HH\} \ , \ B = \{HT, TH\} $ An empty set \emptyset The entire set (any outcome): Ω
Event Space	${\cal F}$	The space of all possible events	$\{HH\}, \{HT\}, \{TH\}, \{TT\}, \{\emptyset\}, \{\Omega\}$
Probability	P, Pr	A function $P:\mathcal{F} o [0,1]$ which assigns a probability to each event	$egin{aligned} P(HT) &= rac{1}{4} \ P(\emptyset) &= 0 \ P(\Omega) &= 1 \end{aligned}$

Joint Probability

- Joint Probability Pr(A,B) the probability the both event A and event B happen ($Pr(A,B) \geq 0$)
- Marginal Distributions -
- Law of Total Probability suppose the events B_1, B_2, \dots, B_k are mutually exclusive (intersection of all events is zero) and form a partition of the sample space (i.e. one of them must occur), then for any event Pr(A):

$$Pr(A) = \sum_{i=1}^k Pr(A|B_j)P(B_j)$$

- Conditioning if A and B are events and Pr(B)>0, the conditional probability of A given B is: Pr(A|B)
 - $ullet Pr(A|B) = rac{P(A,B)}{P(B)}$
 - ightharpoonup Pr(A,B) = Pr(A|B)Pr(B)
 - The chain rule in the general case:

$$Pr(igcap_i A_i) = \prod_{i=n}^1 Pr(A_i | A_{i-1}, \dots, A_1)$$

- $\circ \ Pr(A,B,C) = P(A|B,C)P(B,C) = P(A|B,C)P(B|C)P(C)$
- \circ Is that the only option? No! Pr(A,B,C) = P(C|A,B)P(A,B) = P(C|A,B)P(B|A)P(A)
- · Independence -
 - Two events A and B are independent iff
 - $\circ Pr(A|B) = Pr(A)$
 - Pr(A, B) = Pr(A)Pr(B)
 - For a set of events $\{A_i\}$, independence:
 - $\circ \ Pr(\bigcap_i A_i) = \prod_i Pr(A_i)$
- Conditional Independence Events A and B are conditionally independent given C:
 - Pr(A,B|C) = Pr(A|C)Pr(B|C)
 - Pr(A|B,C) = Pr(A|C)



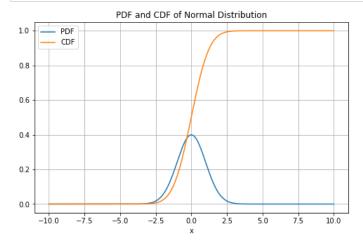
Continuous Random Variables

Assume X is a continuous random variable. We define the following:

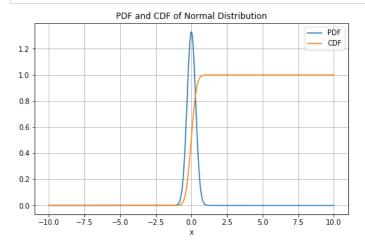
- Cumulative Distribution Function (CDF) $F(x) = P(X \le x)$
 - The CDF is monotonically non-decreasing
 - $P(a < X \le b) = F(b) F(a)$
 - $\lim_{a o \infty} F_x(a) = 1$
 - $\lim_{a \to 0} F_x(a) = 0$
- Probability Density Function (PDF) $f(x) = rac{d}{dx} F(x)$
 - $lacksquare P(a < X \leq b) = \int_a^b f(x) dx$
- All we have seen for discrete variables hold for continuous by replacing the sum with an integral

```
In [10]: def plot_normal_pdf_cdf(mu=0, sigma=1):
              x = np.linspace(-10, 10, 1000)
             x_pdf = (1 / np.sqrt(2 * np.pi * sigma ** 2)) * np.exp(- (x - mu) ** 2 / (2 * sigma ** 2))
             x_cdf = np.cumsum(x_pdf) / (len(x) / (np.max(x) - np.min(x))) # normalization
             fig = plt.figure(figsize=(8,5))
             ax = fig.add_subplot(1,1,1)
             ax.plot(x, x_pdf, label='PDF')
             ax.plot(x, x_cdf, label='CDF')
             ax.grid()
             ax.legend()
             ax.set xlabel('x')
             ax.set title('PDF and CDF of Normal Distribution')
```

In [11]: plot_normal_pdf_cdf(mu=0, sigma=1)



In [12]: plot_normal_pdf_cdf(mu=0, sigma=0.3)
notice how the pdf can be larger than 1



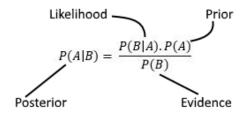
Bayes Rule

Suppose that the events B_1, \ldots, B_k are mutually exclusive and form a partition of the sample space (i.e. one of them must occur), then for any event Pr(A), Bayes Rule:

$$Pr(B_i|A) = \frac{Pr(A,B_i)}{Pr(A)} = \frac{Pr(A|B_i)Pr(B_i)}{Pr(A)} = \frac{Pr(A|B_i)Pr(B_i)}{\sum_{j=1}^{k} Pr(A|B_j)Pr(B_j)}$$

- Posterior Distribution $Pr(B_i|A)$
- Liklihood Distribution $Pr(A|B_i)$
- Prior Distribution $Pr(B_i)$
- Evidence Pr(A)





• Image Source (https://www.analyticsvidhya.com/blog/2019/06/introduction-powerful-bayes-theorem-data-science/)

Mean (Expectation) & Variance

Mean (Expectation) - μ

The mean is the probability weighted average of all possible values.

- Discrete Variables:

 - $\begin{array}{l} \bullet \ \mathbb{E}[X] = \sum_{x \in X} x p(x) \\ \bullet \ \mathbb{E}[f(X)] = \sum_{x \in X} f(x) p(x) \end{array}$
- Continuous Variables:
 - ${\mathbb E}[X]=\int_x x p(x)$
- $\mathbb{E}[f(X)] = \int_{x \in X}^x f(x) p(x)$ Example: the mean of a fair six-sided dice:

$$\mathbb{E}[X] = 1 * \frac{1}{6} + 2 * \frac{1}{6} + 3 * \frac{1}{6} + 4 * \frac{1}{6} + 5 * \frac{1}{6} + 6 * \frac{1}{6} = 3.5$$

• Empirical Mean: if $X \sim P(x)$ and we are given N i.i.d. samples of X, the empirical mean:

$$\overline{X}_N = rac{1}{N} \sum_{i=1}^N X_i$$

- The empirical mean is also R.V. as a sum of RVs is also an RV.
- It converges to the actual mean as we will see shortly.
 - What does this mean that the "random variable converges?" It is not a number! (but a random variable).
- The Law of Total Expectation (Smoothing Theorem):

$$\mathbb{E}_x[X] = \mathbb{E}_y\left[\mathbb{E}_x[X|Y]\right]$$

$$\bullet \text{ Proof: } \mathbb{E}\big[\mathbb{E}[X|Y]\big] = \mathbb{E}\big[\sum_x x \cdot P(X=x|Y)\big] = \sum_y \big[\sum_x x \cdot P(X=x|Y)\big] \cdot P(Y=y) = \sum_y \big[\sum_x x \cdot P(X=x|Y) \cdot P(Y=y)\big] = \sum_y \big[\sum_x x \cdot P(X=x,Y=y)\big] = \sum_x x \cdot \big[\sum_y \cdot P(X=x,Y=y)\big] = \sum_x x \cdot \big[P(X=x)\big] = \mathbb{E}[X]$$

• Example: Suppose that two factories supply light bulbs to the market. Factory X's bulbs work for an average of 5000 hours, whereas factory Y's bulbs work for an average of 4000 hours. It is known that factory X supplies 60% of the total bulbs available. What is the expected length of time that a purchased bulb will work for?

$$\mathbb{E}[L] = \mathbb{E}\big[\mathbb{E}[L|factory]\big] = \mathbb{E}[L|X] \cdot P(X) + \mathbb{E}[L|Y] \cdot P(Y) = 5000 \cdot 0.6 + 4000 \cdot 0.4 = 4600$$

Variance - σ^2

The variance is a measure of the "spread" of the distribution (can also be considered as confidence).

•
$$var[X]=\mathbb{E}[(X-\mu)^2]=\sum (x-\mu)^2p(x)=\sum x^2p(x)+\mu^2\sum p(x)-2\mu\sum xp(x)=\mathbb{E}[X^2]-\mu^2$$
 • The Standard Deviation - $std[X]=\sqrt{var[X]}$

- · Example: the variance of a fair six-sided dice:

$$egin{aligned} var[X] &= \sum_{i=1}^6 rac{1}{6}(i-3.5)^2 \ E[X^2] &= 1^2 * rac{1}{6} + 2^2 * rac{1}{6} + 3^2 * rac{1}{6} + 4^2 * rac{1}{6} + 5^2 * rac{1}{6} + 6^2 * rac{1}{6} = rac{91}{6} \ var[X] &= E[X^2] - \mu^2 = rac{91}{6} - 3.5^2 pprox 2.92 \end{aligned}$$

Vectors of Random Variables

- Let \overline{X} be a d-dimensional random vector

$$oldsymbol{\overline{X}} = [x_1, x_2, \ldots, x_d]$$

- The d-dimensional **mean vector** $\overline{\mu}$ is:

$$oldsymbol{ar{\mu}} = \mathbb{E}[\overline{X}] = [\mathbb{E}[x_1], \mathbb{E}[x_2], \dots, \mathbb{E}[x_d]] = [\mu_1, \mu_2, \dots, \mu_d]$$

• $\overline{\mu}=\mathbb{E}[\overline{X}]=[\mathbb{E}[x_1],\mathbb{E}[x_2],\dots,\mathbb{E}[x_d]]=[\mu_1,\mu_2,\dots,\mu_d]$ • The **covariance matrix** Σ is defined as the (**square**) matrix, where each component σ_{ij} is the covariance of x_i,x_j :

$$\sigma_{ij} = \mathbb{E}[(x_i - \mu_i)(x_j - \mu_j)]$$

$$\Sigma = egin{pmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,d} \ \sigma_{2,1} & \sigma_2^2 & \cdots & \sigma_{2,d} \ dots & dots & \ddots & dots \ \sigma_{d,1} & \sigma_{d,2} & \cdots & \sigma_d^2 \end{pmatrix}$$

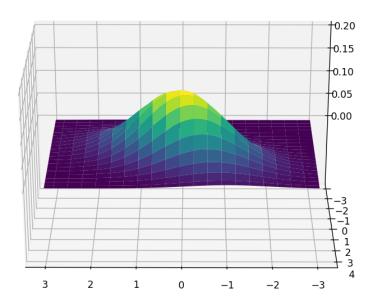


Multivariate Normal Distribution

•
$$x \sim N_d(\mu, \Sigma)$$

$$f(x) = rac{1}{\left(2\pi
ight)^{rac{d}{2}}|\Sigma|^{rac{1}{2}}}e^{-rac{1}{2}(x-\mu)^T\Sigma^{-1}(x-\mu)}$$

```
In [5]: # Our 2-dimensional distribution will be over variables X and Y
                                 %matplotlib notebook
                                 N = 60
                                 X = np.linspace(-3, 3, N)
                                 Y = np.linspace(-3, 4, N)
                                 X, Y = np.meshgrid(X, Y)
                                 # Mean vector and covariance matrix
                                 mu = np.array([0., 1.])
                                 Sigma = np.array([[ 1. , -0.5], [-0.5, 1.5]])
                                 # Pack X and Y into a single 3-dimensional array
                                 pos = np.empty(X.shape + (2,))
                                 pos[:, :, 0] = X
pos[:, :, 1] = Y
                                 F = multivariate_normal(mu, Sigma)
                                 Z = F.pdf(pos)
                                 # Create a surface plot and projected filled contour plot under it.
                                 fig = plt.figure(figsize=(8,5))
                                 ax = fig.gca(projection='3d')
                                 \verb|ax.plot_surface(X, Y, Z, rstride=3, cstride=3, linewidth=1, antialiased=| \textbf{True}, anti
                                                                                                cmap=cm.viridis)
                                 # cset = ax.contourf(X, Y, Z, zdir='z', offset=-0.15, cmap=cm.viridis)
                                 # Adjust the limits, ticks and view angle
ax.set_zlim(-0.15,0.2)
                                 ax.set_zticks(np.linspace(0,0.2,5))
                                 ax.view_init(27, -21)
                                 plt.tight_layout()
                                 # plt.show()
```



Lagrange Multipliers

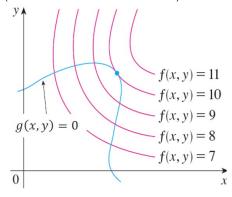
- · A method for optimization with equality constraints (can also be inequalities)
- · The general case:

$$\min f(x,y) \ s.t. \ (subject \ to) : g(x,y) = 0$$

- Alternatively, can be defined as a maximization problem (max)
- The Lagrange function (Lagrangian) is defined by:

$$\mathcal{L}(x,y,\lambda) = f(x,y) - \lambda \cdot g(x,y)$$

• Geometric Intuition: let's look at the following figure (here we maximize instead of minimize) -



- The blue line shows the constraint g(x, y) = 0
- The red lines are contours of f(x, y) = c
- The point where the blue line tangentially touches a red contour is the maximum of f(x, y) = c that satisfy the constraint g(x, y) = 0
- ullet To maximize f(x,y) subject to g(x,y)=0 is to find the largest value $c\in\{7,8,9,10,11\}$ such that the level curve (contour) f(x,y)=cintersects with g(x,y)=0
- It happens when the curves just touch each other
 - When they have a common tangent line
- Otherwise, the value of c should be increased
- Since the gradient of a function is **perperndicular** to the contour lines:
 - \circ The *contour lines* of f and g are **parallel** iff the *gradients* of f and g are **parallel**
 - \circ Thus, we want points (x,y) where g(x,y)=0 and

$$abla_{x,y}f(x,y)=\lambda
abla_{x,y}g(x,y)$$

 \circ λ - The Lagrange Multiplier is required to adjust the **magnitudes** of the (parallel) gradient vectors.



Multiple Constraints

- · Extenstion of the above for problems with multiple constraints using a similar argument
- The general case: minimize f(x) s.t. $g_i(x) = 0, i = 1, 2, \dots, m$
- The Lagrangian is a weighted sum of objective and constraint functions:

$$\mathcal{L}(x,\lambda_1,\dots,\lambda_m) = f(x) - \sum_{i=1}^m \lambda_i g_i(x)$$

- ullet λ_i is the Lagrange multipler associated with $g_i(x)=0$
- The **solution** is obtained by solving the (unconstrained) optimization problem:

The **solution** is obtained by solving the (unconstrained) optimization problem:
$$\nabla_{x,\lambda_1,\dots,\lambda_m}\mathcal{L}(x,\lambda_1,\dots,\lambda_m)=0\iff \begin{cases} \nabla_x\big[f(x)-\sum_{i=1}^m\lambda_ig_i(x)=0\big]\\ g_1(x)=\dots=g_m(x)=0 \end{cases}$$
 • Amounts to solving $d+m$ equations in $d+m$ unkowns
$$\cdot d=|x| \text{ is the dimension of } x$$

- - $\circ \ d = |x|$ is the dimension of x

Maximize $H(P) = -\sum_{i=1}^d p_i \log p_i$ subject to $\sum_{i=1}^d p_i = 1$



· The Lagrangian is:

$$L(P,\lambda) = -\sum_{i=1}^d p_i \log p_i - \lambda ig(\sum_{i=1}^d p_i - 1ig)$$

- Find stationary point for L:

 $\forall i, \frac{\partial L(P,\lambda)}{\partial p_i} = -\log p_i 1 \lambda = 0 \rightarrow p_i = e^{-\lambda 1}$ $\frac{\partial L(P,\lambda)}{\partial \lambda} = -\sum_{i=1}^d p_i + 1 = 0 \rightarrow \sum_{i=1}^d e^{-\lambda 1} = 1 \rightarrow e^{-\lambda 1} = \frac{1}{d} = p_i$ The Max Entropy distribution is the **uniform distribution**.

Useful Inequalities

• Markov Inequality - for a non-negative R.V (Random Variable) $X \geq 0$ and for any positive number $\lambda > 0$:

$$Pr(X \geq \lambda) \leq \frac{\mathbb{E}[X]}{\lambda}$$

$$Pr(X \geq \lambda) \leq \frac{\mathbb{E}[X]}{\lambda}$$

$$\mathbb{E}[X] = \sum_{i=1}^n x_i \cdot Pr(X = x_i) \geq \sum_{i=j}^n x_i \cdot Pr(X = x_i) \geq \sum_{i=j}^n \lambda \cdot Pr(X = x_i) = \lambda \cdot \sum_{i=j}^n Pr(X = x_i) = \lambda \cdot Pr(X \geq \lambda)$$

- Chebyshev Inequality - for any R.V (Random Variable) $X \geq 0$ and for any positive number $\lambda > 0$:

$$Pr(|X - \mathbb{E}[X]| \geq \lambda) \leq rac{Var(X)}{\lambda^2}$$

- Proof using the Markov Inequality.
- Hoeffding Inequality Let X_1,\dots,X_n be i.i.d. random variables, bounded by the intervals $a_i \leq X_i \leq b_i$. Let the empirical mean be defined according to $\overline{X} = rac{1}{n} \sum_{i=1}^n X_i$. It holds that:

$$P(|\overline{X} - \mathbb{E}[\overline{X}]| \geq \epsilon) \leq 2e^{-rac{2n^2\epsilon^2}{\sum_{i=1}^n(a_i-b_i)^2}}$$



Recommended Videos



- · These videos do not replace the lectures and tutorials.
- · Please use these to get a better understanding of the material, and not as an alternative to the written material.

Video By Subject

- Basic Probability Math Antics Basic Probability (https://www.youtube.com/watch?v=KzfWUEJjG18)
- Probability for ML Machine Learning 1/5: Probability (https://www.youtube.com/watch?v=wG_gQpXJNGU)
- Lagrange Multipliers Lagrange Multipliers I Geometric Meaning & Full Example (https://www.youtube.com/watch?v=8mjcnxGMwFo)
- Hoefdding's Inequality Chernoff, Hoeffding, etc. bounds II @ CMU II Lecture 5c of CS Theory Toolkit (https://www.youtube.com/watch?v=zz4C-xEClp4)
- Markov and Chebyshev Inequalities MIT 6.041SC Probability Bounds (https://www.youtube.com/watch?v=s8geHBRvSos)



- Icons from Icon8.com (https://icons8.com/) https://icons8.com (https://icons8.com)
- Datasets from Kaggle (https://www.kaggle.com/ (htt