CEE 616: Probabilistic Machine Learning

Lecture 1a: Foundations: Probability

Jimi Oke

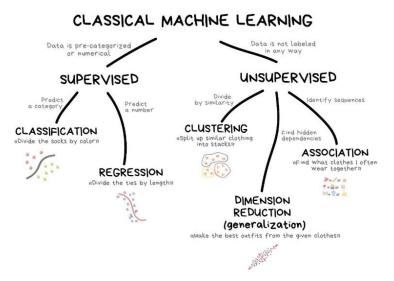
UMassAmherst

College of Engineering

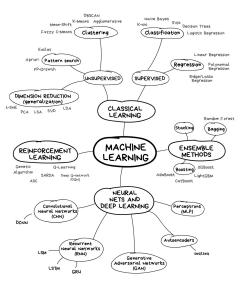
Feb 8, 2023

Outline

What is machine learning?



Machine learning—alternate illustration



Source: https://i.vas3k.ru/7vx.jpg

Machine learning flow

The "learning" refers to the search for **optimal parameters** as a function of the data.

- Inputs (data, domain knowledge/human)
- Learning (computer/algorithm)
- Outputs (predictions, information/inference)

Supervised vs. unsupervised learning

Supervised learning

Goal: fit a model characterizing relationship between predictor(s) X and response(s) Y (i.e. known outputs)

- regression (linear, nonlinear, logistic, etc)
- boosting/bagging/random forests
- support vector machines

Unsupervised learning

Goal: infer relationships between/among variables or observations (outputs/target unknown)

- dimensionality reduction (principal components, factor analysis)
- cluster analysis

 Semi-supervised learning occurs when responses are available for a subset of the observations

Notation

Symbol Meaning

n number of observations (distinct data points)

p number of variables

 x_{ij} value of jth variable for ith observation

So, we can write the $n \times p$ matrix \boldsymbol{X} as:

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

where the rows of \boldsymbol{X} are: x_1, x_2, \dots, x_n and the columns are written $\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_p$

Notation (cont.)

We will denote y as the *response* variable vector.

Summary of notation conventions

- Scalar: lower case italic (e.g. b)
- Vector: lower case bold (e.g $\mathbf{x}_j \in \mathbb{R}^n$), except for feature vectors of length p)
- Matrix: upper case bold (e.g. $\mathbf{X} \in \mathbb{R}^{n \times p} 1$)
- Random variable: upper case italic (e.g. $Y \sim \mathcal{N}(\mu, \sigma)$)

Learning framework

Given a set of inputs X_j ($j \in \{1, ..., p\}$) and a given output Y, "learning" refers to the techniques used in estimating the functional relationship between X_i and Y for the purposes of *prediction* and *inference*.

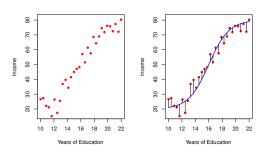


Figure: Estimating the functional relationship between income and educational attainment in a data set

Model equation

$$Y = f(X) + \epsilon \tag{1}$$

where f is an unknown function and ϵ is the random error (independent of X with zero mean)

Prediction

We predict Y using:

$$\hat{Y} = \hat{f}(X) \tag{2}$$

where \hat{f} is the estimate of f and \hat{Y} is the predicted value of Y.

Reducible and irreducible error

The prediction accuracy depends on *reducible error* and *irreducible error* (noise—intrinsic variability in the data)

$$E\left[(Y - \hat{Y})^2\right] = E\left[f(X) + \epsilon - \hat{f}(X)\right]^2$$

$$= \left[f(X) - \hat{f}(X)\right]^2 + \text{Var}(\epsilon)$$
(3)

Inference

This refers to the process of determining the nature of the relationship between the inputs (X) and outputs (Y).

In other words, if Y = f(X), then what is f?

Questions relating to inference

- What is the elasticity^a of a certain input in relation to an output?
- What are the important *predictors* of a certain outcome?
- What is the correlation between X and Y?

^aCan be defined as the percentage change in Y for a 1% change in X.

Parametric methods

These methods require an assumption of the structure of the relationship between X and Y.

Step 1: assume functional form (e.g. linearity in coefficients):

$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots$$
 (4)

Step 2: fit model, i.e. *estimate* the parameters/coefficients:

$$Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots \tag{5}$$

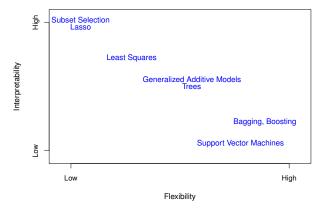
The estimation procedure can be a method of choice, e.g. OLS (ordinary least squares), WLS (weighted least squares), etc.

Non-parametric methods

- The assumption of linearity is a strong one and may result in a poor fit if f is very different from \hat{f} .
- Non-parametric methods allow flexible functional forms (although the danger of overfitting is real).
- For accuracy, however, non-parametric models require many more observations compared to the parametric case.

Tradeoff between accuracy and interpretability

A simpler model is more interpretable in its parameters. A highly complicated model may operate more like a blackbox.



CORE PRINCIPLES IN RESEARCH



OCCAM'S RAZOR

"WHEN FACED WITH TWO POSSIBLE EXPLANATIONS, THE SIMPLER OF THE TWO IS THE ONE MOST LIKELY TO BE TRUE."



OCCAM'S PROFESSOR

"WHEN FACED WITH TWO POSSIBLE WAYS OF DOING SOMETHING, THE MORE COMPLICATED ONE IS THE ONE YOUR PROFESSOR WILL MOST LIKELY ASK YOU TO DO."

WWW. PHDCOMICS. COM

CARGE CHAIN IN 2001

Theory of probability

Three axioms of probability:

$$P(E) \geq 0$$
 and $P(E) \leq 1$ for given event E
$$P(S) = 1$$

$$P(E_1 \cup E_2 \cup \cdots \cup E_n) = P(E_1) + P(E_2) + \cdots + P(E_n) \text{ (Mutually exclusive)}$$

- Addition rule: $P(A \cup B) = P(A) + P(B) P(AB)$
 - For mutually exclusive events: $P(A \cup B) = P(A) + P(B)$ (Axiom 3)
- Counting events:
 - Fundamental principle of counting: number of outcomes for $1, \ldots, k$ events, each with n_1, \ldots, n_k possibilities is $n_1 \times \cdots \times n_k$
 - Permutations (arrangements) of *n* objects: $n! = n(n-1)(n-2)\cdots(2)(1)$
 - Permutations of a subset of k items chosen from set of n items: n!/(n-k)!
 - Combinations (distinct; order not important) of group of k items chosen from set of n items: n!/(k!(n-k)!)

Conditional probability

Conditional probability:

$$P(A|B) = \frac{P(AB)}{P(B)} \tag{6}$$

Independent events:

$$P(AB) = P(A)P(B) \tag{7}$$

 Generally, the joint probability (intersection) of any number of independent events is the product of their individual probabilities:

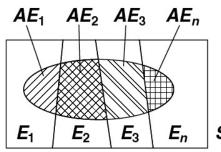
$$P(E_1 \cap E_2 \cap \dots \cap E_n) = P(E_1)P(E_2) \dots P(E_n)$$
(8)

Multiplication rule:

$$P(AB) = P(A|B)P(B) = P(B|A)P(A)$$
(9)

Total probability

Useful in situations where the probability of an event cannot be directly determined but its conditional probabilities are known.



$$P(A) = P(AE_1) + P(AE_2)$$

+ $P(AE_3) + \cdots + P(AE_n)$
Note that:

Note that: $P(AE_1) = P(A|E_1)P(E_1)$, etc.

Theorem of total probability

The probability of an event A conditioned on the mutually exclusive and collectively exhaustive events E_1, E_2, \ldots, E_n is given by

$$P(A) = P(A|E_1)P(E_1) + P(A|E_2)P(E_2) + \dots + P(A|E_n)P(E_n)$$
 (10)

Derivation of Bayes' theorem

Recall from the multiplication rule that:

$$P(AB) = P(A|B)P(B) \tag{11}$$

Equivalently:

$$P(AB) = P(B|A)P(A)$$
 (12)

We combine both equations to obtain:

$$P(A|B)P(B) = P(B|A)P(A)$$
(13)

Then, we obtain the **inverse probability** of the conditioning event:

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)} \tag{14}$$

Bayes' theorem

Bayes' Theorem allows for the computation of an inverse probability, e.g. given P(A|B), can we find P(B|A)?

$$P(E_i|A) = \frac{P(A|E_i)P(E_i)}{\sum_{j=1}^{n} P(A|E_j)P(E_j)} = \frac{P(A|E_i)P(E_i)}{P(A)}$$
(15)

- posterior probability: $P(E_i|A)$
- likelihood: $P(A|E_i)$
- prior: $P(E_i)$
- evidence (total probability): P(A)

If the event A can be conditioned on only two events E_1 and E_2 , then:

$$P(E_1|A) = \frac{P(A|E_1)P(E_1)}{P(A|E_1)P(E_1) + P(A|E_2)P(E_2)}$$
(16)

$$P(E_2|A) = \frac{P(A|E_2)P(E_2)}{P(A|E_1)P(E_1) + P(A|E_2)P(E_2)}$$
(17)

Example 1: Construction supplies

Aggregates for the construction of a reinforced concrete building are supplied by two companies. Company a delivers 600 truckloads a day while Company b delivers 400 truckloads a day. From prior experience, 3% of Company a's material is expected to be substandard while 1% of Company b's material is expected to be substandard.

We define:

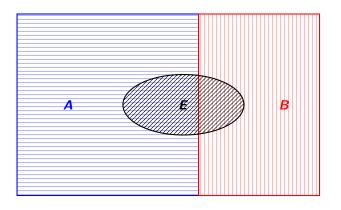
A = aggregates supplied by Company a

B = aggregates supplied by Company b

E = aggregates are substandard

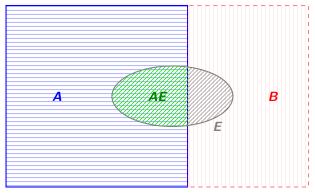
- **3** Draw a Venn diagram and convince yourself that P(A) = 0.60, P(B) = 0.40, P(E|A) = 0.03, P(E|B) = 0.01
- **b** Find the probability P(A|E) = 0.82.

3 Draw a Venn diagram and convince yourself that P(A) = 0.60, P(B) = 0.40, P(E|A) = 0.03, P(E|B) = 0.01



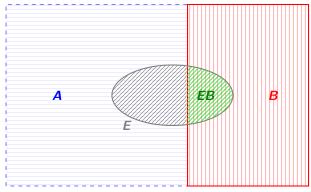
$$P(A) = 0.60, P(B) = 0.40, P(E|A) = 0.03, P(E|B) = 0.01$$

 $P(E|A) = \frac{P(EA)}{P(A)}$



$$P(A) = 0.60, P(B) = 0.40, P(E|A) = 0.03, P(E|B) = 0.01$$

 $P(E|B) = \frac{P(EB)}{P(B)}$



b Find the probability P(A|E) = 0.82.

First, we find the evidence:

$$P(E) = P(E|A)P(A) + P(E|B)P(B)$$

$$= (0.03)(0.6) + (0.01)(0.4)$$

$$= 0.018 + 0.004 = 0.022$$

Then we use Bayes':

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

$$= \frac{P(E|A)P(A)}{P(E)} \text{ (Denominator: total probability)}$$

$$= \frac{0.03 \times 0.60}{0.022} \equiv \frac{\text{likelihood} \times \text{prior}}{\text{evidence}}$$

$$= 0.818 \approx \boxed{0.82}$$

Random variables

A random variable is a function that uniquely maps events in a sample space to the set of real numbers.

A random variable X may be:

- Discrete
- Continuous
- Mixed (probability defined over both discrete and range of continuous values)

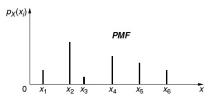
Probability mass function (PMF)

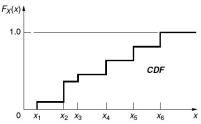
The PMF is given by

$$p_X(x_i) \equiv P(X = x_i) \quad \forall x$$
 (18)

CDF of discrete random variable

$$F_X(x) = \sum_{x_i \le x} P(X = x_i)$$
$$= \sum_{x_i \le x} p_X(x_i)$$





The probability masses in a PMF sum up to 1.

Probability density function (PDF)

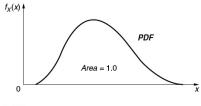
The PDF is denoted $f_X(x)$ such that the probability of X in the interval (a, b] is:

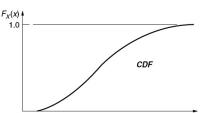
$$P(a < X \le b) = \int_a^b f_X(x) dx \quad (19)$$

CDF of continuous random variable

$$F_X(x) = P(X \le x)$$
$$= \int_{-\infty}^x f_X(\tau) d\tau$$

It follows that the PDF is the derivative of the CDF:





The total area under a PDF is 1.

Central values

These include the mean, median and mode.

• Mean: weighted average (by probability of occurence) or expected value

$$\mathbb{E}(X) = \mu_X = \sum_i x_i p_X(x_i) \text{ discrete case}$$
 (21)

$$\mathbb{E}(X) = \mu_X = \int_{-\infty}^{\infty} x f_X(x) dx \quad \text{continuous case}$$
 (22)

Generalized expectation

The mathematical expectation can be defined for a function g of random variable X:

$$\mathbb{E}[g(X)] = \sum_{i} g(x_i) p_X(x_i) \quad \text{discrete case}$$
 (23)

$$\mathbb{E}[g(X)] = \int_{-\infty}^{\infty} g(x) f_X(x) dx \quad \text{continuous case}$$
 (24)

Measures of dispersion

Variance

In discrete case:

$$V(X) = \sum_{i} (x_i - \mu_X)^2 p_X(x_i)$$
 (25)

In continuous case:

$$\mathbb{V}(X) = \int_{-\infty}^{\infty} (x - \mu_X)^2 f_X(x) dx$$
 (26)

Expanding both equations results in:

$$\mathbb{V}(X) = \mathbb{E}(X^2) - \mu_X^2 = \mathbb{E}(X^2) - \mathbb{E}(X)^2$$
 (27)

Measures of dispersion (cont.)

Standard deviation

The standard deviation is convenient as it has the same unit as the random variable:

$$\sigma_X = \sqrt{\mathbb{V}(X)} \tag{28}$$

Coefficient of variation

The COV gives the deviation relative to the mean. It is unitless.

$$\delta_X = \frac{\sigma_X}{\mu_X} \tag{29}$$

Mean of a linear function

For a continuous random variable X, the mean is defined as

$$\mathbb{E}(X) = \int_{-\infty}^{\infty} x f_X(x) dx \tag{30}$$

Now, given that Z = aX + bY, then the mean of Z is

$$\mathbb{E}(Z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (aX + bY) f_{X,Y} dx dy$$

$$= a \int_{-\infty}^{\infty} x f_{X}(x) dx + b \int_{-\infty}^{\infty} y f_{Y}(y) dy$$

$$= a \mathbb{E}(X) + b \mathbb{E}(Y)$$

Variance of a linear function

We also recall the variance of an r.v. X:

$$\mathbb{V}(X) = \mathbb{E}[(X - \mu_X)^2] \tag{31}$$

Thus, for Z = aX + bY:

$$V(Z) = \mathbb{E}[((aX + bY) - (a\mu_X + b\mu_Y))^2]$$

$$= \mathbb{E}[(a(X - \mu_X) + b(Y - \mu_Y))^2]$$

$$= \mathbb{E}[a^2(X - \mu_X)^2 + 2ab(X - \mu_X)(Y - \mu_Y) + b^2(Y - \mu_Y)]$$

$$= a^2V(X) + b^2V(Y) + 2abCov(X, Y)$$

Moments

The m-th order moment of a distribution is given by:

$$\mathbb{E}(X^m) = \begin{cases} \sum_i x_i^m \cdot p_X(x_i) & \text{(discrete)} \\ \int x^m \cdot f_X(x) dx & \text{(continuous)} \end{cases}$$
(32)

- *m*-th central moment: $\mathbb{E}[(X \mu_X)^m]$
- Normalized *m*-th central moment: $\left(\frac{\mathbb{E}[(X-\mu_X)^m]}{\sigma^m}\right)$

Examples

- **Mean**: first moment, $\mathbb{E}(X)$
- **Variance**: second central moment, $\mathbb{E}[(X \mu_X)^2]$
- Skewness: normalized third central moment, $\left(\frac{\mathbb{E}[(X-\mu_X)^3]}{\sigma^3}\right)$

Covariance and correlation

Recall that the variance of an r.v. X is given by:

$$\mathbb{V}(X) = \mathbb{E}[(X - \mu_X)^2] = \mathbb{E}(X^2) - \mathbb{E}(X)^2$$
(33)

Then given two r.v.'s X and Y, the *covariance* measures the strength of the linear relationship between them.

Covariance

$$Cov(X,Y) = \mathbb{E}[(X - \mu_X)(Y - \mu_Y)] = \mathbb{E}(XY) - \mathbb{E}(X)\mathbb{E}(Y)$$
 (34)

Correlation coefficient

This is the normalized covariance

$$\rho = \frac{Cov(X, Y)}{\sigma_X \sigma_Y} \tag{35}$$

Joint distributions

Given two random variables X and Y:

Discrete case

The joint PMF is:

$$p_{X,Y}(x_i, y_j) = P(X = x_i, Y = y_j)$$
(36)

The CDF is:

$$F_{X,Y}(x,y) = \sum_{x_i \le x} \sum_{y_i \le y} p_{X,Y}(x_i, y_j)$$
(37)

Continuous case

The joint probability is given by:

$$P(a < X \le b, c < Y \le d) = \int_{a}^{b} \int_{c}^{d} f_{X,Y}(x, y) dy dx$$
 (38)

Conditional distributions of continuous random variables

Recall the definition of conditional probability (multiplication rule):

$$P(A|B) = \frac{P(AB)}{P(B)} \tag{39}$$

$$P(AB) = P(A|B)P(B) = P(B|A)P(A)$$
(40)

Similarly, for two continuous r.v.'s, the conditional PDF of X given Y is:

$$f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)} \tag{41}$$

Joint PDF and CDF of two variables

The joint PDF is given by:

$$f_{X,Y}(x,y) = f_{X|Y}(x|y)f_Y(y) = f_{Y|X}(y|x)f_X(x)$$
 (42)

While the joint CDF is given by:

$$F_{X,Y}(a,b) = P(X \le a, Y \le b) = \int_{-\infty}^{a} \int_{-\infty}^{b} f_{X,Y}(x,y) dy dx$$
 (43)

Marginal distributions of continuous random variables

Recall the theorem of total probability:

$$P(A) = \sum_{i=1}^{n} P(A|E_i)P(E_i)$$
 (44)

Similarly, the marginal PDFs from a joint distribution of two continuous r.v.'s X and Y is given as:

$$f_X(x) = \int_{-\infty}^{\infty} f_{X|Y}(x|y) f_Y(y) dy = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dy$$
 (45)

$$f_{Y}(y) = \int_{-\infty}^{\infty} f_{Y|X}(y|x) f_{X}(x) dx = \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx$$
 (46)

Bernoulli distribution

Let X be an event with only two outcomes $\{1,0\}$. And let the probability of the event be given by:

$$p(X) = \theta, \quad 0 \le \theta \le 1$$

And $p(X = 1) = \theta$ and $p(X = 0) = 1 - \theta$. X is said to be Bernoulli distributed:

$$X \sim \mathrm{Ber}(\theta)$$
 (47)

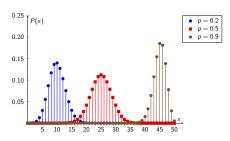
The PMF is then given by:

$$Ber(x|\theta) := \theta^{x} (1 - \theta)^{1 - x}$$
(48)

Binomial distribution

Given a Bernoulli sequence with X random number of occurrences of an event, N trials and θ the probability of occurrence of each event:

- $X \sim \text{Bin}(N, \theta)$
- PMF: $P(X = x) := Bin(x|N,\theta) := \binom{N}{x} p^x (1-\theta)^{N-x}, \quad x = 0,1,2,\ldots,N$
- CDF: $F_X(x) = P(X \le x) = \sum_{k=0}^{x} {N \choose k} \theta^k (1-\theta)^{N-k}$
- Mean: $\mathbb{E}(X) = N\theta$
- Variance: $\mathbb{V}(X) = N\theta(1-\theta)$



Bernoulli, binomial, categorical and multinomial

- ullet The Bernoulli distribution is a special case of the binomial distribution with ${\it N}=1$
- The categorical distribution is generalization of the Bernoulli to more than two outcomes for a single trial (e.g. set of labels $x \in \{1, ..., C\}, C > 2$):

$$\operatorname{Cat}(\mathbf{x}|\boldsymbol{\theta}) := \prod_{c=1}^{C} \theta_{c}^{\mathsf{x}_{c}}$$
 (49)

where x is a one-hot vector (e.g. (1,0,0,0) for class 1 of four classes)

 The multinomial distribution generalizes the categorical distribution for multiple trials:

$$\mathscr{M}(\mathbf{x}|N,\boldsymbol{\theta}) := \binom{N}{N_1 \dots N_C} \prod_{c=1}^C \theta_c^{N_c}$$
 (50)

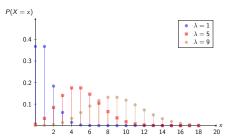
Poisson distribution

- The Poisson distribution is used to model the probability that a number of independent events occur within a fixed time interval (or within a finite space)
- Such events are described as Poisson processes
- The PMF of a Poisson random variable with rate parameter λ is given by:

$$P(X = x) := \operatorname{Poiss}(x|\lambda) := \frac{\lambda^x}{x!} e^{-\lambda}, \quad x \ge 0$$
 (51)

The mean and variance of a Poisson random variable are equal:

$$\mathbb{E}(X) = \mathbb{V}(X) = \lambda \tag{52}$$



Gaussian distribution

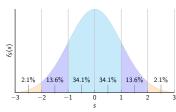
The PDF of a Gaussian (normal) distribution $X \sim \mathcal{N}(\mu, sigma^2)$ is given by:

$$\mathcal{N}(x|\mu,\sigma^2) := \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2\right]$$
 (53)

where μ is the mean and σ^2 is the variance.

$$P(a < X \le b) = \frac{1}{\sigma\sqrt{2\pi}} \int_{a}^{b} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^{2}} dx = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)$$
 (54)

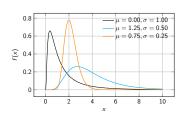
where Φ is the CDF of the standard normal distribution (N(0,1)).



Lognormal distribution

A random variable X that is lognormally distributed with the parameters μ and σ^2 (denoted $X \sim \mathcal{LN}(\mu, \sigma^2)$ has the PDF:

$$\mathscr{LN}(x|\mu,\sigma^2) = \frac{1}{(\sigma x)\sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\ln(x) - \mu}{\sigma}\right)^2\right] \quad x \ge 0$$
 (55)



CDF:
$$F_X(x) = P(X \le x) = \Phi((\ln(x) - \mu)/\sigma)$$

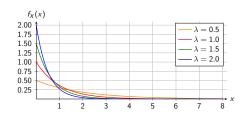
Mean: $\mathbb{E}(X) = e^{\left(\mu + \frac{1}{2}\sigma^2\right)}$

Variance: $\mathbb{V}(X) = (e^{\sigma^2} - 1)e^{(2\mu + \sigma^2)}$

Exponential distribution

A random variable X exponentially distributed with parameter λ has the PDF:

$$\operatorname{Exp}(x|\lambda) = \lambda e^{-\lambda x} \qquad x > 0 \tag{56}$$



CDF:

$$F_X(x) = P(X \le x) = 1 - e^{-\lambda x}, \quad x > 0$$
 (57)

Mean:

$$\mathbb{E}(X) = 1/\lambda \tag{58}$$

Variance:

$$\mathbb{V}(X) = 1/\lambda^2 \tag{59}$$

Multivariate normal distribution (MVN)

The MVN PDF is given by:

$$\mathscr{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) := \frac{1}{(2\pi)^{D/2} |\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right]$$
(60)

where:

- $oldsymbol{\mu} = \mathbb{E}[oldsymbol{x}] \in \mathbb{R}^D$ is the mean vector
- $\Sigma = \text{Cov}[x]$ is the $D \times D$ covariance matrix:

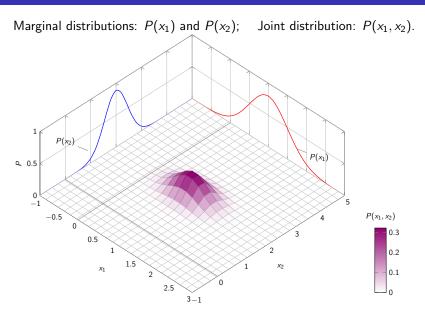
$$Cov[x] := \mathbb{E}\left[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^T \right]$$
(61)

In 2D:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12}^2 \\ \sigma_{21}^2 & \sigma_2^2 \end{pmatrix} = \begin{pmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 \end{pmatrix}$$
 (62)

where ρ is the correlation coefficient.

Bivariate MVN



Reading

- PMLI 1, 2, 3
- PMLCE 1, 3, 4