CEE 616: Probabilistic Machine Learning

Lecture 1a: Foundations: Probability

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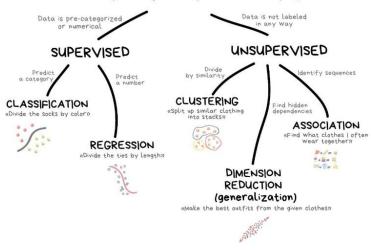
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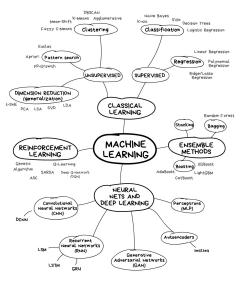
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Introduction

CLASSICAL MACHINE LEARNING





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Introduction
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Introduction

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

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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

Introduction

Notation

Symbol Meaning

number of observations (distinct data points)

number of variables

value of jth variable for ith observation

So, we can write the $n \times p$ matrix **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 **X** are: x_1, x_2, \ldots, x_n and the columns are written x_1, x_2, \dots, x_p

Notation (cont.)

Introduction

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

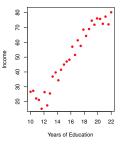
Summary of notation conventions

- 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

Introduction

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*.



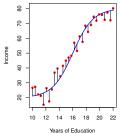


Figure: Estimating the functional relationship between income and educational attainment in a data set

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)
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Introduction

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)

0000000000000 Inference

Introduction

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):

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

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

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

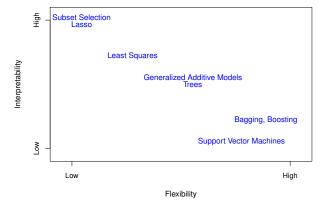
The estimation procedure can be a method of choice, e.g. OLS (ordinary least squares), WLS (weighted least squares), etc.

Introduction 0000000000000

- 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.



Occam's razor

Introduction 000000000000

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."

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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:

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

Independent events:

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

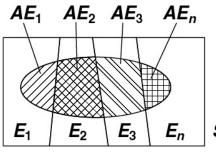
 Generally, the joint probability (intersection) of any number of independent events is the product of their individual probabilities:

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

Multiplication rule:

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

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:

 $P(AE_1) = P(A|E_1)P(E_1),$

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)

etc.

Recall from the multiplication rule that:

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

Equivalently:

$$P(AB) = P(B|A)P(A) \tag{12}$$

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 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

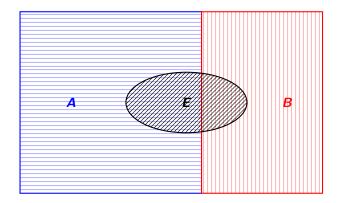
B = aggregates supplied by Company b

E = aggregates are substandard

- a 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.

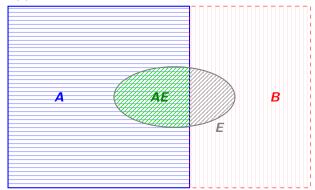
Example 1: Construction supplies (cont.)

① 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



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

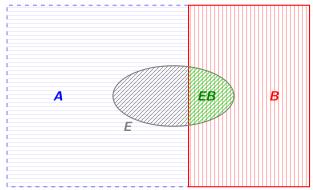
$$P(E|A) = \frac{P(EA)}{P(A)}$$



Example 1: Construction supplies (cont.)

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

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



Example 1: Construction supplies (cont.)

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':

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

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

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

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

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)

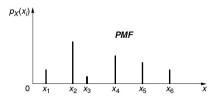
Probability mass function (PMF)

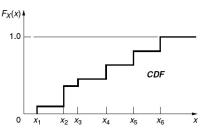
The PMF is given by

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

CDF of discrete random variable

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





The probability masses in a PMF sum up to 1.

Probability density function (PDF)

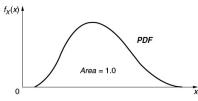
The PDF is denoted $f_X(x)$ such that the probability of X in the interval (a, b] is:

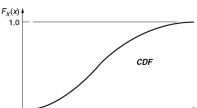
$$P(a < X \le b) = \int_a^b f_X(x) dx \quad (19)$$

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)

Variance

In discrete case:

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

In continuous case:

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

Expanding both equations results in:

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

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

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:

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

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

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

$$= a^2\mathbb{V}(X) + b^2\mathbb{V}(Y) + 2abCov(X, Y)$$

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

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

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:

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

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 Xand 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:

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

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

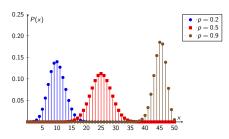
$$X \sim \mathrm{Ber}(\theta) \tag{47}$$

The PMF is then given by:

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

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: $P(X = x) := Bin(x|N,\theta) := \binom{N}{x} p^x (1-\theta)^{N-x}, \quad x = 0, 1, 2, ..., N$
- 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: $\mathbb{V}(X) = N\theta(1-\theta)$



- 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)

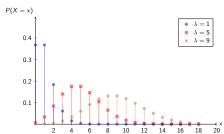
Poisson distribution

- 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:

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

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

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



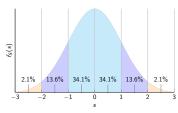
The PDF of a Gaussian (normal) distribution $X \sim \mathcal{N}(\mu, sigma^2)$ is given by:

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

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

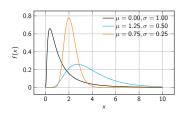
$$P(a < X \le b) = \frac{1}{\sigma\sqrt{2\pi}} \int_{a}^{b} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^{2}} dx = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)$$
 (54)

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



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)



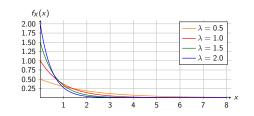
CDF:
$$F_X(x) = P(X \le x) = \Phi((\ln(x) - \mu)/\sigma)$$

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

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

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:

- $\mu = \mathbb{E}[x] \in \mathbb{R}^D$ 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)

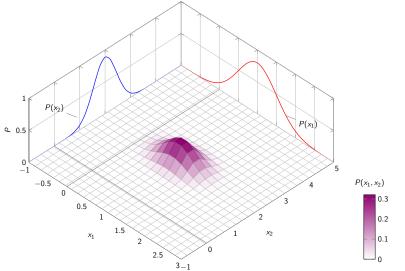
In 2D:

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

where ρ is the correlation coefficient.

Bivariate MVN

Marginal distributions: $P(x_1)$ and $P(x_2)$; Joint distribution: $P(x_1, x_2)$.



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