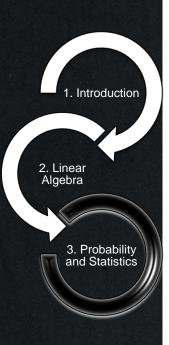
Scientific Machine and Deep Learning for Design and Construction in Civil Engineering





Introduction

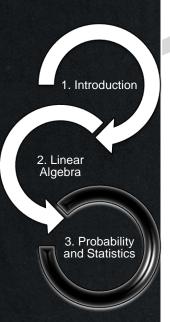
Linear Algebra

- Scalars, Vectors, Matrices
- Matrix Operations
- Norms, Determinant
- Eigenvalues and Eigenvectors

Probability and Statistics

- Random Variables
- Expectation operator
- Bayes
- Important distributions
- Monte Carlo

01. Introduction



Dr. Michael A. Kraus

- PhD with honors 2019

 @ Bundeswehr University Munich
- Post-Doc @ Stanford University
- Post-Doc @ ETH Zürich



Dr. Danielle Griego

- PhD 2020@ ETH Zürich
- Post-Doc @ ETH Zürich
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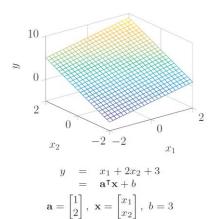
Sophia Kuhn, M.Sc.

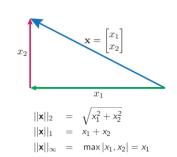
- M.Sc. Civil Engineering 2021
 @ ETH Zürich
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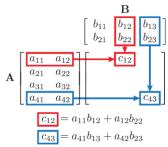


O1. Introduction Content of this Lecture

Linear Algebra

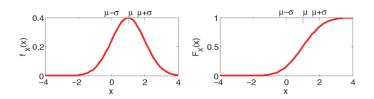






Probability / Statistics

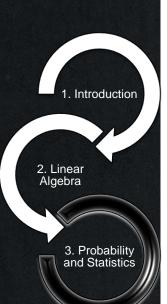
$$\Pr(E_1|A) = \frac{\Pr(A|E_1)\Pr(E_1)}{\Pr(A)}$$



$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]$$

Moment of order m: $\mathbb{E}[X^m]$

$$\mathbb{E}[X^m] = \int_{-\infty}^{\infty} x^m f_X(x) dx$$



02. Linear Algebra Basic Definitions

Notation

we assume, that there is at least some basic linear algebra background prior to this lecture

Relevant Elements from Linear Algebra

- scalars
- vectors
- matrices
- tensors

02. Linear Algebra

Basic Definitions

Notation

Scalar → single number

$$x \in \mathbb{R} = (-\infty; \infty)$$

$$\in \mathbb{R}^+ = (0; \infty)$$

$$\in \mathbb{Z} = (-\infty; \dots -1, 0; 1, \dots, \infty)$$

$$\in (0; 1)$$

$$\in (0; 1]$$

02. Linear Algebra Basic Definitions

Notation

Vector → 1-D array containing numbers or scalars

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

If e.g. each $[x]_i \in \mathbb{R}$, $\forall i = \{1: n\} \rightarrow x \in \mathbb{R}^n$

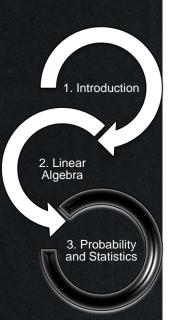
02. Linear Algebra Basic Definitions

Notation

Matrix → 2-D array containing numbers or scalars

$$\boldsymbol{X} = \begin{bmatrix} x_{11} & x_{12} & x_{1n} \\ \vdots & \vdots & \dots & \vdots \\ x_{m1} & x_{m2} & x_{mn} \end{bmatrix}$$

If e.g. each $[X]_{ij} \in \mathbb{R}, \forall i = \{1: m\}, j = \{1: n\}, \rightarrow X \in \mathbb{R}^{m \times n}$



02. Linear Algebra Basic Definitions

Notation

Matrix → 2-D array containing numbers or scalars Special types:

- square matrices: $X \in \mathbb{R}^{n \times n}$

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nn} \end{bmatrix}$$

02. Linear Algebra Basic Definitions

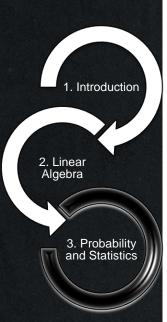
Notation

Matrix \rightarrow 2-D array containing numbers or scalars

Special types:

- square matrices: $X \in \mathbb{R}^{n \times n}$
- diagonal matrices: special square matrices with elements just on diagonal: Y = diag(x)

$$\mathbf{Y} = \operatorname{diag}(\mathbf{x}) = \left[egin{array}{cccc} x_1 & 0 & \cdots & 0 \\ 0 & x_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & x_n \end{array}
ight]_{n \times n}$$



02. Linear Algebra Basic Definitions

Notation

Matrix \rightarrow 2-D array containing numbers or scalars

Special types:

- square matrices: $X \in \mathbb{R}^{n \times n}$
- diagonal matrices: special square matrices with elements just on diagonal: Y = diag(x)
- Identity matrix: special diagonal matrix with just 1 on diagonal

$$oldsymbol{\mathsf{I}} = \left[egin{array}{cccc} 1 & 0 & \cdots & 0 \ 0 & 1 & \cdots & 0 \ dots & dots & \ddots & dots \ 0 & 0 & \cdots & 1 \end{array}
ight]_{n imes n}$$

02. Linear Algebra **Basic Definitions**

Notation

Matrix \rightarrow 2-D array containing numbers or scalars

Special types:

- square matrices: $X \in \mathbb{R}^{n \times n}$
- diagonal matrices: special square matrices with elements just on diagonal: Y = diag(x)
- Identity matrix: special diagonal matrix with just 1 on diagonal
- Block diagonal matrix: concatenates several matrices on diagonal

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix} \qquad \text{blkdiag}(\mathbf{A}, \mathbf{B}) = \begin{bmatrix} 1 & 2 & 0 & 0 & 0 \\ 3 & 4 & 0 & 0 & 0 \\ 0 & 0 & 4 & 5 & 6 \\ 0 & 0 & 7 & 8 & 9 \\ 0 & 0 & 10 & 11 & 12 \end{bmatrix}$$

02. Linear Algebra Basic Definitions

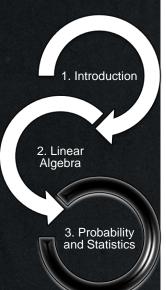
Linear Algebra Operations

Transposition

Matrix multiplication

Matrix inversion

02. Linear Algebra Basic Definitions



Linear Algebra Operations

- Transposition

$$\mathbf{X} = \left[egin{array}{cccc} x_{11} & x_{12} & x_{13} \ x_{21} & x_{22} & x_{23} \end{array}
ight]
ightarrow \ \mathbf{X}^\intercal = \left[egin{array}{cccc} x_{11} & x_{21} \ x_{12} & x_{22} \ x_{13} & x_{23} \end{array}
ight]$$

- Matrix multiplication

$$[\mathbf{X}^{\intercal}]_{ij} = [\mathbf{X}]_{ji}$$

- Matrix inversion

02. Linear Algebra Basic Definitions

Linear Algebra Operations

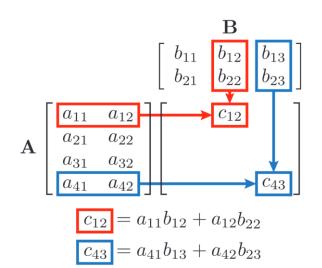
 $\begin{array}{rcl}
\mathsf{C} &=& \mathsf{A}\mathsf{B} \\
&=& \mathsf{A} \times \mathsf{B}
\end{array}$

- Transposition

$$[\mathbf{C}]_{ij} = \sum_{k} [\mathbf{A}]_{ik} \cdot [\mathbf{B}]_{kj}$$

 $\mathbf{C}_{m \times n} = \mathbf{A}_{m \times k} \mathbf{B}_{k \times n}$

- Matrix multiplication



- Matrix inversion

$$A(B+C) = AB+AC$$
 (Distributivity)
 $A(BC) = (AB)C$ (Associativity)
 $AB \neq BA$ (Not commutative)
 $(AB)^T = B^TA^T$ (Conjugate transposability)
 $x^Ty = x \cdot y$ (Inner product)

02. Linear Algebra

Basic Definitions

Linear Algebra Operations

- Transposition

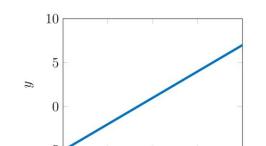
1. Introduction

3. Probability and Statistics

2. Linear Algebra

- Matrix multiplication

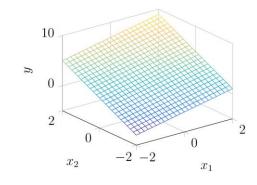
- Matrix inversion



$$y = 3x + 1$$
$$= ax + b$$

$$a = 3, b = 1$$

Example: Linear Systems

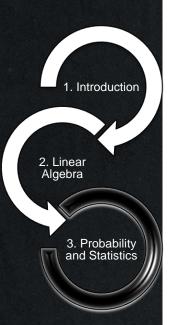


$$y = x_1 + 2x_2 + 3$$

= $\mathbf{a}^{\mathsf{T}}\mathbf{x} + b$

$$\mathbf{a} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \ \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \ b = 3$$

from [2]



02. Linear Algebra Basic Definitions

Linear Algebra Operations

- Transposition

Matrix multiplication

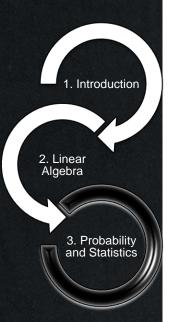
Matrix inversion

Hadamar product element-wise product

$$C = A \odot B$$

$$[\mathbf{C}]_{ij} = [\mathbf{A}]_{ij} \cdot [\mathbf{B}]_{ij}$$

$$C_{m\times n} = A_{m\times n} \odot B_{m\times n}$$



02. Linear Algebra Basic Definitions

Linear Algebra Operations

- Transposition

- Matrix multiplication

- Matrix inversion

To be invertible, a matrix:

- must be square
- must not have linearly dependent rows or columns

$$X^{-1}A = I$$

Systems of linear equations

$$Ax = b$$

$$A^{-1}Ax = A^{-1}b$$

$$Ix = A^{-1}b$$

$$x = A^{-1}b$$

02. Linear Algebra

Basic Definitions

Norms of Vectors and Matrices

Measure how large a vector / matrix is.

 L^p norm is defined as

$$||\mathbf{x}||_{p} = \left(\sum_{i} |[\mathbf{x}]_{i}|^{p}\right)^{\frac{1}{p}} \qquad (L^{p}\text{-norm})$$

$$||\mathbf{x}||_{2} = \sqrt{\sum_{i} [\mathbf{x}]_{i}^{2}} \equiv \sqrt{\mathbf{x}^{\mathsf{T}}\mathbf{x}} \quad (\text{Euclidian norm})$$

$$||\mathbf{x}||_{1} = \sum_{i} |[\mathbf{x}]_{i}| \qquad (\text{Manhattan norm})$$

$$||\mathbf{x}||_{\infty} = \max_{i} |[\mathbf{x}]_{i}| \qquad (\text{Max norm})$$

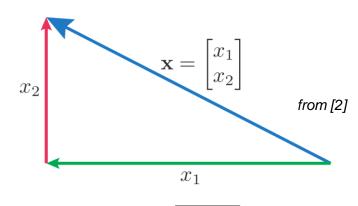
1. Introduction 2. Linear Algebra 3. Probability

and Statistics

02. Linear Algebra Basic Definitions

Norms of Vectors and Matrices

L^2 norm is the most common norm



$$||\mathbf{x}||_2 = \sqrt{x_1^2 + x_2^2}$$

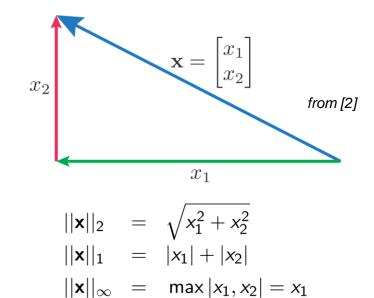
 $||\mathbf{x}||_1 = |x_1| + |x_2|$
 $||\mathbf{x}||_{\infty} = \max |x_1, x_2| = x_1$

Task (2 minutes) draw lines for $||x||_p = 1$ for p = 0.5; 1; 2; 20; ∞

02. Linear Algebra Basic Definitions

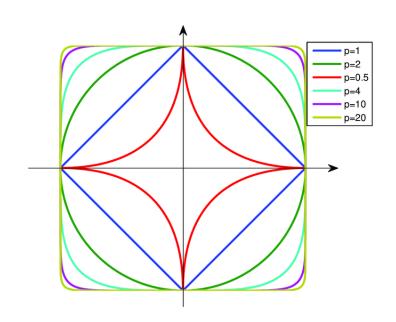
Norms of Vectors and Matrices

L^2 norm is the most common norm



Task (2 minutes)

draw lines for $||x||_p = 1$ for p = 0.5; 1; 2; 20; ∞



02. Linear Algebra Basic Definitions

Norms of Vectors and Matrices

Determinant det(A)

For a square matrix $[A]_{n\times n}$, $\det(A) \to \mathbb{R}$

The determinant measures how much a matrix contracts or expands in space

det(A) = 1: preservers space / volume

det(A) = 0: contracts the space / volume along 1-D

The determinant is the product of the eigenvalues of a matrix

02. Linear Algebra Basic Definitions

Norms of Vectors and Matrices

Eigen Decomposition

A square matrix $[A]_{n\times n}$ can be decomposed in eigenvectors $\{\nu_1, ..., \nu_n\}$ and eigenvalues $\{\lambda_1, ..., \lambda_n\}$. This can be written in matrix form:

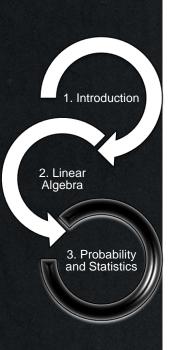
$$V = [v_1, ..., v_n]$$
, $\lambda = [\lambda_1, ..., \lambda_n]^T$
 $A = V \operatorname{diag}(\lambda)V^{-1}$

A matrix is positive definite if all eigenvalues > 0

A matrix is positive semi-definite if all eigenvalues ≥ 0

For positive semidefinite matrices:

 $\forall x, x^T A x \geq 0$



02. Linear Algebra Summary

Matrix transposition

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ x_{21} & x_{22} & x_{23} \end{bmatrix} \rightarrow \mathbf{X}^{\mathsf{T}} = \begin{bmatrix} x_{11} & x_{21} \\ x_{12} & x_{22} \\ x_{13} & x_{23} \end{bmatrix}$$

Matrix multiplication

$$\mathbf{C} = \mathbf{AB}$$

$$= \mathbf{A} \times \mathbf{B}$$

$$[\mathbf{C}]_{ij} = \sum_{k} [\mathbf{A}]_{ik} \cdot [\mathbf{B}]_{kj}$$

$$\mathbf{C}_{m \times n} = \mathbf{A}_{m \times k} \mathbf{B}_{k \times n}$$

Element-wise product

$$\begin{array}{ccc} \mathbf{C} & = & \mathbf{A} \odot \mathbf{B} \\ [\mathbf{C}]_{ij} & = & [\mathbf{A}]_{ij} \cdot [\mathbf{B}]_{ij} \\ \mathbf{C}_{m \times n} & = & \mathbf{A}_{m \times n} \odot \mathbf{B}_{m \times n} \end{array}$$

Matrix inversion

$$\mathsf{A}^{-1}\mathsf{A}=\mathsf{I}$$

Norm of a vector

$$||\mathbf{x}||_2 = \sqrt{\sum_i [\mathbf{x}]_i^2} \equiv \sqrt{\mathbf{x}^\mathsf{T}\mathbf{x}}$$

Determinant

 $det(\mathbf{A}): \mathbb{R}^{n \times n} \to \mathbb{R}$ measures how much the matrix contracts or expands the space

Eigendecomposition

A matrix is **positive semidefinite** if all eigenvalues ≥ 0 . For positive semidefinite (PSD) matrices

$$\forall \mathbf{x}, \mathbf{x}^\mathsf{T} \mathbf{A} \mathbf{x} \geq 0$$

Q & A

Break

03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – univariate random variables

we assume, that there is at least some basic understanding of probability prior to this lecture

Random Phenomena; Experiments

- study of random phenomena
- Experiments have different outcomes ξ_i (random variable / RV)
- A set of all outcomes is $\Omega = \{\xi_1, ..., \xi_K\}$
- An event is a subset of Ω : $E_i \subset \Omega$
- Outcomes have certain underlying patterns about them
- Experiments are conducted under repeatable conditions
- Probability of an event $1 \ge \Pr(E_i) \ge 0$
- Frequentist / Bayesian definition of probability

03. Probability / Statistics Basic Definitions of Probability

Probability mass and density function – univariate random variables

1. Introduction

2. Linear Algebra

3. Probability and Statistics

Description of discrete RV:

Probability Mass Function (PMF)

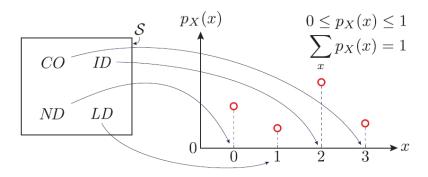
$$Pr(X = x) = Pr(x) = p_X(x) = p(x)$$

$$\mathcal{S} = \left\{ \begin{array}{c} \text{no damage (ND)} \\ \text{light damage (LD)} \\ \text{important damage (ID)} \\ \text{collapse (CO)} \end{array} \right\} \qquad \text{from [2]}$$

Properties

$$0 \le p_X(x) \le 1$$

$$\sum_x p_X(x) = 1$$



Light or important damage: $\{1 \le x \le 2\}$

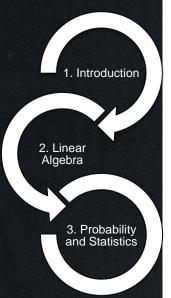
03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – univariate random variables

Description of continuous RV:

Probability Density Function (PDF)



$$f_X(x) = f(x)$$

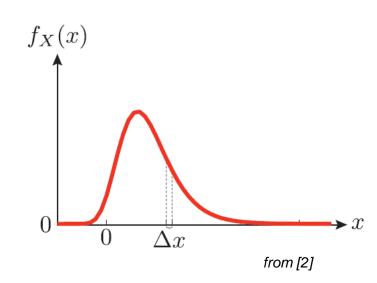
 $Pr(x \le X \le x + \Delta x) = f_X(x)\Delta x$

Properties

$$Pr(X = x) = 0$$

$$f_X(x) \ge 0$$

$$\int_{-\infty}^{\infty} f_X(x) dx = 1$$



03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – univariate random variables

1. Introduction

2. Linear
Algebra

3. Probability and Statistics

Description of RV: Cumulative Distribution Function (CDF)

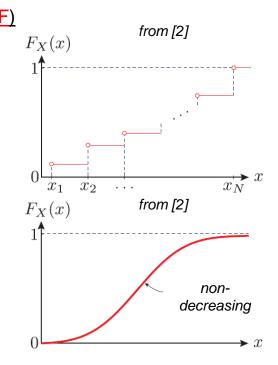
continous
$$F_X(x) = \int_{-\infty}^{x'} f_X(x') dx \Leftrightarrow f_X(x) = \frac{dF_X(x)}{dx}$$

discrete
$$F_X(x) = \Pr(X \le x) = \sum_{x' \le x} p_X(x')$$

Properties

$$F_X(-\infty)=0$$

$$F_X(\infty)=1$$



03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – multivariate random variables

Description of multivariate RV:

Given
$$\mathbf{X} = [X_1, X_2, \cdots, X_n]^{\mathsf{T}} \left\{ \begin{array}{l} \text{vector (column) of} \\ \text{random variables} \end{array} \right.$$

Given
$$\mathbf{x} = [x_1, x_2, \dots, x_n]^\mathsf{T} \left\{ \begin{array}{l} \text{vector describing} \\ \text{the outcomes a} \\ \text{random variable } \mathbf{X} \end{array} \right.$$

X describes the simultaneous realization of several phenomena

03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – multivariate random variables

Description of discrete RV:

Definition: $p_X(x) = \Pr(X_1 = x_1 \cap X_2 = x_2 \cap \dots \cap X_n = x_n)$

$$0 \le p_X(x) \le 1$$

Marginalization

$$\sum_{x_n} p_{X_1...X_n}(x_1,...,x_n) = p_{X_1...X_{n-1}}(x_1,...,x_{n-1})$$

 $p_{X_i}(x_i)$: Marginal PMF

$$\sum_{x_1} \dots \sum_{x_n} p_X(x) = 1$$

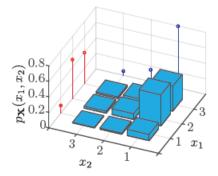
03. Probability / Statistics **Basic Definitions of Probability**

Probability mass and density function – multivariate random variables

Given two discrete R.V. $X_1 \perp X_2$

$$p_{X_1}(x_1) \begin{cases} p_{X_1}(1) = 0.1 \\ p_{X_1}(2) = 0.5 \\ p_{X_1}(3) = 0.4 \end{cases}$$

$$p_{X_2}(x_2) \begin{cases} p_{X_2}(1) = 0.8 \\ p_{X_2}(2) = 0.15 \\ p_{X_2}(3) = 0.05 \end{cases} \qquad p_{X_1X_2}(x_1, x_2) = p_{X_1}(x_1) \cdot p_{X_2}(x_2)$$



$$p_{X_1X_2}(x_1,x_2) = p_{X_1}(x_1) \cdot p_{X_2}(x_2)$$

$$p_{\mathbf{X}}(x_1, x_2) = \begin{cases} x_2 = 1 & x_2 = 2 & x_2 = 3 \\ \hline x_1 = 1 & 0.08 & 0.015 & 0.005 \\ x_1 = 2 & 0.4 & 0.075 & 0.025 \\ x_1 = 3 & 0.32 & 0.06 & 0.02 \end{cases} \begin{array}{c} n=3 \\ \sum_{i=1}^{n=3} p_{\mathbf{X}}(x_1, i) \\ 0.1 \\ 0.5 \\ 0.4 \\ from [2] \end{cases}$$

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. Introduction

3. Probability and Statistics

2. Linear Algebra

03. Probability / Statistics

Basic Definitions of Probability

Probability mass and density function – multivariate random variables

Description of continous RV:

Definition:
$$f_X(x)\Delta x = \Pr(x_1 < X_1 < x_1 + \Delta x_1 \cap \dots \cap x_1 < X_n < x_n + \Delta x_n)$$

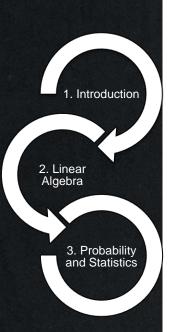
 $0 \le f_X(x)$ (may be larger than 1!!)

Marginalization

$$\int_{-\infty}^{\infty} f_{X_1 \dots X_n}(x_1, \dots, x_n) dx_n = f_{X_1 \dots X_n}(x_1, \dots, x_n)$$

$$\sum_{x_{-}} \dots \sum_{x_{-}} p_X(x) = 1$$

 $p_{X_i}(x_i)$: Marginal PMF



03. Probability / Statistics

Basic Definitions of Probability

Expectation and variance operator

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} x \cdot f_x(x) dx$$

(continuous R.V.)

$$\mathbb{E}[X] = \sum x \cdot p_{x}(x) dx$$

(discrete R.V.)

Moment of order m: $\mathbb{E}[X^m]$

 $\mathbb{E}[X^m] = \int_{-\infty}^{\infty} x^m f_X(x) dx$

For m=1: $\mathbb{E}[X] = \mu_X$

(expectation / center of gravity)

For $m=2: \mathbb{E}[X^2]$

(expectation of the squares)

Centered moments of order m: $\mathbb{E}[(X - \mu_X)^m]$ $\mathbb{E}[(X - \mu_X)^m] = \int_{-\infty}^{\infty} (X - \mu_X)^m f_x(x) dx$

For
$$m=1$$
: $\mathbb{E}[(X - \mu_X)^1] = 0$

For $m=2: \mathbb{E}[(X - \mu_X)^2] = \sigma_X^2 = \text{var}[X]$

(variance / inertia)

03. Probability / Statistics Basic Definitions of Probability

Expectation and variance operator

$$Variance - \mathbb{E}[(X - \mu_X)^2]$$

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

var[X]: The variance measures the dispersion of the probability density function. This s concept is analogue to the inertia of a cross-section.

 σ_{x} : Standard deviation

 $\delta_X = \frac{\sigma_X}{\mu_X}$: coefficient of variation (C.O.V.)

adimensional dispersion metric ($\bigwedge \mu_X \neq 0$)

03. Probability / Statistics

Basic Definitions of Probability

Expectation and variance operator

Covariance –
$$\mathbb{E}[(X - \mu_X) - (Y - \mu_Y)]$$

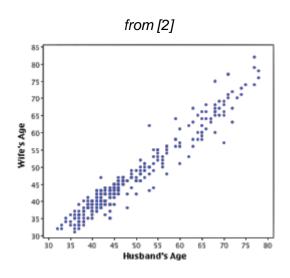
Given two random variables X, Y

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

 ρ_{XY} : correlation coefficient

(quantifies the **linear dependence** between X and Y)

$$\rho_{ij} = \frac{cov[XY]}{\sigma_i \sigma_j}, \quad -1 \le \rho_{XY} \le +1$$



$$\to X \perp\!\!\!\perp Y \Rightarrow \rho_{XY} = 0$$

$$\rightarrow \rho_{XY} = 0 \Rightarrow X \perp \!\!\!\perp Y \wedge$$

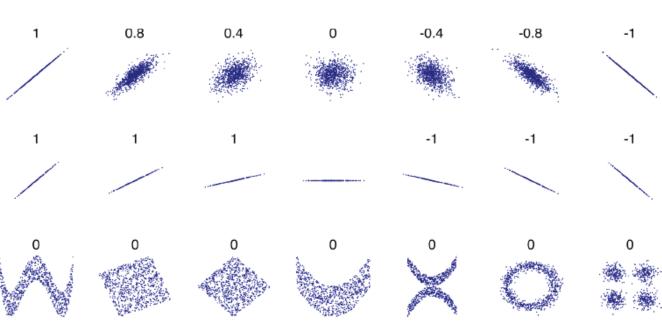
 \rightarrow correlation \Leftrightarrow causality



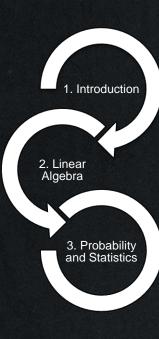
03. Probability / Statistics Basic Definitions of Probability

Variance / Covariance

quantify <u>linear</u> dependence



from [2]



03. Probability / Statistics

Basic Definitions of Probability

Distributions

Parametric Distributions

basic building block: $p(x|\theta)$ defined by parameters θ need to determine θ given a sample $\{x_1, ..., x_N\}$

- Non-Parametric Distributions

are not restricted to specific functional forms

make few assumptions about the shape of the distribution being modelled

03. Probability / Statistics Important Distributions

Bernoulli Distribution

Coin flipping: heads=1, tails=0

$$p(x=1|\mu)=\mu$$

Bernoulli Distribution

Bern
$$(x|\mu) = \mu^x (1 - \mu)^{1-x}$$

$$\mathbb{E}[x] = \mu$$

$$\text{var}[x] = \mu(1 - \mu)$$

03. Probability / Statistics Important Distributions

Binomial Distribution

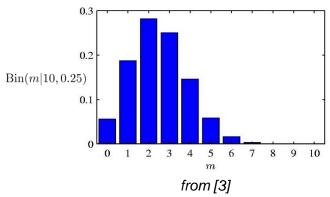
N coin flips: what is the probability of seeing *m* heads

$$p(m \text{ heads}|N, \mu)$$

Binomial Distribution

$$Bin(m|N,\mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}$$

$$\mathbb{E}[m] \equiv \sum_{m=0}^{N} m \text{Bin}(m|N,\mu) = N\mu$$

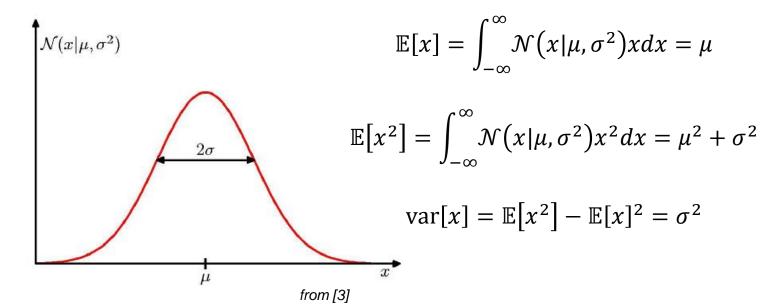


$$var[m] \equiv \sum_{n=0}^{N} (m - \mathbb{E}[m])^{2} Bin(m|N,\mu) = N\mu(1-\mu)$$

03. Probability / Statistics Important Distributions

Normal or Gaussian Distribution (univariate case)

$$\mathcal{N}(x|\mu,\sigma^2) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



Normal or Gaussian Distribution (multivariate case)

5 Parameters:

$$\mu_{X_1}$$
, σ_{X_1} , μ_{X_2} , σ_{X_2} , ρ

 $X \sim \mathcal{N}(x; \mu, \Sigma)$

$$\mu_{X_1}=0$$

. Introduction

3. Probability and Statistics

2. Linear Algebra

$$\mu = \begin{bmatrix} \mu_{X_1} \\ \mu_{X_2} \end{bmatrix}, \qquad \Sigma = \begin{bmatrix} \sigma_{X_1}^2 & \rho \sigma_{X_1} \sigma_{X_2} \\ \rho \sigma_{X_1} \sigma_{X_2} & \sigma_{X_2}^2 \end{bmatrix}$$

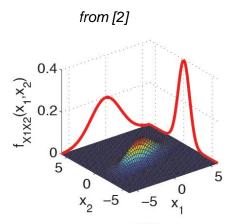
 $\sigma_{X_1}=2$

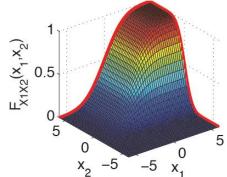
$$\mu_{X_2}=0$$

$$\sigma_{X_2}=1$$

$$\rho = 0.6$$

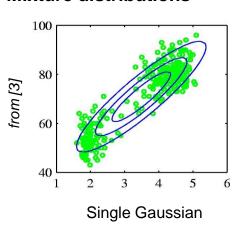
$$F_{X_1,X_2}(X_1,X_2) = \int_{-\infty}^{X_1} \int_{-\infty}^{X_2} f_{X_1,X_2}(X_1,X_2) \partial x \partial y$$

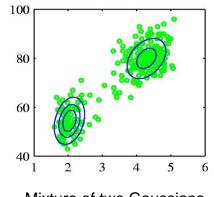




. Introduction 2. Linear Algebra 3. Probability and Statistics

Mixture distributions





(c)

$$P(x) = \sum_{i} P(c = i) P(x|c = i)$$

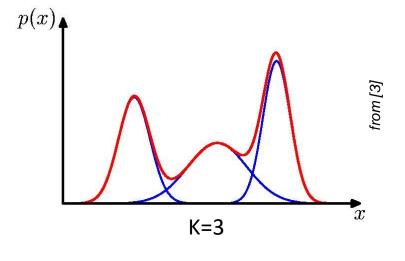
$$p(x) = \sum_{k=1}^{K} \pi_{k} \mathcal{N}(x|\mu_{k} \Sigma_{k})$$
Component
Mixing coefficient

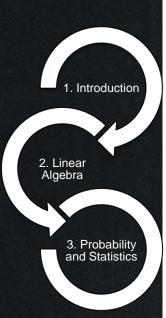
Mixture distributions

Combine simple models into a complex model:

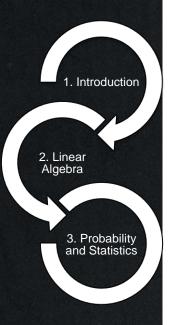
$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x | \mu_k \Sigma_k)$$
Component
Mixing coefficient

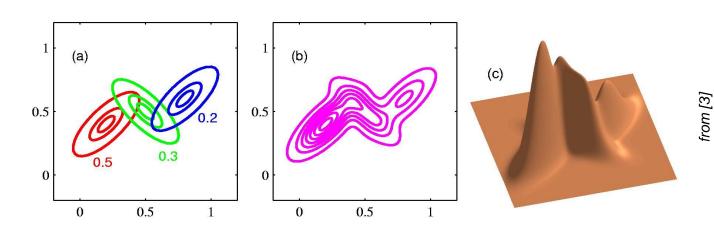
$$\forall k : \pi_k \ge 0 \qquad \sum_{k=1}^K \pi_k = 1$$





Mixture distributions - Example: Mixutre of 3 Gaussians





$$p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x | \mu_k \Sigma_k) \qquad \forall k : \pi_k \ge 0 \qquad \sum_{k=1}^{K} \pi_k = 1$$

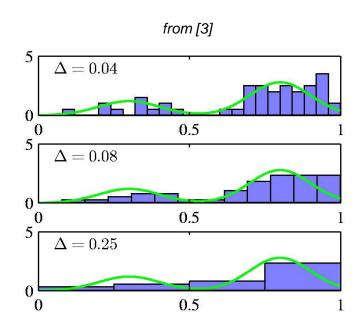
03. Probability / Statistics Important Distributions

Nonparametric Methods

Histogram methods partition the data space in to distinct bins with widths Δ_i and count the number of observations, n_i , in each bin.

$$p_i = \frac{n_i}{N\Delta_i}$$

- often, the same width is used for all bins, $\Delta_i = \Delta$
- Δ acts as a smoothing parameter.



03. Probability / Statistics Important Distributions

Nonparametric Methods

Kernel Density Estimation: fix a volume V and estimate the number of data points K within a certain region R from the data.

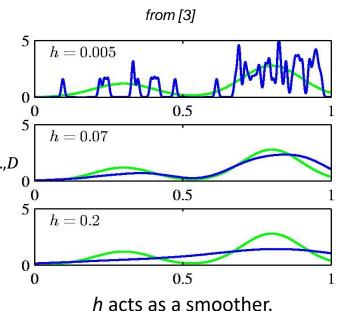
Let *R* be a hypercube centred on *x* and define the kernel function (Parzen window)

$$k((x-x_n)/h) = \begin{cases} 1, & |(x-x_n)/h| \le 1/2, & i=1,...,D \\ 0, & \text{otherwise} \end{cases}$$

$$p(x) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{h^{D}} k\left(\frac{x - x_{n}}{h}\right)$$

To avoid discontinuities in p(x), use a smooth kernel, e.g. a Gaussian

$$p(x) = \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi h^2)^{D/2}} \exp\left\{-\frac{\|x - x_n\|^2}{2h^2}\right\}$$



03. Probability / Statistics Functions of RV

. Introduction 2. Linear Algebra 3. Probability and Statistics

Functions of random variables

Given $\mathbf{X} = [X_1, X_2, ..., X_n]^T$ defined from their joint PDF $f_{\mathbf{X}}(\mathbf{X})$, and given $\mathbf{Y} = [Y_1, Y_2, ..., Y_m]^T$ obtained from a function:

$$\mathbf{Y} = \boldsymbol{g}(\mathbf{X}) = \begin{bmatrix} g_1(\mathbf{X}) \\ g_2(\mathbf{X}) \\ \vdots \\ g_m(\mathbf{X}) \end{bmatrix}$$

3 cases:

1.
$$m = n = 1$$

2.
$$m = n > 1$$

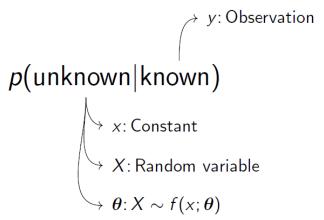
3.
$$m = 1, n > 1$$

Analytical expressions just for linear functions;

Taylor expansion or Monte-Carlo

03. Probability / Statistics Bayes Theorem

Bayes Theorem



Given $\mathbf{X} = [X_1, X_2, \cdots, X_X]^T$ a vector of random varia bles so that $\mathbf{X} \sim f(x)$ and given $\mathbf{D} = \{y_1, y_2, \cdots, y_D\}$ a set of observations corresponding to realizations of $\mathbf{Y} = [Y_1, Y_2, \cdots, Y_D]^T$ so that $\mathbf{Y} \sim f(\mathbf{y})$

$$f(x|y = D) = \frac{f(y = D|x) \cdot f(x)}{f(y = D)}$$

$$\underbrace{f(x|\mathcal{D})}_{\text{posterior}} = \underbrace{\frac{\overbrace{f(\mathcal{D}|x)}^{\text{likelihod}} \cdot \overbrace{f(x)}^{\text{prior}}}{\underbrace{f(\mathcal{D})}_{\text{normalization cte}}}$$

03. Probability / Statistics Bayes Theorem

Bayes Theorem – highly topical example

Given a deadly disease so rare that only one human on Earth has it.

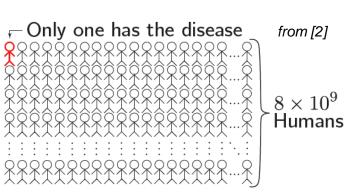
We have a screening test so that

$$test+ \mapsto \begin{cases} Pr(test + | desease) = 0.999 \\ Pr(test + | no desease) = 0.001 \end{cases}$$

If you test positive, should you be worried?

03. Probability / Statistics Bayes Theorem

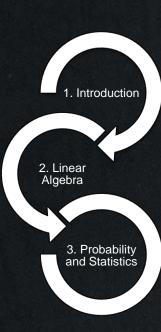
Bayes Theorem – highly topical example



expect $\approx 0.001 \times 8 \times 10^9$ = 8 x 10⁶ false diagnoses

$$Pr(desease|test +) = \frac{1}{8 \cdot 10^6} \approx 2 \cdot Pr(600)$$

If you want to properly extract information from data, you must consider the prior probability of the phenomenon you are interested in.



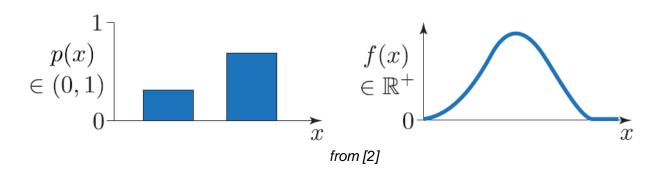
03. Probability / Statistics Bayes Theorem

Bayes Theorem – Prior knowledge

f(x) describes prior knowledge for the values that values x can take.

Prior knowledge can be based on:

- Engineering heuristics (expert knowledge)
- The posterior PDF obtained from previous data
- Non-informative prior (i.e. absence of prior knowledge)



03. Probability / Statistics

Bayes Theorem

Bayes Theorem – Likelihood $f(\mathcal{D}|x)$

 $f(\mathcal{D}|x)$ describes the conditional probability of a set of observations D given the values that x can take.

"how the data is produced"

Examples:

- Hooke's law:
- Parabola:
- Tossing a dice:

$$F = k \cdot w$$

$$y = a \cdot x^2 + b \cdot x + c$$

$$f(\mathcal{D}|x) = 1$$

03. Probability / Statistics Bayes Theorem

Bayes Theorem – Evidence $f(\mathcal{D})$

 $f(\mathcal{D})$ is called the evidence or the normalization constant.

The posterior integral must be equal to 1

$$\underbrace{\sum_{x} p(x|\mathcal{D})}_{\text{discrete case}} \equiv \underbrace{\int f(x|\mathcal{D}) dx}_{\text{continous case}} = 1$$

so that

$$p(\mathcal{D})\underbrace{\sum_{x} p(y|x) \cdot p(x)}_{\text{discrete case}}, \qquad f(\mathcal{D})\underbrace{\int_{x} f(y|x) \cdot f(x) dx}_{\text{continous case}} = 1$$

03. Probability / Statistics Monte Carlo Methods

Monte Carlo Methods – Short Introduction

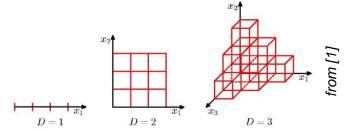
How to estimate integrals (expectations; evidence) for high-dimensional problems?

$$\underbrace{f(\boldsymbol{\theta}|\mathcal{D})}_{\text{posterior}} = \underbrace{\frac{f(\mathcal{D}|\boldsymbol{\theta})f(\boldsymbol{\theta})}{f(\mathcal{D}|\boldsymbol{\theta})f(\boldsymbol{\theta})}}_{\text{unknown normalization cte.}} f(\mathcal{D}) = \int f(\mathcal{D}|\boldsymbol{x}) \cdot f(\boldsymbol{x}) d\boldsymbol{x}$$

$$\approx \sum_{i=1}^{N} f(\mathcal{D}|\boldsymbol{x}_i) \cdot f(\boldsymbol{x}_i) \Delta \boldsymbol{x}_i$$

- standard (numerical) integration techniques are just efficient for few dimension
- # of parameters of a distribution is decisive for complexity of a problem
- Curse of Dimensionality

Solution: Monte Carlo Sampling

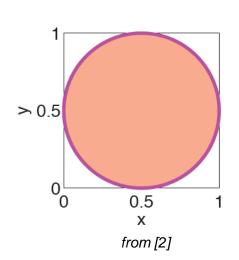


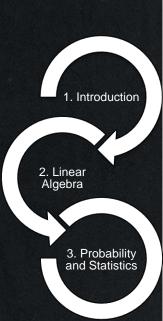
Monte Carlo Methods – Example: Estimate area content of a circle

Consider a circle with diameter D = 1: $(x - 0.5)^2 + (y - 0.5)^2 = r^2$

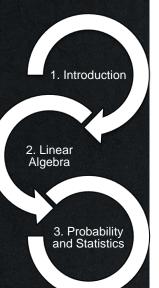
and indicator function
$$I(x,y) = \begin{cases} 1 & \text{if } (x-0.5)^2 + (y-0.5)^2 \le r^2 \\ 0 & \text{else} \end{cases}$$

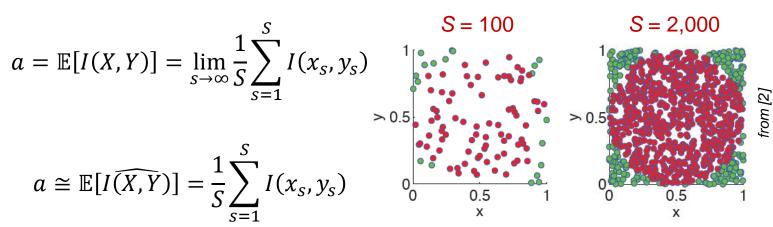
$$\underbrace{a}_{\text{area}} = \iint_{y \mid x} I(x, y) f_{XY}(x, y) \, dx \, dy$$
$$= \mathbb{E}[I(X, Y)]$$





Monte Carlo Methods – Example: Estimate area content of a circle





 $\pi r^2 = 0.785$

Estimation quality:

- $\mathbb{E}[\widehat{I(X,Y)}]$ depends on the number of samples
- Independent of the number of dimensions

03. Probability / Statistics Monte Carlo Methods

Monte Carlo Methods – Metropolis Algorithm

Metropolis algorithm (Metropolis, 1953) developed during WWII within the Manhattan

project (atomic bomb) in Los Alamos.

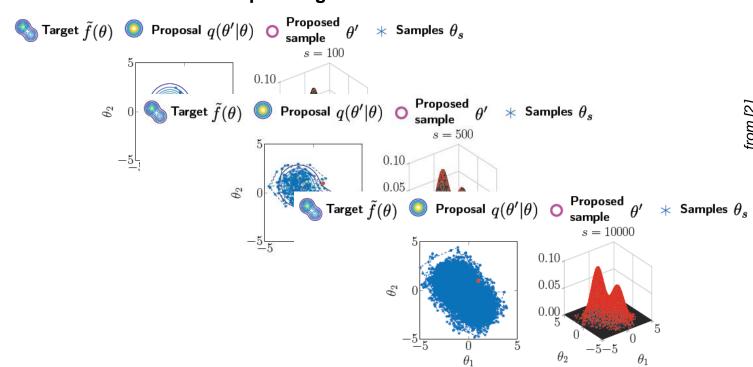
oldest MCMC algorithm

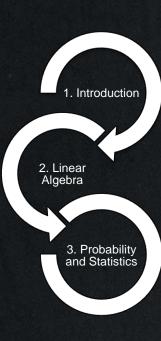
further MCMC samplers:

- Metropolis-Hasting
- Gibbs Sampling
- Slice Sampling

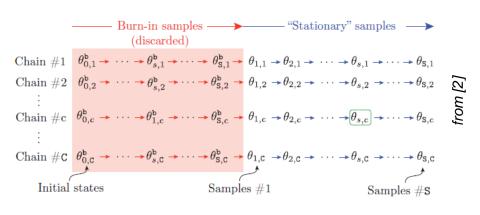
```
Algorithm 1: Metropolis
                                                                             Proposal Distribution
 1 initialize \theta_0;
  2 for s = 0, 1, 2, \cdots do
           define \theta = \theta_s;
                                                              q(\theta'|\theta) = \mathcal{N}\left(\theta'; \theta, \begin{vmatrix} \sigma_{q_1}^2 & 0\\ 0 & \sigma_{q_2}^2 \end{vmatrix}\right)
           sample \theta' \sim q(\theta'|\theta);
           compute \alpha = \frac{\tilde{f}(\theta')}{\tilde{f}(\theta)};
           compute r = \min(1, \alpha);
           sample u \sim \mathcal{U}(0,1);
                                                                                                             from [2]
           if u < r then
                \theta_{s+1} = \theta';
10
           else
                \theta_{s+1} = \theta_s;
11
                                                                      random acceptance
                                                                              or rejection
```

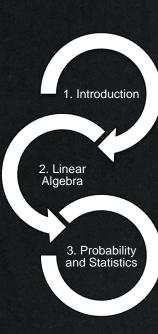
Monte Carlo Methods – Metropolis Algorithm





Monte Carlo Methods – Convergence Monitoring





Monte Carlo Methods – Convergence Monitoring



2. Linear Algebra

> 3. Probability and Statistics

Within-chains

Mean:

$$\overline{ heta}_{\cdot c} = rac{1}{\mathtt{S}} \sum_{s=1}^{\mathtt{S}} heta_{s,c}$$

Variance:
$$W = \frac{1}{C} \sum_{c=1}^{C} \left[\frac{1}{S-1} \sum_{s=1}^{S} (\theta_{s,c} - \overline{\theta}_{\cdot c})^2 \right] \qquad B = \frac{1}{C-1} \sum_{c=1}^{C} (\overline{\theta}_{\cdot c} - \overline{\theta}_{\cdot c})^2$$

Underestimates $Var[\theta_{s,c}]$

Between-chains

Mean:

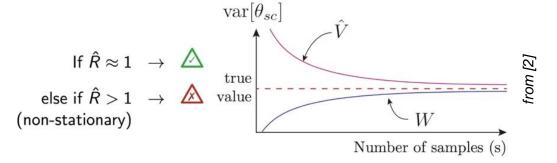
$$\overline{ heta}_{\cdot \cdot} = rac{1}{\mathtt{C}} \sum_{c=1}^{\mathtt{C}} \overline{ heta}_{\cdot c}$$

$$B = \frac{1}{C-1} \sum_{c=1}^{C} (\overline{\theta}_{c} - \overline{\theta}_{c})^{2}$$

Overestimates $Var[\theta_{s,c}]$

$$\widetilde{\widetilde{V}} = \frac{S-1}{S}W + B$$

Convergence
$$\hat{R} = \sqrt{\frac{\hat{V}_{I}}{W}}$$



03. Probability / Statistics Information Theory

Important Measures from Information Theory often used within Al algorithms

(Self-) Information of an event:

(base is exponential e => unit: nats)

$$I(x) = -\log P(x).$$

Entropy:

$$H(\mathbf{x}) = \mathbb{E}_{\mathbf{x} \sim P}[I(x)] = -\mathbb{E}_{\mathbf{x} \sim P}[\log P(x)]$$

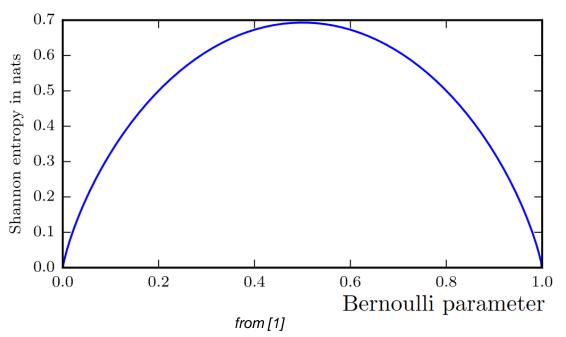
Kullback-Leibler (KL) Divergence:

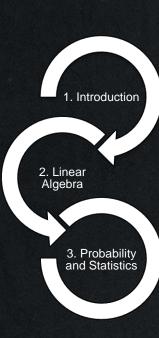
$$D_{\mathrm{KL}}(P||Q) = \mathbb{E}_{\mathbf{x} \sim P} \left[\log \frac{P(x)}{Q(x)} \right] = \mathbb{E}_{\mathbf{x} \sim P} \left[\log P(x) - \log Q(x) \right]$$

03. Probability / Statistics Information Theory

Important Measures from Information Theory often used within Al algorithms

Entropy of a Bernoulli Variable:

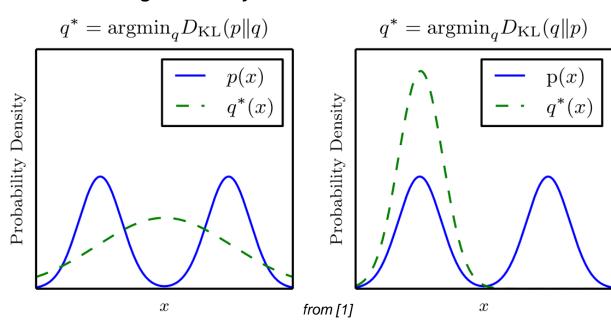


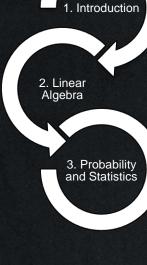


03. Probability / Statistics Information Theory

Important Measures from Information Theory often used within Al algorithms

Note: KL Divergence is Asymmetric





03. Probability / Statistics Summary

Probabilities:

- Probabilities describe our knowledge
- ► The less we know, the more we should employ probability theory

Bayesian interpretation: $Pr(E_i)$ quantifies the likelihood of an event with respect to others in S

Rules/operations events: \cap , \cup , \subset , \subseteq , \in

Fundamental Axioms:

- 1. $0 \le \Pr(E_i) \le 1$
- 2. Pr(S) = 1
- 3. Si E_1 et E_2 are mutually exclusives $Pr(E_1 \cup E_2) = Pr(E_1) + Pr(E_2)$

Inclusion-exclusion rule: $Pr(\bigcup_{i=1}^n E_i) = ...$

Bayes Theorem: $Pr(E_i|A) = \frac{Pr(A|E_i)Pr(E_i)}{Pr(A)}$

Probability distributions: PDF, CDF, PMF, CMF

Multivariate Normal: $\mu_1, \sigma_1, \mu_2, \sigma_2, \rho_{12}$

Multivariate probability density function:

- $ightharpoonup 0 \le f_{\mathbf{X}}(\mathbf{x})$

Conditional probabilities:

- si $p_{X_1|X_2}(x_1|x_2) = p_{X_1}(x_1), X_1 \perp X_2$

General case: $X_1 \not\perp X_2 \rightarrow$ Chain rule

Expectation & Variance:

$$\mathbb{E}[X] = \int x \cdot f_X(x) dx \text{ (Continuous R.V.)}$$

$$\mathbb{E}[(X - \mu_X)^2] = \sigma_X^2 = \text{var}[X] = \mathbb{E}[X^2] - (\mathbb{E}[X])^2$$

Matrix notation: $\Sigma_X = D_X R_X D_X$

Function of random variables: Y = g(X)

$$f_Y(y)dy = f_X(x)dx$$

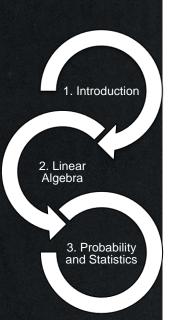
$$M_Y = g(M_X) = AM_X + B$$

$$\Sigma_Y = A\Sigma_X A^T = J_{y,x} \Sigma_X J_{y,x}^T$$

Linearization - First order approximation

$$\begin{array}{ccc} Y = g(\mathbf{X}) & \cong & g(\mathbf{M}_{\mathbf{X}}) + \nabla g(\mathbf{M}_{\mathbf{X}})(\mathbf{X} - \mathbf{M}_{\mathbf{X}}) \\ \mu_{Y} & \cong & g(\mathbf{M}_{\mathbf{X}}) \\ \sigma_{Y}^{2} & \cong & \nabla g(\mathbf{M}_{\mathbf{X}}) \mathbf{\Sigma}_{\mathbf{X}} \nabla g(\mathbf{M}_{\mathbf{X}})^{\mathsf{T}} \end{array}$$

03. Probability / Statistics Summary



Univariate Normal:

$$X \sim \mathcal{N}(x; \mu, \sigma^2), x \in (-\infty, +\infty)$$

if
$$X \sim \mathcal{N}(x; \mu_X, \sigma_X^2), Y \sim \mathcal{N}(y; \mu_Y, \sigma_Y^2)$$

$$Z = X + Y$$

$$\sim \mathcal{N}(z; \mu_Z, \sigma_Z^2)$$

Multivariate Normal:

 $\mathbf{X} \sim \mathcal{N}(\mathbf{x}; \mathbf{M}_{\mathbf{X}}, \mathbf{\Sigma}_{\mathbf{X}})$

Normal conditional:

$$f_{\mathbf{X}_1|\mathbf{X}_2}(\mathbf{x}_1|\mathbf{X}_2=\mathbf{x}_2) = \mathcal{N}(\mathbf{x}_1;\mathbf{M}_{1|2},\mathbf{\Sigma}_{1|2})$$

Univariate Lognormal:

$$X \sim \ln \mathcal{N}(x; \lambda, \zeta), x \in (0, +\infty)$$

 $X \sim \ln \mathcal{N}(x; \lambda_X, \zeta_X^2), Y \sim \ln \mathcal{N}(y; \lambda_Y, \zeta_Y^2)$

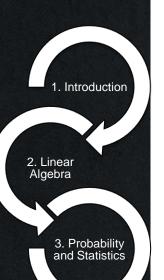
$$Z = X \cdot Y$$

$$\sim \ln \mathcal{N}(z; \lambda_Z, \zeta_Z^2)$$

Beta:

$$X \sim \text{Beta}(x; \alpha, \beta), x \in (0, 1)$$

03. Probability / Statistics Summary



Bayes's rule:
$$\underbrace{f(\mathbf{x}|\mathcal{D})}_{\text{posterior}} = \underbrace{\frac{f(\mathcal{D}|\mathbf{x}) \cdot f(\mathbf{x})}{f(\mathcal{D})}}_{\text{normalization cte.}}$$

Prior – f(x), $f(\theta)$: based on: Engineering heuristics, Previous posterior PDF, Non-informative prior

Likelihood – $f(\mathcal{D}|\mathbf{x})$ or $f(\mathcal{D}|\theta)$: Conditional probability of a set of observations \mathcal{D} given the values that \mathbf{x} or $\boldsymbol{\theta}$ can take

Evidence – $f(\mathcal{D})$:

$$f(\mathcal{D}) = \underbrace{\int f(\mathbf{y}|\mathbf{x}) \cdot f(\mathbf{x}) d\mathbf{x}}_{\text{continuous case}} = 1$$

MC sampling from the prior

$$f(\mathcal{D}) \approx \frac{1}{S} \sum_{s=1}^{S} \left[\prod_{j=1}^{D} f(y_{j} | \mathbf{x}_{s}) \right]$$

$$\mathbb{E}[\mathbf{x} | \mathcal{D}] \approx \frac{1}{S} \sum_{s=1}^{S} \left[\mathbf{x}_{s} \cdot \frac{\prod_{j=1}^{D} f(y_{j} | \mathbf{x}_{s})}{f(\mathcal{D})} \right]$$

$$\operatorname{var}[\mathbf{x} | \mathcal{D}] \approx \frac{1}{S} \sum_{s=1}^{S} \left[(\mathbf{x}_{s} - \mathbb{E}[\mathbf{x} | \mathcal{D}])^{2} \cdot \frac{\prod_{j=1}^{D} f(y_{j} | \mathbf{x}_{s})}{f(\mathcal{D})} \right]$$

Limited to simple cases → MCMC Module

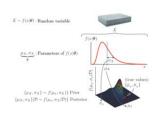
Posterior – $f(x|\mathcal{D})$: When the number of independent observations $D \to \infty$

$$f(\mathbf{x}|\mathcal{D}) = \frac{f(\mathcal{D}|\mathbf{x})f(\mathbf{x})}{f(\mathcal{D})} \to \underbrace{\delta(\check{\mathbf{x}})}_{\text{Dirac delta PDF}}$$

$$f(\boldsymbol{\theta}|\mathcal{D}) = \frac{f(\mathcal{D}|\boldsymbol{\theta})f(\boldsymbol{\theta})}{f(\mathcal{D})} \to \underbrace{\delta(\widecheck{\boldsymbol{\theta}})}_{\text{Dirac delta PD}}$$

Posterior Predictive – $f(x|\mathcal{D})$

$$f(x|\mathcal{D}) = \int f(x; \boldsymbol{\theta}) f(\boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta}$$



Conjugate priors: For specific combinaisons of prior distribution and likelihood function, the posterior PDF follows the same type of distribution than the prior PDF

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