Machine Learning A Bayesian and Optimization Perspective

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Chapter 2 Probability and Stochastic Processes

Version I

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Machine Learning,

The Notion of a Random Variable

- A random variable, x, is a variable whose variations are due to chance/randomness. A random variable can be considered as a function, which assigns a value to the outcome of an experiment. For example, in a coin tossing experiment, the corresponding random variable, x, can assume the values x₁ = 0 if the result of the experiment is "heads" and x₂ = 1 if the result is "tails."
- We will denote a random variable with a lower case roman, such as x, and the values it takes once an experiment has been performed, with mathmode italics, such as x.
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• Relative Frequency Definition: The probability, P(A), of an event, A, is the limit

$$P(A) = \lim_{n \to \infty} \frac{n_A}{n},$$

where n is the total number of trials and n_A the number of times event A occurred.

In practice, one can use

$$P(A) \approx \frac{n_A}{n},$$

for large enough values of n. However, care must be taken on how large n must be, especially when P(A) is very small.

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- Axiomatic Definition: This definition of probability is traced back to 1933 to the work of Andrey Kolmogorov, who found a close connection between probability theory and the mathematical theory of sets and functions of a real variable, in the context of measure theory.
 - **1** The probability of an event A, P(A) is a nonnegative number

 $P(A) \ge 0.$

2 The probability of an event C, which is certain to occur, is equal to one,
P(C) = 1



 $P(A \cup B) = P(A) + P(B).$

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• These three defining properties (axioms), suffice to develop the rest of the theory.

• A discrete random variable, x, can take any value from a finite or a countably infinite set, \mathcal{X} . The probability of an event " $\mathbf{x} = x$ " is denoted as

$$P(\mathbf{x} = x)$$
 or simply $P(x)$.

 Assuming that no two values in X can occur simultaneously and that an experiment always returns a value, we have that

$$\sum_{x \in \mathcal{X}} P(x) = 1,$$

- Joint probability: The joint probability of two events A and B to occur simultaneously is denoted as P(A, B).
- Given two random variables $x \in \mathcal{X}$ and $y \in \mathcal{Y}$, the following sum rule is obtained

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• Conditional probability: The conditional probability of an event A given another event B, is denoted as P(A|B) and it is defined as

$$P(A|B) := \frac{P(A,B)}{P(B)}$$

- The above definition gives rise to the following product rule $P(A,B) = P(A|B)P(B). \label{eq:product}$
- Expressed in terms of two random variables, x and y, we have $P(x,y) = P(x|y)P(y). \label{eq:prod}$
- P(x) and P(y) are also known as the marginal probabilities to be distinguished from the joint and the conditional ones.
- Statistical independence: Two random variables, x and y, are said to be statistically independent if and only if

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• Bayes Theorem: This important and elegant theorem is a direct consequence of the product rule and the symmetry property of the joint probability, i.e., P(x, y) = P(y, x), and it is given by the following two equations,

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This theorem plays a very important role in Machine Learning.

• What this theorem says is that, our uncertainty as expressed by the conditional probability P(y|x) of an output variable, say y, given the value of an input, x, can be expressed the other way round; that is, in terms of the (uncertainty) conditional, P(x|y) and the two marginal probabilities, P(x) and P(y).

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- A continuous random variable, x, can take values anywhere in an in interval in the real axis $\mathbb R.$
- The starting point to develop tools for describing such variables is to build bridges with what we know from the discrete random variables case.
- The cumulative distribution function (cdf) is defined as

 $F_{\mathbf{x}}(x) := P(\mathbf{x} \le x).$

That is, cdf is the probability of the discrete event: "x takes any value less or equal to x".

Thus, we can write

$$P(x_1 < x \le x_2) = F_x(x_2) - F_x(x_1).$$

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• Assuming $F_x(x)$ to be differentiable, the probability density function (pdf), denoted with lower case p, is defined as $p_x(x) := \frac{dF_x(x)}{r}.$

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• Then, it is readily seen that

$$P(x_1 < \mathbf{x} \le x_2) = \int_{x_1}^{x_2} p_{\mathbf{x}}(x) dx,$$

and

$$F_{\mathbf{x}}(x) = \int_{-\infty}^{x} p_{\mathbf{x}}(z) dz.$$

- Since an event is certain to occur in $-\infty < x < +\infty$, we have that $\int_{-\infty}^{+\infty} e^{-x} dx = 1$
- The previously stated rules, for the discrete random variables case, are also valid for the continuous ones, i.e.,

$$p(x|y) = \frac{p(x,y)}{p(y)}, \quad p_{\mathbf{x}}(x) = \int_{-\infty}^{+\infty} p(x,y)dy.$$

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- Two of the most useful quantities associated with a random variable, x, are:
 - The mean value, which is defined as:

$$\mathbb{E}[\mathbf{x}] := \int_{-\infty}^{+\infty} x p(x) dx.$$

• The variance, which is defined as:

$$\sigma_x^2 := \int_{-\infty}^{+\infty} \left(x - \mathbb{E}[\mathbf{x}] \right)^2 p(x) dx,$$

with integrations substituted by summations for the case of discrete variables, e.g.,

$$\mathbb{E}[\mathbf{x}] := \sum_{x \in \mathcal{X}} x P(x).$$

More general, when a function f is involved, we have,

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 It can readily be deduced from the respective definitions that, the mean value with respect to two random variables can be written as:

$$\mathbb{E}[\mathbf{x},\mathbf{y}] := \mathbb{E}_{\mathbf{x}} \big[\mathbb{E}_{\mathbf{y}|\mathbf{x}}[f(\mathbf{x},\mathbf{y})] \big].$$

Given two random variables, x, y, their covariance is defined as

 $\operatorname{cov}(\mathbf{x}, \mathbf{y}) := \mathbb{E} [(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{y} - \mathbb{E}[\mathbf{y}])].$

• Their correlation is defined as

$$r_{x,y} := \mathbb{E}[xy] = \operatorname{cov}(x, y) - \mathbb{E}[x]\mathbb{E}[y].$$

A random vector is a collection of random variables,
 x := [x₁,..., x_l]^T and their joint pdf is denoted as

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$$p(\mathbf{x}) = p(x_1, \dots, x_l), \ \mathbf{x} = [x_1, \dots, x_l]^T.$$
• The covariance matrix of a random vector, $\mathbf{x} \in \mathbb{R}^l$, is defined as

$$\mathsf{Cov}(\mathbf{x}) := \mathbb{E} \left[(\mathbf{x} - \mathbb{E}[\mathbf{x}])(\mathbf{x} - \mathbb{E}[\mathbf{x}])^T \right],$$
$$\mathsf{Cov}(\mathbf{x}) = \left[\begin{array}{ccc} \mathsf{cov}(\mathbf{x}_1, \mathbf{x}_1) & \dots & \mathsf{cov}(\mathbf{x}_1, \mathbf{x}_l) \\ \vdots & \ddots & \vdots \\ \mathsf{cov}(\mathbf{x}_l, \mathbf{x}_1) & \dots & \mathsf{cov}(\mathbf{x}_l, \mathbf{x}_l) \end{array} \right].$$

• Similarly, the correlation matrix of a random vector, \mathbf{x} , is defined as $P_{\mathbf{x}} := \mathbb{R} \left[m_{\mathbf{x}}^{T} \right]$

or

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$$R_x = \begin{bmatrix} \mathbb{E}[\mathbf{x}_1, \mathbf{x}_1] & \dots & \mathbb{E}[\mathbf{x}_1, \mathbf{x}_l] \\ \vdots & \ddots & \vdots \\ \mathbb{E}[\mathbf{x}_l, \mathbf{x}_1] & \dots & \mathbb{E}[\mathbf{x}_l, \mathbf{x}_l] \end{bmatrix}$$
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- Important Property: The covariance as well as the correlation matrices are positive semidefinite.
- A matrix \boldsymbol{A} is called positive semidefinite, if

 $\boldsymbol{y}^T A \boldsymbol{y} \geq 0, \; \forall \boldsymbol{y} \in \mathbb{R}^l,$

and it is called **positive definite** if the inequality is a strict one.

• **Proof:** For the covariance matrix, we have

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where "*" denotes complex conjugation.

The latter definition leads to the variance of a complex variable,

$$\sigma_{z}^{2} = \mathbb{E}\left[\left|\mathbf{z} - \mathbb{E}[\mathbf{z}]\right|^{2}\right] = \mathbb{E}\left[\left|\mathbf{z}\right|^{2}\right] - \left|\mathbb{E}\left[\mathbf{z}\right]\right|^{2}$$

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where $x_i, y_i, i = 1, 2, ..., l$, are the components of the involved real vectors, respectively.

• The covariance and correlation matrices are similarly defined, in terms of the Hermitian transposition,

$$\operatorname{Cov}(\mathbf{z}) := \mathbb{E}\left[\left(\mathbf{z} - \mathbb{E}[\mathbf{z}]\right)\left(\mathbf{z} - \mathbb{E}[\mathbf{z}]\right)^{H}\right], \ R_{z} := \mathbb{E}[\mathbf{z}\mathbf{z}^{H}].$$

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• Let **x**, **y** be two random vectors, which are related via a transform,

$$\mathbf{y} = \boldsymbol{f}(\mathbf{x}).$$

The vector function *f* is assumed to be invertible. That is, there
is a uniquely defined vector function, denoted as *f*⁻¹, so that,

$$\mathbf{x} = \boldsymbol{f}^{-1}(\mathbf{y}).$$

• Given the pdf, $p_{\mathbf{x}}(oldsymbol{x})$, of \mathbf{x} , it can be shown that,

$$p_{\mathbf{y}}(\boldsymbol{y}) = \frac{p_{\mathbf{x}}(\boldsymbol{x})}{\left|\det(J(\mathbf{y};\mathbf{x}))\right|} \bigg|_{\boldsymbol{x} = \boldsymbol{f}^{-1}(\boldsymbol{y})}$$

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Example

• Let the two random vectors **x** and **y** be related by a linear transform, via an invertible matrix *A*,

$$\mathbf{y} = A\mathbf{x}.$$

 Then, it is easily checked out that the Jacobian matrix is equal to the matrix A,

$$J(\mathbf{y}; \mathbf{x}) = A.$$

Thus, we readily obtain that,

$$p_{\mathbf{y}}(\boldsymbol{y}) = \frac{p_{\mathbf{x}}(A^{-1}\boldsymbol{x})}{|\mathsf{det}A|}.$$

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• The Bernoulli distribution: A random variable is said to be distributed according to a Bernoulli distribution, if it is binary, $\mathcal{X} = \{0, 1\}$, with

$$P(\mathbf{x} = 1) = p, P(\mathbf{x} = 0) = 1 - p.$$

• In a more compact way, we write that $\mathrm{x}\sim \mathsf{Bern}(x|p)$ where $P(x)=\mathsf{Bern}(x;p):=p^x(1-p)^{1-x}.$

Its mean value is equal to:

$$\mathbb{E}[\mathbf{x}] = 1p + 0(1-p) = p.$$

Its variance is equal to:

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• The Binomial Distribution: A random variable, x, is said to follow a binomial distribution, with parameters n, p and we write $x \sim Bin(x|n, p)$, if $\mathcal{X} = \{0, 1, ..., n\}$ and

$$P(\mathbf{x} = k) := \mathsf{Bin}(k|n, p) = \binom{n}{k} p^k (1-p)^{n-k}, \ k = 0, 1, \dots, n.$$

- For example, this distribution models the times that head occurs in *n* successive trials, where *P*(Head) = *p*.
- The binomial is a generalization of the Bernoulli distribution, which results if we set n = 1.
- The mean and variance of the binomial distribution are:

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• The two figures below show he probability mass function and the corresponding CDF for the binomial distribution, for p = 0.4 and n = 9.



 Observe that in the case of discrete variables, the cdf function has a step-wise form.

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- The Multinomial Distribution: This is a generalization of the binomial distribution, if the outcome of each experiment is not binary, but it can take one out of K possible values. For example, instead of tossing a coin, a die with K sides is thrown.
- Each one of the possible K outcomes has probability P_1, P_2, \ldots, P_K to occur, and we denote

$$\boldsymbol{P} = [P_1, P_2, \dots, P_K]^T.$$

• After *n* experiments, assume that x_1, x_2, \ldots, x_K times sides $x = 1, x = 2, \ldots, x = K$ occurred, respectively.

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$$\begin{pmatrix} n \\ x_1, x_2, \dots, x_K \end{pmatrix} = \frac{n!}{x_1! x_2! \dots x_K!}.$$

• Note that the variables, x_1, \ldots, x_K , are subject to the constraints

$$\sum_{k=1}^{K} \mathbf{x}_k = n, \ \sum_{k=1}^{K} P_K = 1.$$

- For the multinomial distribution:
 - the mean values is given by,

$$\mathbb{E}[\mathbf{x}] = n\boldsymbol{P},$$

• the variances by

$$\sigma_k^2 = nP_k(1 - P_k), \ k = 1, 2, \dots, K,$$

and the covariances by

$$\operatorname{cov}(\mathbf{x}_i, \mathbf{x}_j) = -nP_iP_j, \ i \neq j.$$

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Typical Distributions for Continuous Variables

• The Uniform Distribution: A random variable, x, is said to follow a uniform distribution in an interval [a, b] and we write $x \sim U(a, b)$, with $a > -\infty$ and $b < +\infty$, if

$$p(x) = \begin{cases} \frac{1}{b-a}, & \text{if } a \le x \le b, \\ 0 & \text{otherwise.} \end{cases}$$

- The distribution is shown in the figure below:
 - The mean value and the variance are equal to

$$\mathbb{E}[\mathbf{x}] = \frac{a+b}{2}, \ \sigma_x^2 = \frac{1}{12}(b-a)^2$$
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• The Gaussian Distribution: The Gaussian or normal distribution is one among the most widely used distributions in all scientific disciplines. We say that a random variable, x, is Gaussian or normal with parameters μ and σ^2 , and we write $x \sim \mathcal{N}(\mu, \sigma^2)$ or $\mathcal{N}(x|\mu, \sigma^2)$, if

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

- The distribution is shown in the figure below:
 - The mean value and the variance are equal to:

$$\mathbb{E}[\mathbf{x}] = \mu, \ \sigma_x^2 = \sigma^2.$$

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• **Proof of the mean value**: By the definition of the mean value, we have that,

$$\begin{aligned} \mathbb{E}[\mathbf{x}] &= \frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} x \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx \\ &= \frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} (y+\mu) \exp\left(-\frac{y^2}{2\sigma^2}\right) dy. \end{aligned}$$

Due to the symmetry of the exponential function, performing the integration involving y gives zero and the only surviving term is due to μ . Taking into account that a pdf integrates to one, we obtain the result.

• Proof of the variance: For the variance, we have that,

$$\int_{-\infty}^{+\infty} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \sqrt{2\pi}\sigma.$$

• Taking the derivative of both sides with respect to σ , we obtain

$$\int_{-\infty}^{+\infty} \frac{(x-\mu)^2}{\sigma^3} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \sqrt{2\pi}$$

$$\frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} (x-\mu)^2 \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \sigma^2$$

which proves the claim.

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$$\int_{-\infty}^{+\infty} \frac{(x-\mu)^2}{\sigma^3} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \sqrt{2\pi},$$

or

$$\frac{1}{\sqrt{2\pi\sigma}} \int_{-\infty}^{+\infty} (x-\mu)^2 \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx = \sigma^2,$$

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• Multivariate Gaussian: This is the generalization of the Gaussian to vector variables, $\mathbf{x} \in \mathbb{R}^{l}$. We write $\mathbf{x} \sim \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$, with parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$, and it is defined as

$$p(\boldsymbol{x}) = \frac{1}{(2\pi)^{l/2} |\Sigma|^{1/2}} \exp\Big(-\frac{1}{2} (\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\Big),$$

where $|\cdot|$ denotes the determinant of a matrix. It can be shown that, $\mathbb{P}[z_{1}] = z_{2} \text{ and } C_{2} z_{3} = \Sigma$

$$\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu}$$
 and $\mathsf{Cov}(\mathbf{x}) = \boldsymbol{\Sigma}.$

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• Isovalue curves of multivariate Gaussians: The isovalue curves are formed by all the points which correspond to the same value of the pdf, i.e., p(x) = c,

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) = \text{constant} = c.$$

 The isovalue curves are of a quadric nature: circles (hyperspheres) or ellipses (hyperellipsoids) centered at the mean value. The minor/major axes are determined by the eigenstructure of the corresponding covariance matrix Σ.

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• Proof for the shape of the contours: All points $x \in \mathbb{R}^l$, lying on a isovalue contour satisfy

$$(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu}) = \text{constant} = c.$$

The covariance matrix is symmetric, \$\sum 2 = \Sum T\$. Thus, its eigenvalues are real and the corresponding eigenvectors can be chosen to form an orthonormal basis, which leads to its diagonalization, i.e.,

$$arsigma = U^T \Lambda U, ext{ with } U := [oldsymbol{u}_1, \dots, oldsymbol{u}_l],$$

where u_i , i = 1, 2, ..., l, are the corresponding orthonormal eigenvectors, and

$$\Lambda := \mathsf{diag}\{\lambda_1, \ldots, \lambda_l\},\$$

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• Assuming Σ to be invertible, all eigenvalues are positive (being a positive definite matrix, it has positive eigenvalues). Due to the orthonormality of the eigenvectors, matrix U is unitary, i.e., $UU^T = U^T U = I$. Thus, we can now write

$$\boldsymbol{y}^T \Lambda^{-1} \boldsymbol{y} = c, \text{ where } \boldsymbol{y} := U(\boldsymbol{x} - \boldsymbol{\mu}),$$
 (1)

which corresponds to a rotation of the axes by U and a translation of the origin to μ .

Equation (1) can be written as

$$\frac{y_1^2}{\lambda_1} + \ldots + \frac{y_l^2}{\lambda_l} = c.$$

The last equation is describing a (hyper)ellipsoid in the R^l. It is centered at μ and the major axes of the ellipsoid are parallel to u₁,..., u_l. The size of the respective axes are controlled by the values of the corresponding eigenvalues.

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• Properties of the Gaussian distribution: If the covariance matrix is diagonal,

$$\varSigma = \mathsf{diag}\{\sigma_1^2, \dots, \sigma_l^2\},\$$

that is, when the covariance of all the elements $cov(x_i, x_j) = 0, i, j = 1, 2, ..., l$, then the random variables comprising x are statistically independent. This is not true in general. Uncorrelated variables do not necessarily mean that they are independent. Independence is a much stronger condition.

• Indeed, if the covariance matrix is diagonal, then the multivariate Gaussian is written as,

$$p(\boldsymbol{x}) = \prod_{i=1}^{l} \frac{1}{\sqrt{2\pi\sigma_i}} \exp\Big(-\frac{(x_i - \mu_i)^2}{2\sigma_i^2}\Big).$$

In other words,

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• The Central Limit Theorem: Consider N mutually independent random variables, each following its own distribution with mean values μ_i and variances σ_i^2 , i = 1, 2, ..., N. Define a new random variable as their sum, i.e.,

$$\mathbf{x} = \sum_{i=1}^{N} \mathbf{x}_i.$$

Then, the mean and variance of the new variable are given by,

$$\mu = \sum_{i=1}^N \mu_i, ext{ and } \sigma_x^2 = \sum_{i=1}^N \sigma_i^2.$$

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$$\mathbf{z} = \frac{\mathbf{x} - \boldsymbol{\mu}}{\sigma},$$

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- The Central Limit Theorem is one of the most important theorems in probability and statistics and it partly explains the popularity of the Gaussian distribution.
- In practice, even summing up a relatively small number of random variables, one can obtain a good approximation to a Gaussian. For example, if the individual pdfs are smooth enough and the random variables are identically and independently distributed (iid), a number between 5 to 10 may be sufficient.

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 The Exponential Distribution: We say that a random variable follows an exponential distribution with parameter λ > 0, if

$$p(x) = \begin{cases} \lambda \exp(-\lambda x), & \text{if } x \ge 0, \\ 0, & \text{otherwise.} \end{cases}$$

• The distribution has been used, for example, to model the time between arrivals of telephone calls or of a bus at a bus stop.

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• The mean value and the variance are equal to:

$$\mathbb{E}[\mathbf{x}] = \frac{1}{\lambda}, \quad \sigma_x^2 = \frac{1}{\lambda^2}.$$

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The Beta Distribution: We say that a random variable, x ∈ [0, 1], follows a beta distribution with positive parameters, a, b, and we write, x ~ Beta(x|a, b,), if

$$p(x) = \begin{cases} \frac{1}{B(a,b)} x^{a-1} (1-x)^{b-1}, & \text{if } 0 \le x \le 1, \\ 0 & \text{otherwise,} \end{cases}$$

where B(a, b) is the beta function, defined as,

$$B(a,b) := \int_0^1 x^{a-1} (1-x)^{b-1} dx, \text{ and } B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)},$$

where $\Gamma(\cdot)$ is the gamma function defined as,

$$\Gamma(a) = \int_0^\infty x^{a-1} e^{-x} dx.$$

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The mean value and the variance are equal to:



• The graphs of the pdfs of the Beta distribution for different values of the parameters. a) The dotted line corresponds to a = 1, b = 1, the gray line to a = 0.5, b = 0.5 and the red one to a = 3, b = 3. b) The gray line corresponds to a = 2, b = 3 and the red one to a = 8, b = 4. For values a = b, the shape is symmetric around 1/2. For a < 1, b < 1 it is convex. For a > 1, b > 1, it is zero at x = 0 and x = 1. For a = 1 = b, it becomes the uniform distribution. If a < 1, p(x) → ∞, x → 0 and if b < 1, p(x) → ∞, x → 1.</p>

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The Gamma Distribution: A random variable follows the gamma distribution with positive parameters a, b, and we write x ~ Gamma(x|a, b), if



The gamma distribution also takes various shapes by varying the parameters. For a < 1, it is strictly decreasing and p(x) → ∞ as x → 0 and p(x) → 0 as x → ∞.</p>

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The gamma distribution also takes various shapes by varying the parameters. For a < 1, it is strictly decreasing and p(x) → ∞ as x → 0 and p(x) → 0 as x → ∞.

• The Dirichlet Distribution: The Dirichlet distribution can be considered as the multivariate generalization of the beta distribution. Let $\mathbf{x} = [\mathbf{x}_1, \dots, \mathbf{x}_K]^T$ be a random vector, with components such as

$$0 \le \mathbf{x}_k \le 1, \ k = 1, 2, \dots, K, \text{ and } \sum_{k=1}^K \mathbf{x}_k = 1.$$

In other words, the random variables lie on (K-1)-dimensional simplex, as shown below



• We say that the random vector, \mathbf{x} , follows a Dirichlet distribution with parameters $\boldsymbol{a} = [a_1, \dots, a_K]^T$, and we write $\mathbf{x} \sim \text{Dir}(\boldsymbol{x}|\boldsymbol{a})$, if

$$p(\boldsymbol{x}) = \mathsf{Dir}(\boldsymbol{x}|\boldsymbol{a}) := \frac{\Gamma(\bar{a})}{\Gamma(a_1)\dots\Gamma(a_K)} \prod_{k=1}^K x_k^{a_k-1}, \quad \bar{a} := \sum_{k=1}^K a_k.$$

• The mean, variance and covariances of the involved random variables are given by,

$$\mathbb{E}[\mathbf{x}] = \frac{1}{\bar{a}}\boldsymbol{a}, \quad \sigma_k^2 = \frac{a_k(\bar{a} - a_k)}{\bar{a}^2(\bar{a} + 1)}, \quad \mathsf{cov}(\mathbf{x}_i, \mathbf{x}_j) = -\frac{a_i a_j}{\bar{a}^2(\bar{a} + 1)}.$$

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Typical Distributions for Continuous Variables-Dirichlet

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 The mean, variance and covariances of the involved random variables are given by,

$$\mathbb{E}[\mathbf{x}] = \frac{1}{\bar{a}}a, \quad \sigma_k^2 = \frac{a_k(\bar{a} - a_k)}{\bar{a}^2(\bar{a} + 1)}, \quad \operatorname{cov}(\mathbf{x}_i, \mathbf{x}_j) = -\frac{a_i a_j}{\bar{a}^2(\bar{a} + 1)}.$$

The Dirichlet distribution over the 2D-simplex for a) (0.1,0.1,0.1), b) (1,1,1) and c) (10,10,10).

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- The notion of a stochastic process is used to describe random experiments where the outcome of each experiment is a function or a sequence; in other words, the outcome of each experiment is an infinite number of values. Our focus will be on sequences. Thus, the result of a random experiment is a sequence, u_n (or sometimes denoted as u(n)), n ∈ Z, where Z is the set of integers. Usually, n is interpreted as a time index, and u_n is called a time series or in the signal processing jargon a discrete-time signal. In contrast, if the outcome is a function, u(t), it is called a continuous-time signal.
- We are going to use u_n to denote the specific sequence resulting from a single experiment and the roman font, u_n , to denote the corresponding discrete-time random process; that is, the rule that assigns a specific sequence as the outcome of an experiment.

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- A stochastic process can be considered as a family or ensemble of sequences. The individual sequences are known as sample sequences or simply as realizations.
- Note that fixing the time to a specific value, e.g., $n = n_0$, then u_{n_0} is a random variable. Indeed, for each random experiment, which we perform, a single value results at time instant n_0 . From this perspective, a random process can be considered as the collection of infinite many random variables, i.e., $\{u_n, n \in \mathbb{Z}\}$.

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The outcome of each experiment, associated with a discrete-time stochastic process, is a sequence of values. For each one of the realizations, the corresponding values obtained at any instant, e.g., n or m, comprise the outcomes of a corresponding random variable, un or um respectively.

• First and Second Order Statistics: For a stochastic process to be fully described, one must know the joint pdfs (pmfs for discrete-valued random variables)

 $p(u_n, u_m, \ldots, u_r),$

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$$\mu_n := \mathbb{E}[\mathbf{u}_n] = \int_{-\infty}^{+\infty} u_n p(u_n) du_n.$$

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 Strict Sense Stationarity: A stochastic process, u_n, is said to be strict-sense stationary (SSS) if its statistical properties are invariant to a shift of the origin, i.e., if ∀k ∈ Z

$$p(u_n, u_m, \ldots, u_r) = p(u_{n-k}, u_{m-k}, \ldots, u_{r-k}),$$

and for *any* possible combination of time instants, n, m, \ldots, r . In other words, the stochastic processes u_n and u_{n-k} are described by the same joint pdfs of all orders.

• A weaker version of stationarity is that of the *m*th order stationarity, where joint pdfs involving up to *m* variables, are invariant to the choice of the origin. For example, for a second order (m = 2) stationary process, we have that $p(u_n) = p(u_{n-k})$ and $p(u_n, u_r) = p(u_{n-k}, u_{r-k}), \ \forall n, r, k \in \mathbb{Z}.$

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- Ergodicity: A stochastic process is said to be ergodic, if the complete statistics can be determined by any one of the realizations.
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- For second order ergodic processes, the following are true:

$$\mathbb{E}[\mathbf{u}_n] = \mu = \lim_{N \to \infty} \hat{\mu}_n, \text{ where } \hat{\mu}_n := \frac{1}{2N+1} \sum_{n=-N}^N u_n.$$

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where the limits are in the mean square sense; that is,

$$\lim_{N \to \infty} \mathbb{E}\left[|\hat{\mu}_N - \mu|^2 \right] = 0,$$

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 In summary, when ergodic processes are involved, ensemble averages "across the process" can be obtained as time averages "along the process".



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Example

• The goal of this example is to construct a process which is WSS, yet it is not ergodic. Let a WSS process, x_n, i.e.,

$$\mathbb{E}[\mathbf{x}_n] = \mu$$
, and $\mathbb{E}[\mathbf{x}_n \mathbf{x}_{n-k}] = r_x(k)$.

Define the process,

 $\mathbf{z}_n := \mathbf{a} \mathbf{x}_n,$

where a is a random variable taking values in $\{0, 1\}$, with probabilities P(0) = P(1) = 0.5. Moreover, a and x_n are statistically independent. Then, we have that

$$\mathbb{E}[\mathbf{z}_n] = \mathbb{E}[\mathbf{a}\mathbf{x}_n] = \mathbb{E}[\mathbf{a}]\mathbb{E}[\mathbf{x}_n] = 0.5\mu,$$

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• Thus, z_n is WSS. However, it is not covariance-ergodic. Indeed, some of the realizations will be equal to zero (when a = 0), and the mean value and autocorrelation will be zero, which is different from the ensemble average.

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$$r(k) = r^*(-k), \ \forall k \in \mathbb{Z}.$$

Proof: This property is a direct consequence of the invariance with respect to the choice of the origin. Indeed,

$$r(k) = \mathbb{E}[\mathbf{u}_n \mathbf{u}_{n-k}^*] = \mathbb{E}[\mathbf{u}_{n+k} \mathbf{u}_n^*] = r^*(-k).$$

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• (Properties continued)

 $r(0)\geq |r(k)|, \; \forall k\neq 0.$

In other words, the correlation of the variables, corresponding to two different time instants, cannot be larger (in magnitude) than r(0). This property is essentially the Cauchy-Schwartz inequality for the inner products.

The autocorrelation of a stochastic process is a positive definite sequence. That is,

 $\sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m^* r(n,m) \ge 0, \ \forall a_n \in \mathbb{C}, \ n = 1, 2, \dots, N, \ \forall N \in \mathbb{Z}.$

Proof: The proof is easily obtained by the definition of the autocorrelation,

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• (Properties continued)

 ${f 0}$ Let u_n and v_n be two WSS processes. Define the new process

$$\mathbf{z}_n = \mathbf{u}_n + \mathbf{v}_n.$$

Then,

$$r_z(k) = r_u(k) + r_v(k) + r_{uv}(k) + r_{vu}(k),$$

where the cross-correlation between two jointly WSS stationary stochastic processes is defined as

$$r_{uv}(k) := \mathbb{E}[\mathbf{u}_n \mathbf{v}_{n-k}^*], \ k \in \mathbb{Z}.$$

The proof is a direct consequence of the definition. Note that if the two processes are *uncorrelated*, i.e., $r_{uv}(k) = r_{vu}(k) = 0$, then

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Obviously, this is also true if the processes u_n and v_n are independent and of zero mean value, since then $\mathbb{E}[u_n v_{n-k}] = \mathbb{E}[u_n]\mathbb{E}[v_{n-k}] = 0$. Note that, uncorelateness is a weaker condition and it does not necessarily imply independence; the opposite is true, for zero mean values.

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Power Spectral Density

• Power Spectral Density: Given a WSS stochastic process, u_n , its power spectral density (PSD) (or simply the power spectrum) is defined as the Fourier transform of its autocorrelation sequence, i.e., ∞

$$S(\omega) := \sum_{k=-\infty} r(k) \exp\left(-j\omega k\right).$$

The autocorrelation sequence is obtained via the inverse Fourier transform, i.e., $t = c + \pi$

$$r(k) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} S(\omega) \exp\left(j\omega k\right) d\omega.$$
⁽²⁾

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Autocorrelation Sequence: Properties

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(2)

• The PSD of a WSS stochastic process is a real and non-negative function of $\omega.$

Proof: Indeed, we have that,

$$\begin{aligned} &= \sum_{k=-\infty}^{+\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + \sum_{k=-\infty}^{-1} r(k) \exp\left(-j\omega k\right) + \sum_{k=1}^{\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + \sum_{k=1}^{+\infty} r^*(k) \exp\left(j\omega k\right) + \sum_{k=1}^{\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + 2 \sum_{k=1}^{+\infty} \operatorname{Real}\left(r(k) \exp\left(-j\omega k\right)\right), \end{aligned}$$

which proves the claim that PSD is a real number. In the proof, Property 1 of the autocorrelation sequence has been used. We defer the proof for the non-negative part for later on.

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Proof: Indeed, we have that,

$$\begin{split} S(\omega) &= \sum_{k=-\infty}^{+\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + \sum_{k=-\infty}^{-1} r(k) \exp\left(-j\omega k\right) + \sum_{k=1}^{\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + \sum_{k=1}^{+\infty} r^*(k) \exp\left(j\omega k\right) + \sum_{k=1}^{\infty} r(k) \exp\left(-j\omega k\right) \\ &= r(0) + 2 \sum_{k=1}^{+\infty} \operatorname{Real}\left(r(k) \exp\left(-j\omega k\right)\right), \end{split}$$

which proves the claim that PSD is a real number. In the proof, Property 1 of the autocorrelation sequence has been used. We defer the proof for the non-negative part for later on.

• The area under the graph of $S(\omega)$ is equal to the power of the stochastic process, i.e.,

$$\mathbb{E}[|\mathbf{u}_n|^2] = r(0) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} S(\omega) d\omega,$$

which is obtained from (2) if we set k = 0. We will come to the physical meaning of this property very soon.

• Transmission through a linear system: We will now derive the relation between the PSDs of the input and output in a linear filtering operation, expressed via the convolution sum,

$$\mathbf{d}_n = w_n * \mathbf{u}_n := \sum_{k=-\infty}^{+\infty} w_k^* \mathbf{u}_{n-k}$$

where $\ldots, w_0, w_1, w_2, \ldots$ are the parameters comprising the impulse response describing the filter.

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• In case the impulse response is of finite duration, for example, $w_0, w_1, \ldots, w_{l-1}$, then the convolution can be written as

$$\mathbf{d}_n = \sum_{k=0}^{l-1} w_k^* \mathbf{u}_{n-k} = \boldsymbol{w}^H \mathbf{u}_n,$$

$$\boldsymbol{w} := [w_0, w_1, \dots, w_{l-1}]^T, \ \mathbf{u}_n := [\mathbf{u}_n, \mathbf{u}_{n-1}, \dots, \mathbf{u}_{n-l+1}]^T \in \mathbb{R}^l.$$



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• The random vector at the input

$$\mathbf{u}_n := [\mathbf{u}_n, \mathbf{u}_{n-1}, \dots, \mathbf{u}_{n-l+1}]^T \in \mathbb{R}^l.$$

is known as the input vector of order l and at time n. Note that its elements are part of the stochastic process at successive time instants. This imposes on the respective autocorrelation matrix a rich structure, which can be exploited to develop efficient computational algorithms for its inversion.

Moreover, observe that, if the impulse response of the system is zero for negative values of the time index, n, this guarantees causality. That is, the output depends only on the values of the input at the current and previous time instants only, and there is no dependence on future values.

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• Theorem: The power spectral density of the output, d_n, of a linear time invariant system, when it is excited by a WSS stochastic process, u_n, is given by,

$$S_d(\omega) = |W(\omega)|^2 S_u(\omega),$$

where

$$W(\omega) := \sum_{n=-\infty}^{+\infty} w_n \exp\left(-j\omega n\right).$$

Proof: First, it is shown that,

 $r_d(k) = r_u(k) * w_k * w_{-k}^*.$

Then the claim is proved by taking the Fourier transform of both sides. Two well known properties of the Fourier transform have been used, i.e.,

 $r_u(k) * w_k \longmapsto S_u(\omega)W(\omega), \text{ and } w_{-k}^* \longmapsto W^*(\omega).$

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• Physical Interpretation of the PSD: The following figure shows the Fourier transform of the impulse response of a very narrow bandpass filter.



An ideal bandpass filter. The output contains frequencies only in the range of $|\omega - \omega_0| < \Delta \omega/2$.

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• We assume that $\Delta\omega$ is very small. Then, for this special case, the input-output PSD relation can be written as

$$\Delta P := \mathbb{E}\left[|\mathbf{d}_n|^2\right] = r_d(0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} S_d(\omega) d\omega \approx S_u(\omega_o) \frac{\Delta \omega}{\pi}$$

where real data have been assumed, which guarantees the symmetry of the (magnitude) of the Fourier transform $(S_u(\omega) = S_u(-\omega))$. Hence,

In other words, the value $S_u(\omega_o)$ can be interpreted as the power density (power per frequency interval) in the frequency (spectrum) domain.

This also establishes what was said before: the PSD is a non-negative real function, for any value of ω ∈ [-π, +π] (The PSD, being the Fourier transform of a sequence, is periodic with period 2π).

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Example: White Noise Sequence

• A stochastic process, η_n, is said to be white noise if the mean and its autocorrelation sequence satisfy the following:

$$\mathbb{E}[\eta_n] = 0 \text{ and } r(k) = \begin{cases} \sigma_\eta^2 & \text{if } k = 0, \\ 0, & \text{if } k \neq 0, \end{cases}$$

where σ_{η}^2 is its variance.

- In other words, all variables at different time instants are uncorrelated. If, in addition, they are independent, we say that it is strictly white noise.
- It is readily seen that its PSD is given by

$$S_{\eta}(\omega) = \sigma_{\eta}^2.$$

That is, it is constant and this is the reason it is called white noise, in analogy to the white light whose spectrum is equally spread over all the wavelengths.

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• Autoregressive Models: Autoregressive processes are one among the most popular and widely used models. An autoregressive process of order *l*, denoted as AR(*l*), is defined via the following recursion

 $\mathbf{u}_n + a_1 \mathbf{u}_{n-1} + \ldots + a_l \mathbf{u}_{n-l} = \mathbf{\eta}_n,$

where η_n is a white noise process with variance σ_n^2 .

- To generate samples, one starts form some initial conditions. The input samples here correspond to the white noise sequence and the initial conditions are set equal to zero, $u_{-1} = \dots u_{-l} = 0$.
- This is not a stationary process. Indeed, time instant n = 0 is distinctly different form all the rest, since it is the time that initial conditions are applied in.
- The effects of the initial conditions tend asymptotically to zero, if all the roots of the corresponding characteristic polynomial,

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 Autocorrelation sequence of an AR process: Multiplying both sides of the defining equation with u_{n-k}, k > 0, and taking the expectation, we obtain

$$\sum_{i=0}^{l} a_i \mathbb{E}[\mathbf{u}_{n-i}\mathbf{u}_{n-k}] = \mathbb{E}[\mathbf{\eta}_n \mathbf{u}_{n-k}], \ k > 0, \text{ where } a_0 := 1, \text{ or}$$
$$\sum_{i=1}^{l} a_i r(k-i) = 0.$$

We have used the fact that $\mathbb{E}[\eta_n u_{n-k}]$, k > 0 is zero. Indeed, u_{n-k} depends recursively on $\eta_{n-k}, \eta_{n-k-1} \dots$, which are all uncorrelated to η_n , since this is a white noise process.

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• Yule-Walker equations: Combining the previous two equations, we end up with the elegant linear system of equations:

$$\begin{bmatrix} r(0) & r(1) & \dots & r(l) \\ r(1) & r(0) & \dots & r(l-1) \\ \vdots & \vdots & \vdots & \vdots \\ r(l) & r(l-1) & \dots & r(0) \end{bmatrix} \begin{bmatrix} 1 \\ a_1 \\ \vdots \\ a_l \end{bmatrix} = \begin{bmatrix} \sigma_\eta^2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

These are known as the Yule-Walker equations, whose solution results in the values, $r(0), \ldots, r(l)$, which are then used as the initial conditions to solve the corresponding difference equation and obtain r(k), $\forall k \in \mathbb{Z}$.

- Observe the special structure of the matrix in the linear system. This type of matrices are known as Toeplitz. All the elements along any diagonal are equal.
- Moving Average (MA) models: These are defined by the recursion,

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 $\mathbf{u}_n + a\mathbf{u}_{n-1} = \mathbf{\eta}_n.$

Following the general methodology explained before, we have

$$r(k) + ar(k-1) = 0, \ k = 1, 2, \dots$$

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Considering the first equation for k = 1 together with the second one readily results in

$$r(0) = \frac{\sigma_{\eta}^2}{1 - a^2}.$$

Plugging this value in the difference equation, we recursively obtain

$$r(k) = (-a)^{|k|} \frac{\sigma_{\eta}^2}{1-a^2}, \ k = 0, \pm 1, \pm 2, \dots,$$

where we used the property, r(k) = r(-k).

• Remark: Observe that if |a| > 1, r(0) < 0 which is meaningless. Also, |a| < 1 guarantees that the magnitude of the root of the characteristic polynomial $(z_* = -a)$ is smaller than one. Moreover, |a| < 1 guarantees that $r(k) \longrightarrow 0$ as $k \longrightarrow \infty$. This is in line with common sense, since random variables which are far away in time must be uncorrelated.

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$$r(k) + ar(k-1) = 0, \ k = 1, 2, \dots$$

$$r(0) + ar(1) = \sigma_{\eta}^{2}.$$

Considering the first equation for k = 1 together with the second one readily results in ____2

$$r(0) = \frac{\sigma_{\eta}^2}{1 - a^2}.$$

Plugging this value in the difference equation, we recursively obtain

$$r(k) = (-a)^{|k|} \frac{\sigma_{\eta}^2}{1-a^2}, \ k = 0, \pm 1, \pm 2, \dots,$$

where we used the property, r(k) = r(-k).

• Remark: Observe that if |a| > 1, r(0) < 0 which is meaningless. Also, |a| < 1 guarantees that the magnitude of the root of the characteristic polynomial $(z_* = -a)$ is smaller than one. Moreover, |a| < 1 guarantees that $r(k) \longrightarrow 0$ as $k \longrightarrow \infty$. This is in line with common sense, since random variables which are far away in time must be uncorrelated.

• Plots of a realization (left) and the autocorrelation sequence (right) corresponding to the value a = -0.9.
• Plots of a realization (left) and the autocorrelation sequence (right) corresponding to the value a = -0.9.



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• Plots of a realization (left) and the autocorrelation sequence (right) corresponding to the value a = -0.4. Compared to the value of a = -0.9, the variables at different time instants are less correlated an the autocorrelation sequence fades to zero much faster.

• Plots of a realization (left) and the autocorrelation sequence (right) corresponding to the value a = -0.4. Compared to the value of a = -0.9, the variables at different time instants are less correlated an the autocorrelation sequence fades to zero much faster.



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• Plots of the PSDs for the two previous cases (left). To the right, a realization of a white noise sequence is given for the sake of comparison with the previously plotted ones.

 Plots of the PSDs for the two previous cases (left). To the right, a realization of a white noise sequence is given for the sake of comparison with the previously plotted ones.



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