EG2080 Monte Carlo Methods
in Engineering

Theme 2

RANDOM VARIABLES AND RANDOM NUMBERS

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BASIC DEFINITIONS

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- An experiment (or trial) is an observation of a phenomenon, the result of which is random.
- The result of an experiment is called its outcome.
- The set of possible outcomes for an experiment is called its sample space.

Examples:
- Throwing a die: Integer between 1 and 6.
- Sum of throwing two dice: Integer between 2 and 12.
- The weight of a person: Real number larger than 0.

NOTATION

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Random variables

Upper-case Latin letter, for example X, Y, Z.

Sometimes more than one letter is used (for example NI in the Ice-cream Company).

Observation (outcome) of a random variable

Lower-case counterpart of the symbol of the corresponding random variable, for example x, y, z.

Can sometimes be indexed to differentiate observations, for example x_i, y_i, z_i.

NOTATION

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Probability distribution

Latin f in lower or upper case (depending on interpretation) and an index showing the corresponding symbol of the random variable.

- Density function: f_X, f_Y, f_Z.
- Distribution function: F_X, F_Y, F_Z.

The index makes it easier to differentiate the probability distributions when one is dealing with more than one random variable.

NOTATION

Statistical properties of a probability distribution

Lower-case greek letter and an index showing the corresponding symbol of the random variable:

- Expectation value (mean): μ_X, μ_Y, μ_Z.
- Standard deviation: σ_X, σ_Y, σ_Z.

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NOTATION

Estimates

Latin counterpart of the greek symbol that is estimated. Can be upper-case or lower-case depending on interpretation.

- Estimated expectation value: m_X, m_Y, m_Z.
- Estimated standard deviation: s_X, s_Y, s_Z.

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RANDOM VARIABLES - Concept

- A random variable is a way to represent a sample space by assigning one or more numerical values to each outcome.
- If each outcome produces one value, the probability distribution is univariate.
- If each outcome produces more than one value, the probability distribution is multi-variate.
- If the sample space is finite or countable infinite, the random variable is discrete– otherwise, it is continuous.

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RANDOM VARIABLES - Probability Distributions

- A probability distribution describes the sample space of a random variable.
- A probability distribution can be described in several different ways.
  - Frequency function/density function.
  - Distribution function.
  - Population (set of units).

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RANDOM VARIABLES - Frequency function

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Definition 1: The probability of the outcome x for a univariate discrete random variable X is given by the frequency function $f_X(x)$, i.e.,

$$P(X = x) = f_X(x).$$

RANDOM VARIABLES - Density Function

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The probability that the outcome is exactly x is infinitesimal for a continuous random variable. Therefore, we use a density function to represent the probability that the outcome is approximately equal to x.

Definition 2: The probability of the outcomes $\mathcal{X}$ for a univariate continuous random variable X is given by the density function $f_X(x)$, i.e.,

$$P(X \in \mathcal{X}) = \int_{\mathcal{X}} f_X(x)dx.$$

RANDOM VARIABLES - Frequency and Density Functions

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Lemma: Frequency functions and density functions have the following property:

$$\sum_{x=-\infty}^{\infty} f_X(x) = 1 \text{ or } \int_{-\infty}^{\infty} f_X(x)dx = 1.$$

RANDOM VARIABLES - Distribution Function

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Definition 3: The probability that the outcome of a univariate random variable X is less than or equal to some arbitrary level x is given by the distribution function $F_X(x)$, i.e.,

$$P(X \le x) = F_X(x).$$

RANDOM VARIABLES - Distribution Function

Lemma: A distribution function has the following properties:

- $\lim_{x \to -\infty} F_X(x) = 0.$
- $\lim_{x \to +\infty} F_X(x) = 1.$
- $x_1 < x_2 \Rightarrow F_X(x_1) < F_X(x_2).$ (Increasing)
- $\lim_{h \to 0^+} F_X(x+h) = F_X(x).$ (Right-continuous)

RANDOM VARIABLES - Density, frequency and distribution functions

Lemma: The relation between distribution functions and frequency/density functions can be written as

$$F_X(x) = \sum_{\xi = -\infty}^{x} f_X(\xi) \text{ or } F_X(x) = \int_{-\infty}^{x} f_X(\xi)d\xi.$$

RANDOM VARIABLES - Multivariate Distributions

The definitions 1–3 can easily be extended to the multivariate case.

Examples:

- Discrete, three-dimensional distribution:
  $P((X, Y, Z) = (x, y, z)) = f_{X, Y, Z}(x, y, z).$
- Continuous, two-dimensional distribution:
  $$P(X \le x, Y \le y) = F_{X, Y}(x, y) = \int_{-\infty}^{x}\int_{-\infty}^{y} f_{X, Y}(\xi, \psi)d\xi d\psi.$$

POPULATIONS

For analysis of Monte Carlo simulation it can be convenient to consider observations of random variables as equivalent to selecting an individual from a population.

- The random variable X can be represented by the population $\mathcal{X}$.
- An individual in the population $\mathcal{X}$ is referred to as a unit.
- Unit i is associated to the value x_i. The values of the units do not have to be unique, i.e, it is possible that $x_i = x_j$ for two units i and j.

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POPULATIONS

- The population $\mathcal{X}$ has the units $\chi_1, \ldots, \chi_N$, i.e., $\mathcal{X}$ is a set with N elements.
- It is possible that N is infinite.
- A random observation of X is equivalent to randomly selecting a unit from the population $\mathcal{X}$.
- The probability of selecting a particular unit is $1/N$. Hence,

$$F_X(x) = \frac{N_{\{\chi_i \in \mathcal{X}:\, \chi_i \le x\}}}{N}. \qquad (1)$$

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EXAMPLE 2 - Discrete r.v.

Let X be the result of throwing a fair six-sided die once.

a) State the frequency function $f_X(x)$.

b) State the distribution function $F_X(x)$.

c) Enumerate the population $\mathcal{X}$.

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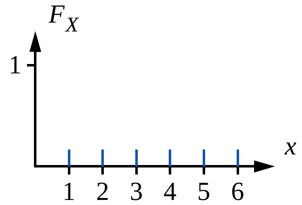
EXAMPLE 2 - Discrete r.v.

Solution:

a)



$$f_X(x) = \begin{cases} \frac{1}{6} & x = 1, 2, 3, 4, 5, 6, \\ 0 & \text{all other } x. \end{cases}$$

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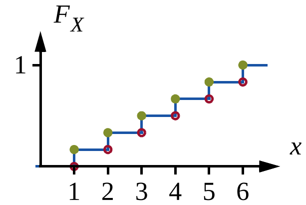
EXAMPLE 2 - Discrete r.v.

Solution (cont.)

b)

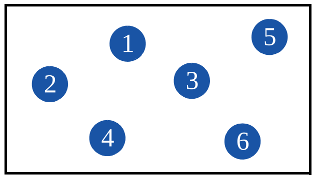
$$F_X(x) = \begin{cases} 0 & x < 1, \\ 1/6 & 1 \le x < 2, \\ 2/6 & 2 \le x < 3, \\ 3/6 & 3 \le x < 4, \\ 4/6 & 4 \le x < 5, \\ 5/6 & 5 \le x < 6, \\ 1 & 6 \le x. \end{cases}$$



EXAMPLE 2 - Discrete r.v.

Solution (cont.)

c) $\mathcal{X} = \{1, 2, 3, 4, 5, 6\}$.



EXAMPLE 3 - Continuous r.v.

Let X be a random variable which is uniformly distributed between 10 and 20.

a) State the frequency function $f_X(x)$.

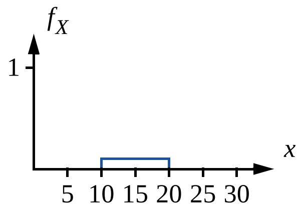
b) State the distribution function $F_X(x)$.

c) Enumerate the population $\mathcal{X}$.

EXAMPLE 3 - Continuous r.v.

Solution:

a)

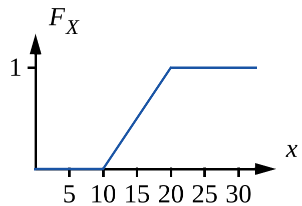


$$f_X(x) = \begin{cases} 0.1 & 10 \le x \le 20, \\ 0 & \text{all other } x. \end{cases}$$

EXAMPLE 3 - Continuous r.v.

Solution (cont.)

b)



$$F_X(x) = \begin{cases} 0 & x \le 10, \\ 0.1x - 1 & 10 \le x \le 20, \\ 1 & 20 \le x. \end{cases}$$

EXAMPLE 3 - Continuous r.v.

Solution (cont.)

c) The population has one unit for each real number between 10 and 20.

EXPECTATION VALUE

The expectation value of a random variable is the mean of the all possible outcomes weighted according to their probability:

Definition 4: The expectation value of the random variable X is given by

$$E[X] = \sum_{x=-\infty}^{\infty} x f_X(x) \text{ (discrete)},$$

EXPECTATION VALUE

Definition 4 (cont.)

$$E[X] = \int_{-\infty}^{\infty} x f_X(x) dx \text{ (continuous)},$$

or

$$E[X] = \frac{1}{N} \sum_{i=1}^{N} x_i \text{ (population)}.$$

EXPECTATION VALUE

Not all random variables have an expectation value!

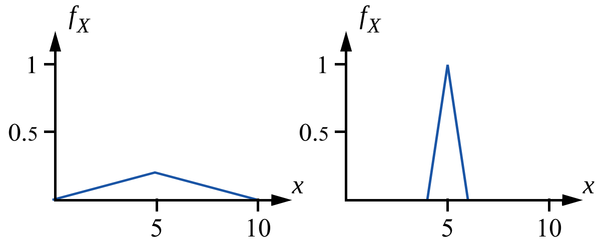
Example (St. Petersburg paradox): A player tosses a coin until a tail appears. If a tail is obtained for the first time in the j:th trial, the player wins 2^{j-1} €.

Let X be the payout when playing this game. The probability that trial j is the first trial where the tail appears is 2^{-j}, $j = 1, 2, 3, \ldots$. Hence we get

$$E[X] = \sum_{j=1}^{\infty} 2^{-j} \cdot 2^{j-1} = \sum_{j=1}^{\infty} \frac{1}{2}.$$

VARIANCE

The expectation value provided important information about a random variable, but in many cases we need to know more than the expected average, for example the spread.



VARIANCE

A common measure of the spread is the variance, i.e., the expected quadratic deviation from the expectation value.

Definition 5: The variance of the random variable X is given by

$$Var[X] = E[(X - E[X])^2] =$$
$$= E[X^2] - (E[X])^2 \text{ (general)},$$

$$Var[X] = \sum_{x=-\infty}^{\infty} (x - E[X])^2 f_X(x) \text{ (discrete)},$$

VARIANCE

Definition 5 (cont.)

$$Var[X] = \int_{-\infty}^{\infty} (x - E[X])^2 f_X(x) dx \text{ (continuous)},$$

or

$$Var[X] = \frac{1}{N} \sum_{i=1}^{N} (x_i - E[X])^2 \text{ (population)}.$$

STANDARD DEVIATION

It is in many cases convenient to have a measure of the spread which has the same unit as the expectation value. Therefore, the notion standard deviation has been introduced:

Definition 6: The standard deviation of the random variable X is given by

$$\sigma_X = \sqrt{Var[X]}.$$

COVARIANCE

For multivariate distributions it is sometimes necessary to describe how the random variables interact:

Definition 7: The covariance of two random variables X and Y is given by

$$Cov[X, Y] = E[(X - E[X])(Y - E[Y])] = = E[XY] - E[X]E[Y].$$

Lemma: $Cov[X, Y] = Cov[Y, X]$, $Cov[X, X] = Var[X]$.

COVARIANCE

A covariance matrix, $\Sigma_{\mathbf{X}}$, states the covariance between all random variables in a multivariate distribution:

$$\Sigma_{\mathbf{X}} = \begin{bmatrix} Var[X_1] & Cov[X_1, X_2] \cdots Cov[X_1, X_k] \\ Cov[X_2, X_1] & Var[X_2] & \\ \vdots & & \ddots \\ Cov[X_k, X_1] & & & Var[X_k] \end{bmatrix}$$

CORRELATION COEFFICIENT

The covariance is an absolute measure of the interaction between two random variables. Sometimes it is preferable to use a relative measure:

Definition 8: The correlation coefficient of two random variables X and Y is given by

$$\rho_{X, Y} = \frac{Cov[X, Y]}{\sqrt{Var[X]Var[Y]}}.$$

CORRELATION COEFFICIENT

We can conclude from definition 8 that the correlation coefficient always is in the interval $[-1, 1]$.

- $\rho_{X, Y} > 0 \Rightarrow X$ and Y positively correlated
  If the outcome of X is low then it is likely that the outcome of Y is also low and vice versa.
- $\rho_{X, Y} < 0 \Rightarrow X$ and Y are negatively correlated.
  If the outcome of X is low then it is likely that the outcome of Y is high and vice versa.
- $\rho_{X, Y} = 0 \Leftrightarrow Cov(X, Y) = 0 \Rightarrow X$ and Y uncorrelated

INDEPENDENT RANDOM VARIABLES

A very important special case when studying multivariate distributions is when the random variables are independent.

Definition 9: X and Y are independent random variables if it holds for each x and y that

$$f_{X,Y}(x,y) = f_X(x)f_Y(y) \Leftrightarrow F_{X,Y}(x,y) = F_X(x)F_Y(y).$$

INDEPENDENT RANDOM VARIABLES

Theorem 1: If X and Y are independent then

$$E[XY] = E[X]E[Y].$$

Theorem 2: If X and Y are independent then they are also uncorrelated.

Warning! Correlations are easily misunderstood!

CORRELATIONS

- X and Y being uncorrelated does not have to imply that they are independent.
  Example: Y uniformly distributed between -1 and 1, $X = Y^2 \Rightarrow \rho_{X,Y} = 0$, although X is dependent of Y.
- A correlation only indicates that *there is* a relation, but does not say anything about the *cause* of the relation.
  Example: $X = 1$ if a driver wears pants, otherwise 0, $Y = 1$ if driver involved in an accident, otherwise 0. The conclusion if $\rho_{X,Y} > 0$ should not be that wearing pants increases the risk of traffic accidents. In reality such a correlation would probably be due to a more indirect relation.

ARITHMETICAL OPERATIONS

Theorem 3:

i) $E[aX] = aE[X]$

ii) $E[g(X)] = \int_{-\infty}^{\infty} g(x)f_X(x)dx$ (continuous),

$E[g(X)] = \sum_x g(x)f_X(x)$ (discrete),

$E[g(X)] = \frac{1}{N}\sum_{i=1}^{N} g(x_i)$ (population).

ARITHMETICAL OPERATIONS

Theorem 3 (cont.)

iii) $E[X+Y] = E[X] + E[Y]$

iv) $$E[g(X,Y)] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(x,y) f_{XY}(x,y)\,dx\,dy$$ (continuous),

$$E[g(X,Y)] = \sum_{x}\sum_{y} g(x,y) f_{XY}(x,y)$$ (discrete).

ARITHMETICAL OPERATIONS

Theorem 3 (cont.)

$$E[g(X,Y)] = \frac{1}{N}\sum_{i=1}^{N} g(x_i, y_i)$$ (population)

Theorem 4:

i) $Var[aX] = a^2 Var[X]$

ii) $Var[X+Y] =$
$= Var[X] + Var[Y] + 2Cov[X,Y]$

ARITHMETICAL OPERATIONS

Theorem 4 (cont.)

iii) $Var[X-Y] =$
$= Var[X] + Var[Y] - 2Cov[X,Y]$

iv) $$Var\left[\sum_{i=1}^{k} X_i\right] = \sum_{i=1}^{k}\sum_{j=1}^{k} Cov[X_i, X_j]$$

ARITHMETICAL OPERATIONS

Theorem 5: If X and Y are independent random variables and $Z = X + Y$ then the probability distribution of Z can be calculated using a convolution formula, i.e.,

$$f_Z(x) = \int_{-\infty}^{\infty} f_X(t) f_Y(x-t)\,dt$$

or

$$f_Z(x) = \sum_{t} f_X(t) f_Y(x-t).$$

PROBABILITY DISTRIBUTIONS

- Probability distributions can be defined arbitrarily, but there are also general probability distributions which appear in many practical applications.
- Density function, distribution functions, expectation values and variances for many general probability distributions can be found in mathematical handbooks. The English version of Wikipedia also provides a lot of information.

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RANDOM NUMBERS

- A random number generator is necessary to create random samples for a computer simulation.
- A random number generator is a mathematical function that generate a sequence of numbers.

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RANDOM NUMBERS

- Modern programming languages have built-in functions for generating random numbers from $U(0, 1)$-distributions and some other distributions.
- The underlying formula behind the most common random number generators is the following:

$$X_{i+1} = aX_i \pmod{m}.^* \tag{2}$$

* The operator $\bmod m$ denotes the remainder when dividing by m.

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RANDOM NUMBERS

- Starting with a certain seed, X_0, the equation (2) will generate a deterministic sequence of numbers, $\{X_i\}$.
- The sequence will eventually repeat itself (at least after m numbers).
- The sequence $U_i = X_i/m$ will imitate a real sequence of $U(0, 1)$-distributed random numbers if the constants a and m are chosen appropriately.

  Example: $a = 7^5 = 16\,807$ and $m = 2^{31} - 1$.

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RANDOM NUMBERS

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- The designation pseudo-random numbers is sometimes used to stress that the sequence of numbers is actually deterministic.
- One method to make it more or less impossible to predict a sequence of pseudo-random numbers it to use the internal clock of the computer as seed.
- An advantage of pseudo-random numbers is that a simulation can be recreated by using the same seed again.

RANDOM NUMBERS

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A good random number generator will generate a sequence of random numbers which

- is as long as possible (before it repeats itself)
- is distributed as close to a $U(0, 1)$-distribution as possible
- has a negligible correlation between the numbers in the sequence.

RANDOM NUMBERS

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How do we generate the inputs Y to a computer simulation?

- A pseudo-random number generator provides $U(0, 1)$-distributed random numbers.
- Y generally has some other distribution.

There are several methods to transform $U(0, 1)$-distributed random numbers to an arbitrary distribution.

In this course we will use the inverse transform method.

INVERSE TRANSFORM METHOD

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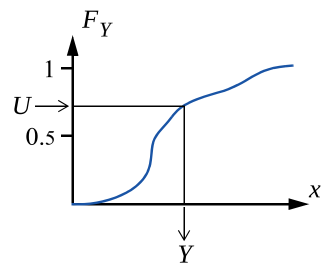
Theorem 6: If a random variable U is $U(0, 1)$-distributed then $Y = F_Y^{-1}(U)$ has the distribution function $F_Y(x)$.



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EXAMPLE 4 - Inverse transform method

A pseudo-random number generator providing $U(0, 1)$-distributed random numbers has generated the value $U = 0.40$.

a) Transform U to a result of throwing a fair six-sided die.

b) Transform U to a result from a $U(10, 20)$-distribution.

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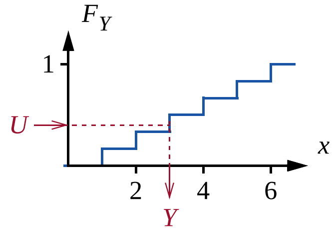
EXAMPLE 4 - Inverse transform method

Solution:

a) Graphic solution:



In the general case, a discrete inverse distribution function can be calculated using a search algorithm.

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EXAMPLE 4 - Inverse transform method

Solution (cont.)

b) The inverse distribution function is given by

$$F_Y^{-1}(x) = \begin{cases} 10 & x \le 0, \\ 10x + 10 & 0 \le x \le 1, \\ 20 & 1 \le x. \end{cases}$$

$$\Rightarrow Y = F_Y^{-1}(0.4) = 14.$$

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NORMALLY DISTRIBUTED RANDOM NUMBERS

The normal distribution does not have an inverse distribution function! However, it is possible to use an approximation:*

> *Theorem 7:* If a random variable U is $U(0, 1)$-distributed then Y is $N(0, 1)$-distributed if Y is calculated as follows:

* This method is therefore referred to as the "*approximative inverse transform method*".

NORMALLY DISTRIBUTED RANDOM NUMBERS

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Theorem 7 (cont.)

$$Q = \begin{cases} U & \text{if } 0 \le U \le 0.5, \\ 1 - U & \text{if } 0.5 < U \le 1, \end{cases}$$

$$t = \sqrt{-2 \ln Q},$$

NORMALLY DISTRIBUTED RANDOM NUMBERS

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Theorem 7 (cont.)

$$z = t - \frac{c_0 + c_1 t + c_2 t^2}{1 + d_1 t + d_2 t^2 + d_3 t^3}$$

$$c_0 = 2.515\,517, \quad d_1 = 1.432\,788,$$
$$c_1 = 0.802\,853, \quad d_2 = 0.189\,269,$$
$$c_2 = 0.010\,328, \quad d_3 = 0.001\,308,$$

NORMALLY DISTRIBUTED RANDOM NUMBERS

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Theorem 7 (cont.)

$$Y = \begin{cases} -z & \text{if } 0 \le U < 0.5, \\ 0 & \text{if } U = 0.5, \\ z & \text{if } 0.5 < U \le 1. \end{cases}$$

CORRELATED RANDOM NUMBERS

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- It is convenient if the inputs Y in a computer simulation are independent, because then the random variables can be generated separately.
- However, it is also possible to generate correlated random numbers.
  - Correlated normally distributed numbers.
  - General method.

CORRELATED RANDOM NUMBERS - Normal distribution

Theorem 8: Let $X = [X_1, \ldots, X_K]^T$ be a vector of independent $N(0, 1)$-distributed components. Let $\boldsymbol{B} = \Sigma^{1/2}$, i.e., let λ_i and g_i be the i:th eigenvalue and the i:th eigenvector of Σ and define the following matrices:

$$\boldsymbol{P} = [g_1, \ldots, g_K],$$

$$\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_K),$$

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CORRELATED RANDOM NUMBERS - Normal distribution

Theorem 8 (cont.)

$$\boldsymbol{B} = \boldsymbol{P}\Lambda^{1/2}\boldsymbol{P}^T.$$

Then $Y = \mu + \boldsymbol{B}X$ is a random vector where the elements are normally distributed with the mean μ and the covariance matrix Σ.

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CORRELATED RANDOM NUMBERS - General method

Consider a multivariate distribution $Y = [Y_1, \ldots, Y_K]$ with the density function f_Y.

- Step 1. Calculate the density function of the first element, f_{Y1}.
- Step 2. Randomise the value of the first element according to f_{Y1}.
- Step 3. Calculate the conditional density function of the next element, i.e.,

$$f_{Yk|[Y_1, \ldots, Y_{k-1}] = [\psi_1, \ldots, \psi_{k-1}]}.$$

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CORRELATED RANDOM NUMBERS - General method

- Step 4. Randomise the value of the k:th element according to the conditional probability distribution obtained from

$$f_{Yk|[Y_1, \ldots, Y_{k-1}] = [\psi_1, \ldots, \psi_{k-1}]}.$$

- Step 5. Repeat step 3–4 until all elements have been randomised.

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CORRELATED RANDOM NUMBERS - Alternative method

- This method is only applicable to discrete probability distributions.

  However, a continuous probability distribution can of course be approximated by a discrete distribution.
- The idea is to use a modified distribution function for the inverse transform method.

CORRELATED RANDOM NUMBERS - Alternative method

Original distribution function: $F_{Y1,\,Y2}(y_1, y_2)$ is the probability that $Y_1 \le y_1$ and $Y_2 \le y_2$.

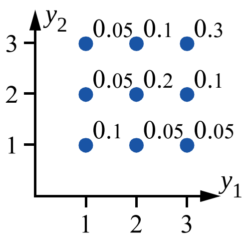
Modified distribution function: Arrange all units in the population in an ordered list; $F_{Y1,\,Y2}(n)$ is now the probability to select one of the n first units in the list.

The order of the list might influence the efficiency of some variance reduction techniques!

EXAMPLE 5 - Correlated discrete random numbers

Consider the multivariate probability distribution $f_{Y1,\,Y2}$ to the right.

According to the definition, we have $\rho_{Y1,\,Y2} \approx 0.4$.



EXAMPLE 5 - Correlated discrete random numbers

a) Apply the general method to randomise values of Y_1 and Y_2 using the two independent random numbers $U_1 = 0.15$ and $U_2 = 0.62$ from a $U(0, 1)$-distribution.

b) Apply the alternative method to randomise values of Y_1 and Y_2 using the random number $U_1 = 0.12$ from a $U(0, 1)$-distribution.

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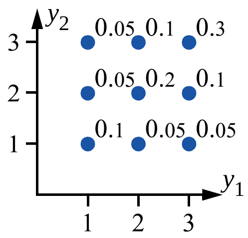
EXAMPLE 5 - Correlated discrete random numbers

Solution: a) The probability distribution of the first element is given by



$$f_{Y1}(y_1) = \sum_{\psi_2} f_{Y1,\,Y2}(y_1, \psi_2) = \begin{cases} 0.2 & y_1 = 1, \\ 0.35 & y_1 = 2, \\ 0.45 & y_1 = 3. \end{cases} \Rightarrow Y_1 = F_{Y1}^{-1}(0.15) = 1.$$

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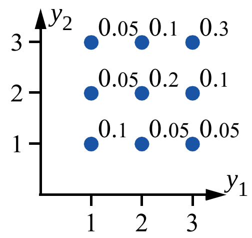
EXAMPLE 5 - Correlated discrete random numbers

Solution (cont.) The conditional distribution of Y_1 is now given by



$$f_{Y2|Y_1 = 1}(y_2) = \frac{f_{Y1,\,Y2}(1, y_2)}{f_{Y1}(1)} = \begin{cases} 0.5 & y_2 = 1, \\ 0.25 & y_2 = 2, \\ 0.25 & y_2 = 3. \end{cases} \Rightarrow Y_2 = F_{Y2|Y_1 = 1}^{-1}(0.62) = 2.$$

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EXAMPLE 5 - Correlated discrete random numbers

Solution: b) Assume that units are listed as follows:

Number	1	2	3	4	5	6	7	8	9
Unit Y_1	1	1	2	1	2	3	2	3	3
Y_2	1	2	1	3	2	1	3	2	3

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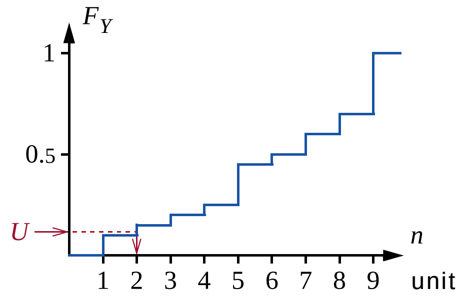
EXAMPLE 5 - Correlated discrete random numbers

Solution(cont.)

The modified distribution function is shown to the right.



The value $U = 0.12$ corresponds to the second unit, i.e., $Y_1 = 1$ and $Y_2 = 2$.