The "mc2d" package.

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Contents

This documentation is intended for readers with:

- A medium level of experience in R. Please refer to the Manual "An Introduction to R" available with R distribution if needed;
- Some knowledge about Monte-Carlo simulation (its basic principles and its utility) and about Quantitative Risk Assessment (QRA).

This documentation will not describe all arguments of the functions. The definitive reference remains the documentation associated with the package.

1 Introduction

1.1 What is `mc2d`?

"`mc2d`" means Two-Dimensional Monte-Carlo (*"Monte-Carlo à Deux Dimensions"*). This package :

- provides additional probability distributions;
- provides tools to construct One-Dimensional and Two-Dimensional Monte-Carlo Simulations;
- provides tools to analyse One-Dimensional and Two-Dimensional Monte-Carlo Simulations.

In a previous version, some tools to fit parametric distributions to data were included. Because these functions are useful for other purposes, they have been moved to a separate package called `fitdistrplus`. Both the `mc2d` and the `fitdistrplus` packages are available at the URL `https://r-forge.r-project.org/projects/riskassessment/`.

`mc2d` was built for QRA in the Food Safety domain but it can be used in other QRA domains.

1.2 What is Two-Dimensional Monte-Carlo Simulation (briefly)?

The following text and Figure 1 are adapted from [4] and [5] where this method was used. The principal reference for Two-Dimensional Monte-Carlo simulation remains [2].

According to international recommendations, a QRA should reflect the "variability" in the risk and calculate the "uncertainty" associated with the risk estimate. The "variability" represents temporal, geographical and/or individual heterogeneity of the risk for a given population. The "uncertainty" is understood as stemming from a lack of perfect knowledge about the QRA model structure and associated parameters[1].

In order to estimate the natural "variability" of the risk, a Monte-Carlo simulation approach may be useful: the empirical distribution of the risk within the population may be estimated from the mathematical combination of distributions reflecting the variability of parameters across the population.

A two-dimensional (or second-order) Monte-Carlo simulation was proposed to estimate the "uncertainty" in the risk estimates stemming from parameter uncertainty [2]. A two-dimensional Monte-Carlo simulation is a Monte-Carlo simulation where the distributions reflecting "variability" and the distributions representing "uncertainty" are sampled separately in the simulation, so that "variability" and "uncertainty" in the output may be estinated separately. It may be described as following (see Figure 1):

1. The parameters of the model should be divided into three categories: the parameters whose distributions reflect "variability only", hereinafter denoted as "variable parameters", the parameters whose distributions reflect "uncertainty only", denoted as "uncertain parameters" and the parameters whose distributions reflect both uncertainty and variability. For this latter category, a hierarchical structure, using "hyper-parameters", should be specified: if a parameter is both uncertain and variable, one should be able to specify an empirical or parametric distribution representing variability. This distribution is conditional upon other parameters for which there is some associated uncertainty. As an example, one should be able to specify a relationship such as $X\,|a,b \sim N\,(a,b)$, where the specified normal distribution represents variability in x conditional upon parameters a and b. Hyperdistributions, such as $a \sim Unif\,(l_a,u_a)$and $b \sim Unif\,(l_b,u_b)$, represent the uncertainty in the parameters a and b;
2. A set of uncertain parameters are randomly sampled from their respective distributions;
3. The QRA is performed using a classical (one-dimensional) Monte-Carlo simulation of size N_v, treating the uncertain parameters as fixed. This QRA takes into account the variability in all variable parameters, and leads to an empirical density function reflecting the variability of exposure/risk across the population, conditional upon the uncertain parameters. Various statistics (*e.g.* the mean, the standard deviation, percentiles) of the resulting empirical density function are evaluated and stored;
4. Steps 2) and 3) are performed a large number (N_u) of times , leading to N_u sets of statistics;
5. As output, the 50^{th} percentile (median) of each statistic is used as a point estimate of this statistic; the 2.5^{th} and 97.5^{th} percentiles of each statistic are used to establish a 95% credible interval (CI95) of this statistic. The median of the N_u estimated values for each of the 101 estimated percentiles allows us to display a "variability cumulative distribution" via a graph. This curve is surrounded by the 2.5th and 97.5th percentiles obtained from the N_u estimates of each of the 101 percentiles.

"`mc2d`" is a set of R functions that will help to develop such two-dimensional Monte-Carlo simulations. The main difference from the procedure described above is that `mc2d` uses arrays of (at least) two dimensions to derive the results: the first dimension will reflect variability, the second will reflect uncertainty. This document will not develop the method further, but will illustrate the practical application of `mc2d`, using a fictitious example.

[1] In the engineering risk community, these concepts are refered as "aleatoric uncertainty" for "variability" and "epistemic uncertainty" for "uncertainty".

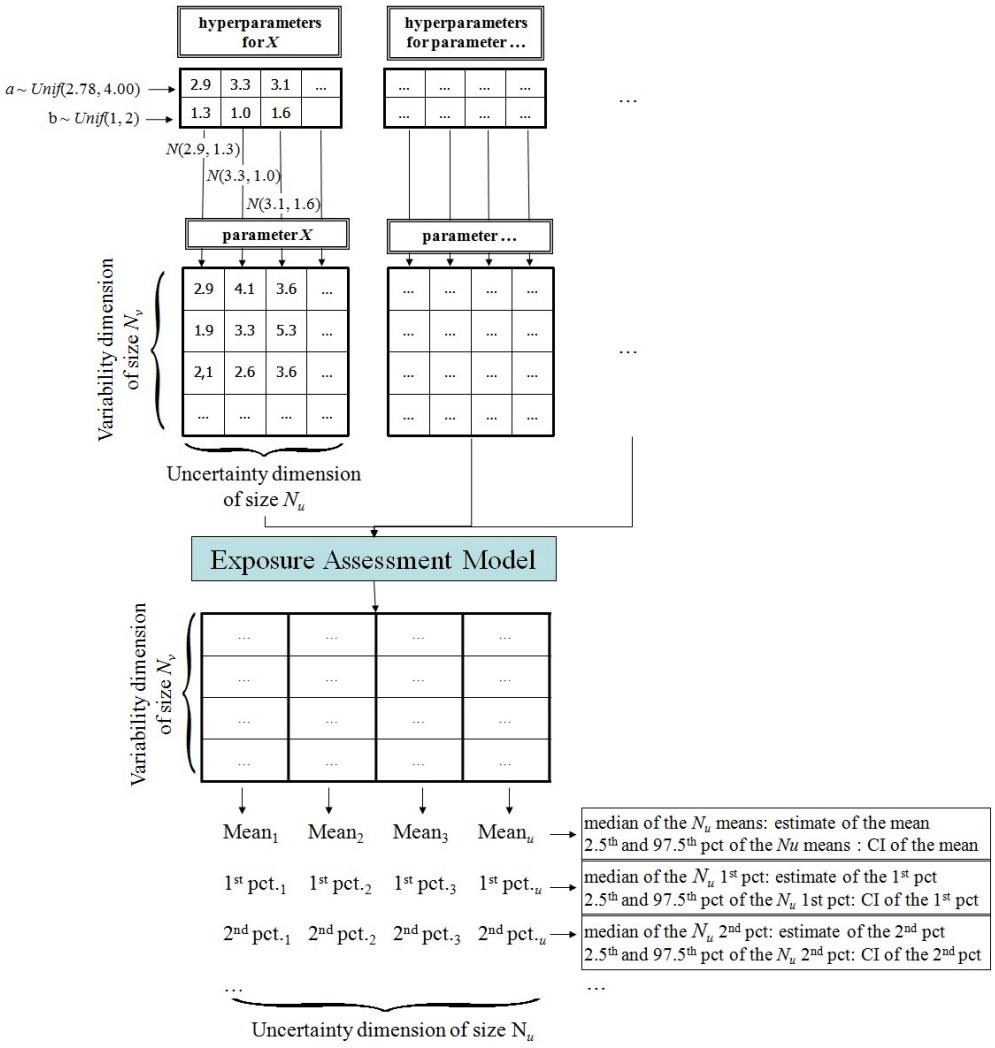


Figure 1: Shematic Representation of a Two-Dimensional Monte-Carlo Simulation.

1.3 A basic example

Quantitative Risk Assessment: *Escherichia coli* O157:H7 infection linked to the consumption of frozen ground beef in <3 year old children.

- We assume that, in a given batch of ground beef, *E. coli* O157:H7 are randomly distributed with a mean concentration of $c = 10$ bacteria (cfu) per gram of product;
- We assume that no bacterial growth occurs in storage, since the product is kept frozen until it is cooked, just before consumption;
- 2.7% of consumers cook their beef "rare", 37.3% "medium" and 60.0% "well done";
- The following bacterial inactivation i is associated with these cooking practices:
  - No inactivation for "rare" cooking;
  - 1/5 surviving bacteria for a "medium" cooking;
  - 1/50 surviving bacteria for a "well done" cooking.
- The variability in steak serving sizes s for <3 year children was estimated in a consumption survey. The "best fit" to the data was a gamma distribution with parameters: $shape = 3.93$, $rate = 0.0806$.
- The dose-response relationship, describing the probability of illness, P, according to the dose is a one-hit model. The probability of illness per hit r is assumed to be constant with $r = 0.001$.

The question is: "*What is the distribution of the risk of illness in the population that consumed the contaminated lot?*"

This distribution will be estimated using Monte-Carlo simulations performed with R via the "`mc2d`" package. First, the model will be developed in a one dimensional framework. Then, in order to include some uncertainties in the model, it will be derived in a two dimensional framework.

1.3.1 One Dimensional Monte-Carlo Simulation

As a first step, we assume that no uncertainty exists in our model. All distributions represent variability only. The model may be written as:

$$\begin{aligned} c &= 10. \\ i &\sim emp\left(\{1, 1/5, 1/50\}, \{0.027, 0.373, 0.600\}\right) \\ s &\sim gamma\left(3.93, 0.0806\right) \\ n &\sim Poisson\left(c \times i \times s\right) \\ P &= 1 - (1 - 0.001)^n \end{aligned}$$

where $emp\left(\boldsymbol{X}, \boldsymbol{P}\right)$ is an empirical distribution wherein each value X_i is associated with a probability P_i.We will use a "classical" one dimensional Monte-Carlo simulation, with 1,000 iterations. Using the "`mc2d`" package, the model may be written as:

```
> library(mc2d)
> ndvar(1000)
```

```
[1] 1000
```

```
> conc <- 10
> cook <- mcstoc(rempiricalD, values = c(1, 1/5, 1/50), prob = c(0.027,
+     0.373, 0.6))
> serving <- mcstoc(rgamma, shape = 3.93, rate = 0.0806)
> expo <- conc * cook * serving
> dose <- mcstoc(rpois, lambda = expo)
> r <- 0.001
> risk <- 1 - (1 - r)^dose
> EC1 <- mc(cook, serving, expo, dose, risk)
> print(EC1)

     node    mode  nsv nsu nva variate  min    mean  median     max Nas type
1    cook numeric 1000   1   1       1 0.02  0.1165  0.0200   1.000   0    V
2 serving numeric 1000   1   1       1 5.17 48.4451 44.0195 219.976   0    V
3    expo numeric 1000   1   1       1 1.03 56.2452 14.1530 935.189   0    V
4    dose numeric 1000   1   1       1 0.00 56.0520 15.0000 938.000   0    V
5    risk numeric 1000   1   1       1 0.00  0.0507  0.0149   0.609   0    V
  outm
1 each
2 each
3 each
4 each
5 each

> summary(EC1)

cook :
       mean    sd  Min 2.5%  25%  50% 75% 97.5% Max  nsv Na's
NoUnc 0.116 0.176 0.02 0.02 0.02 0.02 0.2     1   1 1000    0

serving :
      mean   sd  Min 2.5%  25% 50%  75% 97.5% Max  nsv Na's
NoUnc 48.4 24.3 5.17 14.5 29.8  44 62.6   103 220 1000    0

expo :
      mean   sd  Min 2.5%  25%  50%  75% 97.5% Max  nsv Na's
NoUnc 56.2 96.8 1.03  3.5 8.11 14.2 79.1   229 935 1000    0

dose :
      mean   sd Min 2.5% 25% 50% 75% 97.5% Max  nsv Na's
NoUnc   56 96.3   0    2   7  15  79   226 938 1000    0

risk :
        mean     sd Min  2.5%     25%    50%   75% 97.5%   Max  nsv Na's
NoUnc 0.0507 0.0755   0 0.002 0.00698 0.0149 0.076 0.203 0.609 1000    0
```

This One-Dimensional Monte-Carlo simulation provides an estimate of the mean risk (approximately 5%), as well as some quantiles of the risk distribution (2.5% of the population has a risk of illness greater than 20.3%).

1.3.2 Two dimensional Monte-Carlo Simulation

Assume now that:

- The mean concentration of bacteria in the batch is not known with certainty, but was only a point estimate. Microbiologists think that the uncertainty around this estimate can be represented via a normal distribution with parameters $\mu = 10$ and $\sigma = 2$;
- Epidemiological studies suggest that the r parameter is also uncertain. The uncertainty around the mean value of 0.001 can be represented with a uniform distribution between 0.0005 and 0.0015.

The model could then be written as:

$$\begin{aligned} c &\sim N(10, 2) \\ i &\sim emp(\{1, 1/5, 1/50\}, \{0.027, 0.373, 0.600\}) \\ s &\sim gamma(3.93, 0.0806) \\ n &\sim Poisson(c \times i \times s) \\ r &\sim Unif(0.0005, 0.0015) \\ P &= 1 - (1 - r)^n \end{aligned}$$

Note that the distributions of r and c represent uncertainty, while the distributions of i and s represent variability. n, which is a function of c, i and s, will be both variable *and* uncertain.

We will use a two-dimensional Monte-Carlo simulation, with 1,000 iterations in the variability dimension and 100 iterations in the uncertainty dimension. Using the "`mc2d`" package, the model may be written as:

```
> ndunc(100)

[1] 100

> conc <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
> cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5, 1/50),
+     prob = c(0.027, 0.373, 0.6))
> serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
> expo <- conc * cook * serving
> dose <- mcstoc(rpois, type = "VU", lambda = expo)
> r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
> risk <- 1 - (1 - r)^dose
> EC2 <- mc(conc, cook, serving, expo, dose, r, risk)
> print(EC2, digits = 2)

     node    mode  nsv nsu nva variate     min    mean  median     max Nas type
1    conc numeric    1 100   1       1 5.55771 9.9e+00  9.7214 1.7e+01   0    U
2    cook numeric 1000   1   1       1 0.02000 1.1e-01  0.0200 1.0e+00   0    V
3 serving numeric 1000   1   1       1 2.66586 5.0e+01 45.0430 1.6e+02   0    V
4    expo numeric 1000 100   1       1 0.70535 5.3e+01 13.7118 1.7e+03   0   VU
5    dose numeric 1000 100   1       1 0.00000 5.3e+01 14.0000 1.7e+03   0   VU
6       r numeric    1 100   1       1 0.00051 9.6e-04  0.0009 1.5e-03   0    U
7    risk numeric 1000 100   1       1 0.00000 4.6e-02  0.0136 8.4e-01   0   VU
  outm
1 each
2 each
3 each
4 each
5 each
6 each
7 each
```

```
> summary(EC2)

conc :
       NoVar
median  9.72
mean    9.94
2.5%    5.96
97.5%  14.46

cook :
       mean    sd  Min 2.5%  25%  50% 75% 97.5% Max  nsv Na's
NoUnc 0.107 0.166 0.02 0.02 0.02 0.02 0.2  0.22   1 1000    0

serving :
      mean   sd  Min 2.5% 25% 50%  75% 97.5% Max  nsv Na's
NoUnc 49.7 24.9 2.67 13.6  31  45 64.2   110 161 1000    0

expo :
       mean    sd   Min 2.5%   25%   50%   75% 97.5%  Max  nsv Na's
median 51.9  94.2 1.234 3.06  7.87 13.58  71.8   240  938 1000    0
mean   53.1  96.3 1.261 3.12  8.04 13.89  73.4   245  959 1000    0
2.5%   31.8  57.8 0.756 1.87  4.82  8.33  44.0   147  575 1000    0
97.5%  77.2 140.2 1.836 4.55 11.71 20.21 106.8   357 1396 1000    0

dose :
       mean    sd  Min 2.5%   25%  50%   75% 97.5%  Max  nsv Na's
median 51.9  94.7 0.00    2  7.00 14.0  71.8   242  958 1000    0
mean   53.1  96.7 0.04    2  7.53 14.2  73.4   245  964 1000    0
2.5%   31.7  57.8 0.00    1  4.47  9.0  43.5   146  573 1000    0
97.5%  77.6 140.7 1.00    3 11.00 20.5 107.8   355 1379 1000    0

r :
          NoVar
median 0.000902
mean   0.000962
2.5%   0.000525
97.5%  0.001459

risk :
         mean     sd      Min     2.5%     25%     50%    75%  97.5%   Max  nsv
median 0.0445 0.0703 0.00e+00 0.001713 0.00687 0.01298 0.0645 0.2027 0.589 1000
mean   0.0455 0.0706 3.88e-05 0.001902 0.00717 0.01347 0.0674 0.2061 0.582 1000
2.5%   0.0191 0.0324 0.00e+00 0.000583 0.00282 0.00538 0.0271 0.0841 0.290 1000
97.5%  0.0730 0.1057 7.08e-04 0.004115 0.01226 0.02242 0.1116 0.3259 0.788 1000
       Na's
median    0
mean      0
2.5%      0
97.5%     0
```

Note that the syntax is similar to the earlier model. However, a "`type`" argument is provided for each distribution, indicating whether the parameter distribution represents uncertainty (`type`="`U`"), variability (`type`="V"), or both (`type`="`VU`").

The summary provides estimates of the variability distributions (in rows) but with a measure of their uncertainty, linked to the uncertainty around `conc` and `r`. The estimate of the mean risk is now uncertain. The median of the 100 simulations leads to a "best estimate"of 0.0445, with a 95% "credible interval" of [0.191, 0.0730].

2 Basic Principles and Functions

A typical session of R using "`mc2d`" is as follows:

- From data, expert knowledge, *etc.* an empirical or parametric distribution is chosen for each "parent" parameter. For developing an empirical distribution from data , the "`fitdistrplus`" package is recommended;
- For each parameter, an `mcnode` object is constructed (key functions: `mcdata, mcstoc`);
- Various `mcnode` objects are grouped into an `mc` object (key function: `mc`).
- The `mc` object is studied through summaries, graphs, and sensitivity analysis (key functions: `summary.mc`, `plot.mc`, `tornado`, `tornadounc`).

2.1 Preliminary Step

The "`mc2d`" library should be loaded at the beginning of your R session ("`library(mc2d)`").

The default size of the Monte-Carlo Simulation should be defined using the `ndvar()` function (dimension of variability) and the `ndunc()` function (dimension of uncertainty).

2.2 The `mcnode` Object as an Elementary Object.

2.2.1 `mcnode` Object Structure

An `mcnode` object is the basic element of an `mc` object. It is an array of dimension ($nsv \times nsu \times nvariates$) where nsv is the dimension of variability, nsu is the dimension of uncertainty and $nvariates$ is the number of variates of the `mcnode`[2]. Four types of `mcnode` exist:

- "`V`" `mcnode`, for "*Variability*", is an array of dimension ($nsv \times 1 \times nvariates$). The distribution represents variability in the parameter;
- "`U`" `mcnode`, for "*Uncertainty*", is an array of dimension ($1 \times nsu \times nvariates$). The distribution represents uncertainty in the parameter.
- "`VU`" `mcnode`, for "*Variability and Uncertainty*", is an array of dimension ($nsv \times nsu \times nvariates$). The distribution represents both variability (in the first dimension) and uncertainty (in the second dimension) in the parameter.
- Additionally, a "`0`" `mcnode` is also defined . "`0`" stands for "Neither Variability or Uncertainty". Such nodes are arrays of dimension ($1 \times 1 \times nvariates$). No uncertainty or variability is considered for these nodes. A "`0`" `mcnode` is not necessary in the univariate context (use a scalar instead) but is useful in constructing multivariate nodes (See section 3).

There are 5 ways to construct an `mcnode` object:

[2] In this section, we will only consider `mcnodes` with $nvariates = 1$.

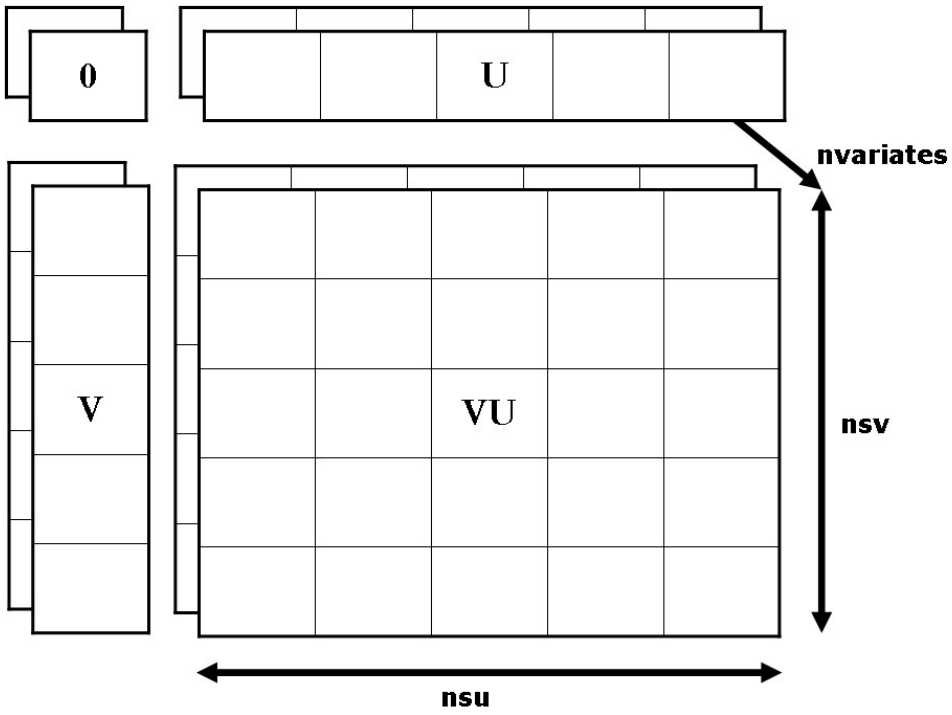


Figure 2: Structure of the various `mcnode` objects.

1. The `mcstoc` function constructs an `mcnode` from random number generating functions;
2. The `mcdata` function constructs an `mcnode` from data sets;
3. `An mcnode` can be constructed directly from operations on `mcnode` objects;
4. `mcprobtree` is a special function that constructs an `mcnode` from other `mcnodes` using a probability tree;
5. Some functions, such as "`==`" or "`>`" , `is.na`, `is.finite` generate a new `mcnode` when applied to an existing `mcnode`.

2.2.2 The `mcstoc` function

The `mcstoc` function is written as[3]:

```
mcstoc(func=runif, type=c("V", "U", "VU", "0"), ..., nsv=ndvar(), nsu=ndunc(),
nvariates=1, outm="each", nsample="n", seed=NULL, rtrunc=FALSE, linf=-Inf, lsup=Inf,
lhs=FALSE)
```

- `func` is a function providing random data or its name as a character. The table 1 provides available distributions from the `stats` and the `mc2d` libraries that can be used in `mcstoc`;
- `type` is the type of requested `mcnode`. By default, `mcstoc` constructs a "`V`" `mcnode`;

[3]as is standard in R, most arguments have logical default values and will be infrequently modified.

Table 1: Available distributions

Package	Distribution	function	Parameter `n`	Other Parameters	trunc	lhs
`stats`	beta	`rbeta`	`n`	`shape1, shape2, ncp`	Y	Y
	binomial	`rbinom`	`n`	`size, prob`	Y	Y
	Cauchy	`rcauchy`	`n`	`location, scale`	Y	Y
	chi-squared	`rchisq`	`n`	`df, ncp`	Y	Y
	exponential	`rexp`	`n`	`rate`	Y	Y
	F	`rf`	`n`	`df1, df2, ncp`	Y	Y
	gamma	`rgamma`	`n`	`shape, rate (or scale)`	Y	Y
	geometric	`rgeom`	`n`	`prob`	Y	Y
	hypergeometric	`rhyper`	`nn`	`m, n, k`	Y	Y
	lognormal	`rlnorm`	`n`	`meanlog, sdlog`	Y	Y
	logistic	`rlogis`	`n`	`location, scale`	Y	Y
	negative binomial	`rnbinom`	`n`	`size, prob (or mu)`	Y	Y
	normal	`rnorm`	`n`	`mean, sd`	Y	Y
	Poisson	`rpois`	`n`	`lambda`	Y	Y
	Student's t	`rt`	`n`	`df, ncp`	Y	Y
	uniform	`runif`	`n`	`min, max`	Y	Y
	Weibull	`rweibull`	`n`	`shape, scale`	Y	Y
	Wilcoxon	`rwilcox`	`nn`	`m,n`	Y	Y
`mc2d`	Bernoulli	`rbern`	`n`	`prob`	Y	Y
	empirical discrete	`rempiricalD`	`n`	`values, prob`	Y	Y
	empirical continuous	`rempiricalC`	n	`min, max, values, prob`	Y	Y
	PERT	`rpert`	`n`	`min, mode, max, shape`	Y	Y
	triangular	`rtriang`	`n`	`min, mode, max`	Y	Y
	generalised beta	`rbetagen`	`n`	`shape1,shape2,min,max,ncp`	Y	Y
	multinomial	`rmultinomial`	`n`	`n, size, prob`	N	N
	Dirichlet	`rdirichlet`	`n`	`alpha`	N	N
	multivariate normal	`rmultinormal`	`n`	`mean, sigma`	N	N

- ... are the arguments to be passed to the function `func`, with the exception of the argument providing the size of the sample. This latter is calculated by the function according to `func`, `type`, `nsv`, `nsu` and `nvariates`. If the name of the argument specifying the size of the sample is not `n` (*e.g.* functions `rhyper` and `rwilcox`, see table 1), the name of this parameter should be provided in the `nsample` argument. *Note that all of the following arguments should be named*;
- `nsv` and `nsu` are the number of samples needed in the variability and uncertainty dimension, respectively. By default, these values are the ones provided by `ndvar()` and `ndunc()`, respectively;
- `nvariates` is the desired number of variates in the `mcnode`;
- `outm` is the default output for multivariate nodes;
- `seed` optionally specifies a seed for the random number generator;
- `rtrunc` allows truncation of a distribution between `linf` and `lsup`. This function is not valid for every distribution (see table 1). See the `rtrunc` function help for further details;
- `lhs` allows Latin hypercube sampling of the node . This function is not valid for every distribution (see table 1). See the `lhs` function help for further details.

In our basic example, `mcstoc` was used to specify `conc` (a normal distribution), `cook` (an empirical discrete distribution), `serving` (a gamma distribution), and `dose` (a Poisson distribution). Note that the argument `lambda` of the Poisson distribution (node `dose`) is itself an `mcnode`.

```
> conc <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
> cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5, 1/50),
+     prob = c(0.027, 0.373, 0.6))
> serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
> ...
> dose <- mcstoc(rpois, type = "VU", lambda = expo)
> r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
> ...
```

A normal distribution with parameters $mean = 2$, $sd = 3$, truncated on the interval [1.5, 2], with samples generated via Latin hypercube sampling could be written[4]:

```
> x <- mcstoc(rnorm, mean = 2, sd = 3, rtrunc = TRUE, linf = 1.5,
+     lsup = 2, lhs = TRUE)
> summary(x)
```

```
node :
      mean    sd Min 2.5%  25%  50%  75% 97.5% Max  nsv Na's
NoUnc 1.75 0.144 1.5 1.51 1.63 1.75 1.88  1.99   2 1000    0
```

For convenience in using `mcstoc`, the following additional distributions have been implemented: the Bernoulli distribution (`rbern`), the empirical discrete distribution (`rempiricalD`), the PERT distribution (`rpert`)[6], the triangular distribution (`rtriang`), the Dirichlet distribution (`rdirichlet`) and the multivariate normal distribution (`rmultinormal`). The multinomial distribution has been adapted (vectorized): `rmultinomial` (library `mc2d`) should be used in place of `rmultinom` (library `stats`). The empirical discrete (*e.g.* for bootstrap), the Dirichlet, the multinomial and the multivariate normal may be used with uncertain and/or variable parameters by specifying multivariate nodes. See section 3.

2.2.3 The `mcdata` function

Another way to construct an `mcnode` object is *via* the `mcdata` function, when data are available.

```
mcdata(data, type=c("V", "U", "VU", "0"), nsv=ndvar(), nsu=ndunc(), nvariates=1,
outm="each")
```

See the documentation associated with this function to see the size/type of data that can be used to construct an `mcnode`. The following example places a `TRUE` value in a "U" node in half of the simulations:

```
> nu <- ndunc()
> tmp <- (1:nu) > (nu/2)
> mcdata(tmp, type = "U")
```

```
  node    mode nsv nsu nva variate min mean median max Nas type outm
1    x logical   1 100   1       1   0  0.5    0.5   1   0    U each
```

[4]Note that the mean and the standard deviation of the untruncatednormal distribution are not preserved in the truncated distribution.

2.2.4 Operations on an mcnode

mcnodes can be automatically constructed using operations on other mcnodes. Rules are used to transfer uncertainty and variability coherently within the model. Logically, the rules are as follows (illustrated here with a "+")[5]:

- "0" + "0" = "0";
- "0" + "V" = "V"
- "0" + "U" = "U";
- "0" + "VU" = "VU";
- "V" + "V" = "V";
- "V" + "U" = "VU": the "U" mcnode is recycled by row, the "V" mcnode is recycled in the standard manner by column;
- "V" + "VU" = "VU": the "V" mcnode is recycled in the standard manner by column;
- "U" + "U" = "U";
- "U" + "VU" = "VU": the "U" mcnode is recycled by row;
- "VU" + "VU" = "VU"

Thus, in our example:

```
> ...
> expo <- conc * cook * serving
> ...
> risk <- 1 - (1 - r)^dose
```

expo is a function of a "U" and two "V" mcnodes: it is a "VU" mcnode with variability in the row dimension and uncertainty in the column dimension . risk is a function of a "U" and a "VU" mcnode: it is therefore a "VU" mcnode.

2.2.5 The mcprobtree function

The mcprobtree function can be used if a "probability tree" is needed to construct an mcnode. Assume that the distribution representing the uncertainty on conc was not itself certain, and that the microbiologists suggest that they are 75% sure that $conc \sim N(10, 2)$ but that they are 25% sure that $conc \sim U(8, 12)$. This could be written using mcprobtree as[6]:

```
> conc1 <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
> conc2 <- mcstoc(runif, type = "U", min = 8, max = 12)
> whichdist <- c(0.75, 0.25)
> concbis <- mcprobtree(whichdist, list(`0` = conc1, `1` = conc2),
+     type = "U")
```

mcprobtree can also be used to generate samples from a mixture distribution for variability .

[5] These rules are not the standard R rules for recycling.

[6] two alternatives for whichdist are whichdist <- mcstoc(rempiricalD, type="U", values=c(0,1), prob=c(75,25)) or whichdist <- mcstoc(rbern,type="U",prob=0.25)

2.2.6 Other functions for constructing an `mcnode`

The functions "==", "<", "<=", ">=", ">", generate an `mcnode` when applied to another `mcnode`.

Special functions `is.na(x)`, `is.nan(x)`, `is.finite(x)`, `is.infinite(x)` are implemented to test if any values are `NA` (missing data), `NaN` ("*Not A Number*"), or finite .

```
> cook < 1
```

```
  node    mode  nsv nsu nva variate min  mean median max Nas type outm
1    x logical 1000   1   1       1   0 0.975      1   1   0    V each
```

```
> tmp <- log(mcstoc(runif, min = -1, max = 1))
> tmp
```

```
  node    mode  nsv nsu nva variate   min  mean median      max Nas type outm
1    x numeric 1000   1   1       1 -8.19 -1.03 -0.699 -0.00167 512    V each
```

```
> is.na(tmp)
```

```
  node    mode  nsv nsu nva variate min  mean median max Nas type outm
1    x logical 1000   1   1       1   0 0.512      1   1   0    V each
```

2.2.7 Specifying a correlation between `mcnodes`

Structural links between sets of parameters may be very important in QRA. In `mc2d`, a Spearman rank correlation structure for 2 or more nodes may be specified with the `cornode` function. This function uses the method of Iman & Conover to generate correlated samples [3]. Assume that a study suggests that people who consume rare ground beef alsoconsume larger serving sizes. We could specify this relation using:

```
> cornode(cook, serving, target = 0.5, result = TRUE)
```

```
output Rank Correlation per variates
variates: 1
[1] 1.0000000 0.3796997 0.3796997 1.0000000
$cook
  node    mode  nsv nsu nva variate  min  mean median max Nas type outm
1    x numeric 1000   1   1       1 0.02 0.107   0.02   1   0    V each

$serving
  node    mode  nsv nsu nva variate  min mean median max Nas type outm
1    x numeric 1000   1   1       1 2.67 49.7     45 161   0    V each
```

Note that the resulting correlation (around 0.4) is obviously an approximation to the desired value of 0.5, because a discrete distribution (`cook`: 3 categories) is correlated with a continuous distribution (`serving`).

It is possible to create such correlations between "V" nodes, between " U" nodes, between "VU" nodes, or between one "V" node and multiple "VU" nodes.

The use of a multivariate normal distribution (`rmultinormal`) is another way to specify correlations among nodes, assuming that the individual nodes are normally distributed.

2.3 The mc Object

Once the mcnode objects are constructed, one should group them into a single object in order to analyse the Monte-Carlo results. The "mc" object is a list of mcnodes. There are three ways to construct an mc object: using the mc function, using the evalmcmod function, or within the evalmccut function.

2.3.1 The mc Function

```
mc(..., name=NULL, devname=FALSE)
```

... are mcnodes or mc objects to be gathered into an mc object. mc value is an mc object with specific methods, e.g. print or summary. In our example, we used:

```
> ...
> EC2 <- mc(conc, cook, serving, expo, dose, r, risk)
> print(EC2)
> summary(EC2)
```

2.3.2 The mcmodel and the evalmcmod Functions

A model may be written in one step using mcmodel (just a wrapper of your model in a function), and then evaluated using evalmcmod. These functions may be used once your model is correct and has been tested using a small number of iterations. For our example:

```
> modelEC3 <- mcmodel({
+     conc <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
+     cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5,
+         1/50), prob = c(0.027, 0.373, 0.6))
+     serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
+     r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
+     expo <- conc * cook * serving
+     dose <- mcstoc(rpois, type = "VU", lambda = expo)
+     risk <- 1 - (1 - r)^dose
+     mc(conc, cook, serving, expo, dose, r, risk)
+ })
> modelEC3

expression({
    conc <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
    cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5,
        1/50), prob = c(0.027, 0.373, 0.6))
    serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
    r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
    expo <- conc * cook * serving
    dose <- mcstoc(rpois, type = "VU", lambda = expo)
    risk <- 1 - (1 - r)^dose
    mc(conc, cook, serving, expo, dose, r, risk)
})
attr(,"class")
[1] "mcmodel"
```

Note that:

- the model is wrapped between "`{`" and "`}`";
- any (valid) R code may be placed in the model[7];
- The model should end with an `mc()` function.

The model is then evaluated using the `evalmcmod` function:

```
evalmcmod(expr, nsv=ndvar(), nsu=ndunc(), seed=NULL)
```

One can re-run the model with various dimensions or random seeds in one line:

```
> EC3 <- evalmcmod(modelEC3, nsv = 100, nsu = 10, seed = 666)
> EC4 <- evalmcmod(modelEC3, nsv = 100, nsu = 1000, seed = 666)
```

2.3.3 The `mcmodelcut` and the `evalmccut` Functions

If evaluating a high-dimensional model, R may exceed its memory limit. `evalmccut` evaluates a 2-dimensional Monte-Carlo model (written with the `mcmodelcut` function) using a loop, and calculates and stores statistics in the uncertainty dimension for further analysis. Readers should refer to the corresponding documentation for further details. Our example would be written as:

```
> modEC4 <- mcmodelcut({
+     {
+         cook <- mcstoc(rempiricalD, type = "V", values = c(0,
+             1/5, 1/50), prob = c(0.027, 0.373, 0.6))
+         serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
+         conc <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
+         r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
+     }
+     {
+         expo <- conc * cook * serving
+         dose <- mcstoc(rpois, type = "VU", lambda = expo)
+         risk <- 1 - (1 - r)^dose
+         res <- mc(zero, conc, cook, serving, expo, dose, r, risk)
+     }
+     {
+         list(sum = summary(res), plot = plot(res, draw = FALSE),
+             minmax = lapply(res, range), tor = tornado(res),
+             et = sapply(res, sd))
+     }
+ })
> evalmccut(modEC4, nsv = 10001, nsu = 101, seed = 666)
```

Note that the use of a `tornado` function in the model should be avoided as it slows the `evalmccut` function considerably. The `tornado` function will be rewritten in the near future to improve its performance.

2.4 Analysing an `mc` Object

As a reminder, the `print` function provides a very basic summary of the `mc` object. It has a `digits` argument (default: 3). Obviously, other more informative functions are provided in the `mc2d` package.

[7] If needed, it is possible to make reference to the simulation dimensions using `ndvar()` and/or `ndunc()`.

2.4.1 The `summary` Function

The `summary` function provides statistics on an `mc` object:

```
summary(object, probs=c(0,0.025,0.25,0.5,0.75,0.975,1), lim=c(0.025,0.975), ...)
```

The mean, the standard deviation and the quantiles provided in the `probs` arguments are evaluated on the variability dimension. Then, the median and the quantiles provided in the `lim` argument are evaluated on these statistics. Of course, these arguments should be changed if other quantiles are needed.

```
> tmp <- summary(EC2, probs = c(0.995, 0.999), digits = 12)
> tmp$risk
```

```
             mean         sd     99.5%     99.9%  nsv Na's
median 0.04446930 0.07028198 0.5016035 0.5573356 1000    0
mean   0.04554518 0.07058057 0.4979376 0.5522955 1000    0
2.5%   0.01914973 0.03243724 0.2380268 0.2771793 1000    0
97.5%  0.07297994 0.10573336 0.7113664 0.7565299 1000    0
attr(,"type")
[1] "VU"
```

2.4.2 The `hist` Function

The `hist` provides a histogram of the different `mcnodes` making up the `mc` object (cf. Figure 3).

```
hist (x, griddim = NULL, xlab = names(x), ylab = "Frequency", main = "", ...)
```

In the current version, uncertainty and variability distributions are collapsed. Thus, the resulting histogram may be meaningless.

```
> hist(EC2)
```

2.4.3 The `plot` function

The `plot` function provides a graph of the empirical distribution function of the estimate (mean or median) of the quantiles.

```
plot (x, prec = 0.01, stat = c("median", "mean"), lim = c(0.025,0.975), na.rm = TRUE,
griddim = NULL, xlab = NULL, ylab = "Fn(x)", main = "", draw = TRUE, ...)
```

For our example, see Figure 4, a default graph.

```
> plot(EC2)
```

Note that `mcnode` objects have the same methods `print`, `summary`, `plot`, and `hist`.

Figure 3: Function `hist`.

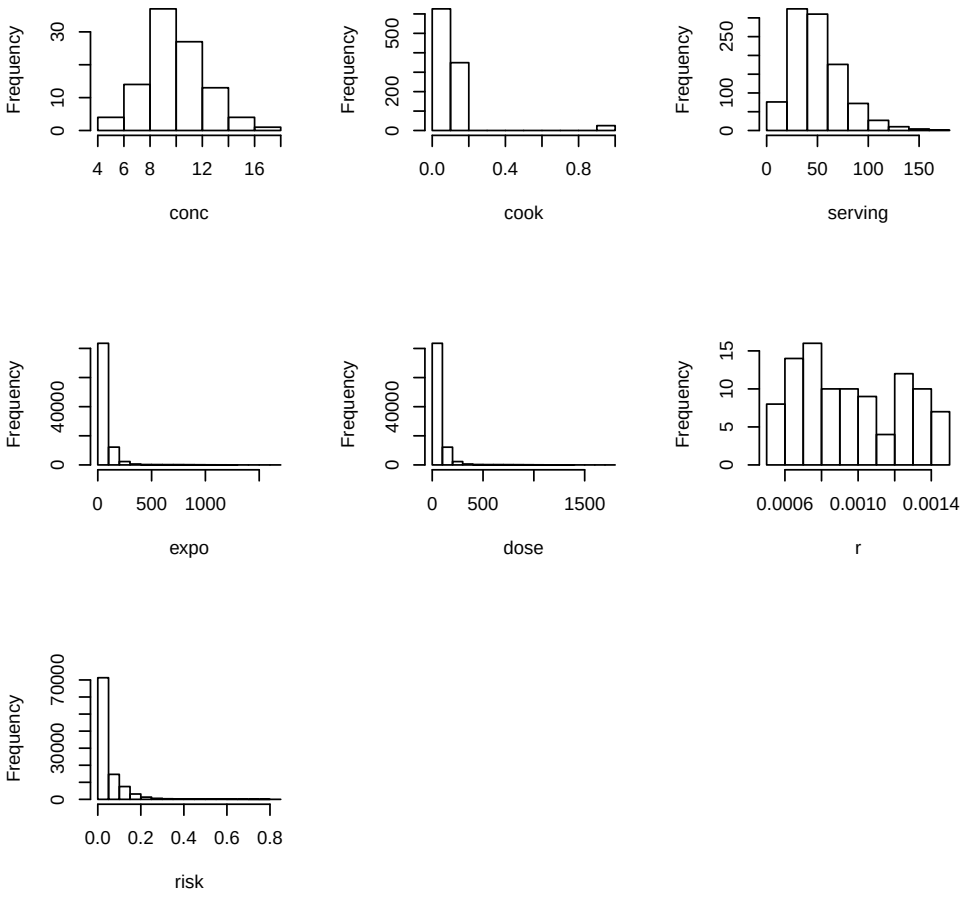


Figure 4: `plot` Function .

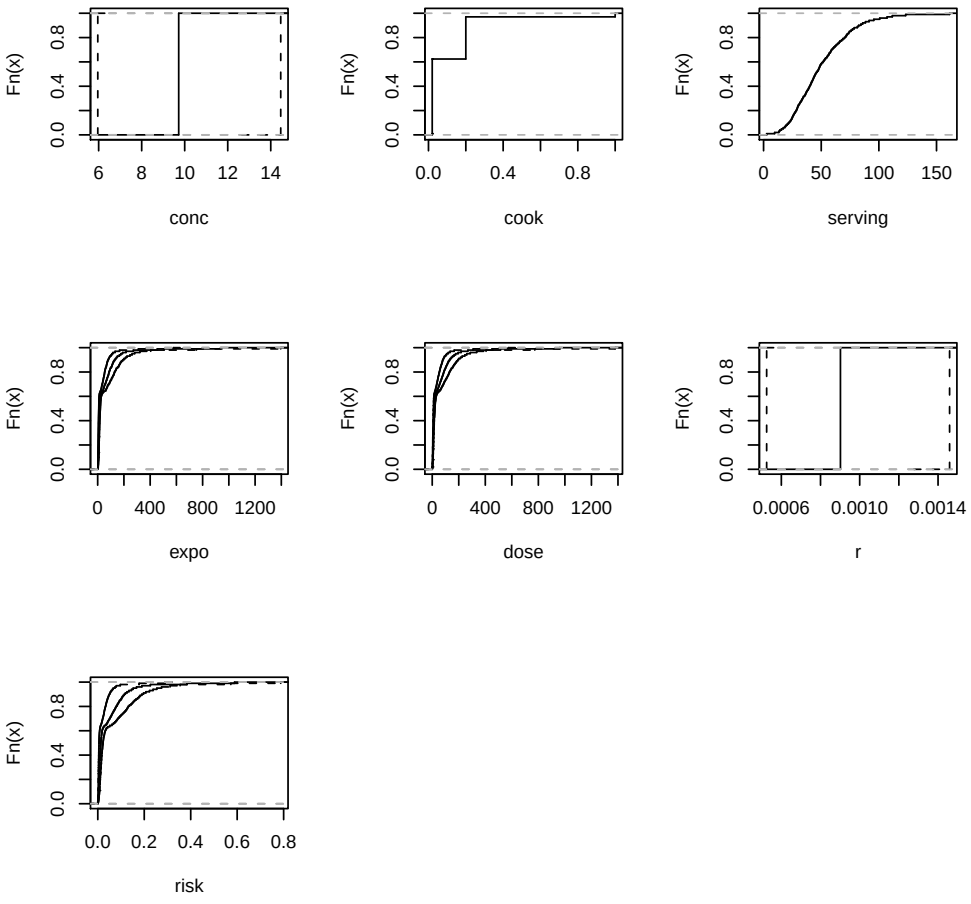
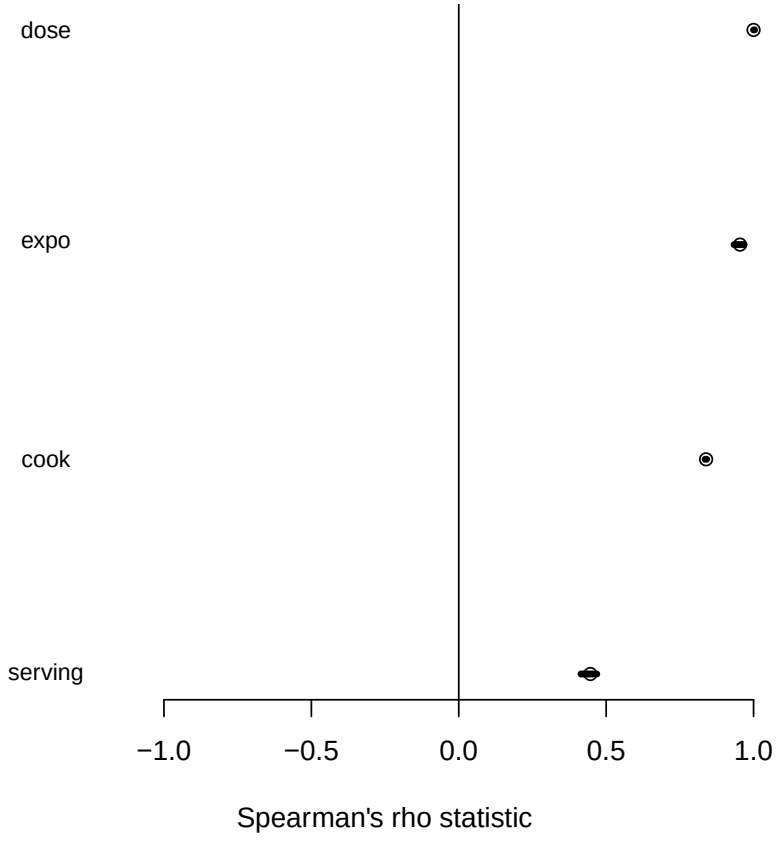


Figure 5: `plot.tornado` Function .



2.4.4 The `tornado` function

The `tornado` function calculates the Spearman (default) rank correlation between nodes of the `mc` object.

```
tornado(x, output=length(x), use="all.obs", method=c("spearman", "kendall","pearson"),
lim=c(0.025, 0.975))
```

where `output` is the `mcnode` (name or rank) of the output (default: the last `mcnode`). Missing data are treated using the `use` arguments (see the reference documentation). `tornado` creates a `tornado` object with a `plot` method (*cf.* Figure 5).

```
> torEC2 <- tornado(EC2)
> plot(torEC2)
```

2.4.5 The `tornadounc` function

The `tornadounc` function examines the impact of the uncertainty on the estimate of an output. It calculates the Spearman (default) rank correlation between statistics of the `mc` object in the variability dimension.

```
tornadounc(mc,output = length(mc), quant=c(0.5,0.75,0.975), use = "all.obs",
method=c("spearman","kendall","pearson"), ...)
```

The `quant` argument indicates which quantiles should be used in the variability dimension. `tornadounc` creates a `tornadounc` object with a `plot` method

```
> tornadounc(EC2, output = "risk", quant = 0.99)

Tornado on uncertainty
Spearman's rho statistic
Output:  risk
$risk
               conc mean expo   sd expo  99% expo mean dose   sd dose  99% dose
mean risk 0.5244044 0.5244044 0.5244044 0.5244044 0.5220402 0.5235644 0.4966712
sd risk   0.5233123 0.5233123 0.5233123 0.5233123 0.5210321 0.5229043 0.4958971
99% risk  0.5233603 0.5233603 0.5233603 0.5233603 0.5214761 0.5233003 0.5088284
                  r
mean risk 0.7727933
sd risk   0.7728413
99% risk  0.7607921
```

The output shows the impact of the uncertain nodes (type "U" nodes) and some statistics (mean, median and, here, the 99$^{\text{th}}$percentile) calculated on the variability dimension (type "V" and type "VU" nodes) of some output statistics .

2.5 Other Functions and `mc` Objects

`mc` objects are simply lists of three dimensional arrays; within each array, values in a given column represent variability in the parameter.

Knowing the structure of the `mc` and the structure of the `mcnode` objects, it is straightforward to apply any R function to these objects. The "`$`" function is helpful for extracting an `mcnode` from an `mc` object. The `unmc` function removes all attributes, classes, and dimensions equal to one, providing a list of vectors, matrices and/or arrays.

Here is a (silly) example building a linear model (in fact `ndunc()` linear models) between the `risk` and the `dose` within each uncertainty dimension and estimating some statistics for the coefficients. This example is here only to illustrate that the entire spectrum of R functionality is available for your analysis.

```
> tmp <- unmc(EC2, drop = TRUE)
> dimu <- ncol(tmp$risk)
> coef <- sapply(1:dimu, function(x) lm(tmp$risk[, x] ~ tmp$dose[,
+     x])$coef)
> apply(coef, 1, summary)

        (Intercept) tmp$dose[, x]
Min.      0.0007991     0.0004028
1st Qu.   0.0038060     0.0005948
Median    0.0064130     0.0007084
Mean      0.0072600     0.0007334
3rd Qu.   0.0092290     0.0008837
Max.      0.0206100     0.0011200
```

3 Multivariate Nodes

The dimension `nvariates` is the third dimension of the `mcnode`. One can ignore it while using `mc2d` . Nevertheless, its use is mandatory to handle some multivariate distributions, and it may be useful in other circumstances. Constructing multivariate nodes is straightforward. We note that the following code:

```
> mcstoc(runif, nvariates = 3, min = c(1, 2, 3), max = 4)
```

will logically not provide a node with 3 variates, each having a different limit. The recycling rule says that `c(1, 2, 3)` will be used in the first dimension, i.e. the variability dimension. Use instead:

```
> lim <- mcdata(c(1, 2, 3), type = "0", nvariates = 3)
> mcstoc(runif, nvariates = 3, min = lim, max = 4)
```

```
  node    mode  nsv nsu nva variate  min mean median max Nas type outm
1    x numeric 1000   1   3       1 1.00 2.54   2.58   4   0    V each
2    x numeric 1000   1   3       2 2.00 3.00   3.00   4   0    V each
3    x numeric 1000   1   3       3 3.00 3.52   3.52   4   0    V each
```

3.1 Multivariate Nodes for Multivariate Distributions

The basic usage of multivariate nodes (and the reason why they have been implemented) is for multivariate distributions such as the Dirichlet distribution, the multinomial distribution, the multivariate normal distribution and, possibly, the empirical distribution

As an example, assume that 3-member families buy 500 g of ground beef. The proportions of steak eaten by the baby, his older brother and his mother follow a Dirichlet (uncertainty) distribution with (vector) parameter $\alpha = (2, 3, 5)$. We want to derive the distribution (variability) of steak eaten by 500 babies sampled from these 500 families.

```
> (p <- mcstoc(rdirichlet, type = "U", nsu = 100, nvariates = 3,
+     alpha = c(2, 3, 5)))
```

```
  node    mode nsv nsu nva variate    min  mean median   max Nas type outm
1    x numeric   1 100   3       1 0.0198 0.196  0.170 0.647   0    U each
2    x numeric   1 100   3       2 0.0389 0.297  0.283 0.685   0    U each
3    x numeric   1 100   3       3 0.1968 0.507  0.512 0.846   0    U each
```

```
> s <- mcstoc(rmultinomial, type = "VU", nsv = 500, nsu = 100,
+     nvariates = 3, size = 500, prob = p)
> summary(s)
```

```
node :
[[1]]
        mean    sd    Min   2.5%   25%   50%   75% 97.5%   Max nsv Na's
median  85.0  8.34  60.50  69.00  79.0  85.0  90.5 101.8 109.5 500    0
mean    98.1  8.16  74.28  82.60  92.5  98.0 103.5 114.2 123.8 500    0
2.5%    15.7  3.68   6.47   8.95  13.4  15.4  17.9  23.4  28.3 500    0
97.5%  249.1 11.29 216.65 226.78 241.5 249.0 256.5 270.8 281.0 500    0

[[2]]
        mean    sd   Min  2.5%   25%   50%   75% 97.5%   Max nsv Na's
```

```
median 141.3 10.06 113.0 121.7 135.0 141.5 148.0 160.3 173.5 500    0
mean   148.5  9.55 120.2 130.3 141.9 148.5 154.9 167.1 178.2 500    0
2.5%    24.4  4.89  11.4  15.6  20.9  23.9  27.4  34.4  38.3 500    0
97.5%  319.8 11.34 289.8 298.9 311.9 320.4 327.9 341.6 351.7 500    0

[[3]]
       mean    sd   Min  2.5% 25% 50% 75% 97.5% Max nsv Na's
median  256 10.78 221.0 234.7 248 256 264   278 290 500    0
mean    253 10.70 221.5 232.7 246 253 261   274 286 500    0
2.5%    114  9.04  88.8  96.7 108 114 121   134 148 500    0
97.5%   380 11.67 347.0 360.3 374 381 387   399 409 500    0
```

Assume that each member of these families eats a "normal" distribution (variability) of steak with mean 100, 150 and 250 g. There is a positive correlation between the servings of the children, and a negative one with the serving of the mother. We want to derive the distribution (variability) of steak eaten by 500 babies.

```
> (x <- mcstoc(rmultinormal, type = "V", nvariates = 3, mean = c(100,
+     150, 250), sigma = c(10, 2, -5, 2, 10, -5, -5, -5, 10)))

  node    mode  nsv nsu nva variate   min mean median max Nas type outm
1    x numeric 1000   1   3       1  88.4  100    100 110   0    V each
2    x numeric 1000   1   3       2 141.3  150    150 160   0    V each
3    x numeric 1000   1   3       3 239.0  250    250 260   0    V each

> cor(x[, 1, ])

           [,1]       [,2]       [,3]
[1,]  1.0000000  0.1822931 -0.4950757
[2,]  0.1822931  1.0000000 -0.4884462
[3,] -0.4950757 -0.4884462  1.0000000
```

In this example, `mean` could be variable or uncertain, as well as `sigma`[8]. You could have used, for an uncertain mean:

```
> m <- mcdata(c(100, 150, 250), type = "0", nvariates = 3)
> mun <- mcstoc(rnorm, type = "U", nvariates = 3, mean = m, sd = 20)
> x <- mcstoc(rmultinormal, type = "VU", nvariates = 3, mean = mun,
+     sigma = c(10, 2, -5, 2, 10, -5, -5, -5, 10))
> cor(x[, 1, ])

           [,1]       [,2]       [,3]
[1,]  1.0000000  0.1817660 -0.5168595
[2,]  0.1817660  1.0000000 -0.4903274
[3,] -0.5168595 -0.4903274  1.0000000
```

The correlation is preserved, but the mean of each category is uncertain.

Finally, multivariate nodes may be useful to derive a nonparametric bootstrap. Assume that, based on a study, you obtained 6 individuals who eat 100 g, 12 individuals who eat 150 g, 6 individuals who eat 170 g and 6 individuals who eat 200 g of ground beef. You want to use a nonparametric bootstrap to derive uncertainty [2], and then select samples from the empirical distribution.

[8] Caution: the use of a varying `sigma` can make the analysis very slow.

```
> (x <- mcstoc(rempiricalD, type = "U", outm = c("min", "mean",
+     "max"), nvariates = 30, values = c(100, 150, 170, 200), prob = c(6,
+     12, 6, 6)))

  node    mode nsv nsu nva variate min mean median max Nas type outm
1    x numeric   1 100  30      NA 100  100    100 100   0    U  min
2    x numeric   1 100  30      NA 143  154    154 168   0    U mean
3    x numeric   1 100  30      NA 200  200    200 200   0    U  max

> mcstoc(rempiricalD, type = "VU", values = x)

  node    mode  nsv nsu nva variate min mean median max Nas type outm
1    x numeric 1000 100   1       1 100  154    150 200   0   VU each
```

Printing the statistics of the 30 variates of `x` is of no interest. Instead, we use the "`outm`" option, which allows us to specify which output we want ("`none`" for none, "`each`", the default, for a series of statistics for each variate, or, as in the example, a vector of functions that are applied over all the 30 variates).

3.2 Multivariate Nodes as a "Third Dimension" for Multiple Options in a Model

The recycling rules in `mc2d` regarding the `nvariate` dimension are as follows: the recycling will be done from `nvariates=1` to `nvariates=n` with $n > 1$. This allows you to use multivariates nodes as a third dimension, in case you want to test various alternatives.

Assume, as in section 2.2.5, that the distribution representing uncertainty in `conc` was not certain, and that the microbiologists suggest that $conc \sim N(10, 2)$ is possible, but that $conc \sim U(8, 12)$ is also possible. We can i) build a "bivariate" node reflecting these two options; ii) transfer these options into the final risk estimate. We obtain a bivariate node for the risk, one using the first hypothesis, the second the second hypothesis.

```
> conc1 <- mcstoc(rnorm, type = "U", mean = 10, sd = 2)
> conc2 <- mcstoc(runif, type = "U", min = 8, max = 12)
> conc <- mcdata(c(conc1, conc2), type = "U", nvariates = 2)
> cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5, 1/50),
+     prob = c(0.027, 0.373, 0.6))
> serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
> expo <- conc * cook * serving
> dose <- mcstoc(rpois, type = "VU", nvariates = 2, lambda = expo)
> r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
> risk <- 1 - (1 - r)^dose
> EC5 <- mc(conc, cook, serving, expo, dose, r, risk)
> summary(EC5)

conc :
[[1]]
       NoVar
median  9.96
mean    9.86
2.5%    6.12
97.5%  13.65

[[2]]
       NoVar
```

```
median  9.95
mean    9.92
2.5%    8.08
97.5%  11.82


cook :
       mean    sd  Min 2.5%  25%  50% 75% 97.5% Max  nsv Na's
NoUnc 0.122 0.182 0.02 0.02 0.02 0.02 0.2     1   1 1000    0

serving :
      mean   sd  Min 2.5%  25%  50%  75% 97.5% Max  nsv Na's
NoUnc 48.8 25.9 5.88 13.2 29.5 44.3 61.9   112 169 1000    0

expo :
[[1]]
       mean    sd  Min 2.5%   25%   50%   75% 97.5%  Max  nsv Na's
median 59.3 100.7 1.17 3.16  7.95 15.00  83.0   312 1000 1000    0
mean   58.7  99.7 1.16 3.13  7.87 14.85  82.1   309  990 1000    0
2.5%   36.5  61.9 0.72 1.94  4.89  9.22  51.0   192  615 1000    0
97.5%  81.3 138.0 1.60 4.33 10.90 20.56 113.7   428 1370 1000    0

[[2]]
       mean    sd  Min 2.5%  25%  50%  75% 97.5%  Max  nsv Na's
median 59.3 100.7 1.17 3.16 7.95 15.0 82.9   312  999 1000    0
mean   59.1 100.4 1.17 3.15 7.92 14.9 82.7   311  996 1000    0
2.5%   48.1  81.7 0.95 2.56 6.45 12.2 67.3   253  811 1000    0
97.5%  70.4 119.5 1.39 3.75 9.44 17.8 98.5   370 1187 1000    0


dose :
[[1]]
       mean    sd  Min 2.5%   25%  50%   75% 97.5%  Max  nsv Na's
median 59.4 101.4 0.00 2.00  8.00 16.0  82.0   312  998 1000    0
mean   58.7 100.1 0.04 1.88  7.61 15.8  81.1   314  990 1000    0
2.5%   36.3  62.1 0.00 1.00  5.00 10.0  49.1   198  633 1000    0
97.5%  81.2 138.0 1.00 3.00 11.00 22.0 110.8   426 1363 1000    0

[[2]]
       mean    sd  Min 2.5%  25%  50%  75% 97.5%  Max  nsv Na's
median 59.3 101.0 0.00 2.00 8.00 16.0 82.2   317 1020 1000    0
mean   59.1 100.7 0.02 1.95 7.63 16.0 81.4   316 1002 1000    0
2.5%   47.8  81.8 0.00 1.00 6.00 13.0 66.1   255  791 1000    0
97.5%  70.7 120.4 0.00 3.00 9.00 19.0 97.0   378 1196 1000    0


r :
          NoVar
median 0.001004
mean   0.001036
2.5%   0.000568
97.5%  0.001435

risk :
```

```
[[1]]
         mean     sd      Min     2.5%     25%    50%    75% 97.5%   Max  nsv
median 0.0546 0.0808 0.000000 0.001936 0.00752 0.0162 0.0811 0.278 0.630 1000
mean   0.0543 0.0796 0.000042 0.001968 0.00787 0.0163 0.0805 0.274 0.622 1000
2.5%   0.0257 0.0408 0.000000 0.000604 0.00357 0.0074 0.0362 0.131 0.358 1000
97.5%  0.0854 0.1175 0.000858 0.003666 0.01292 0.0263 0.1325 0.413 0.812 1000
       Na's
median    0
mean      0
2.5%      0
97.5%     0

[[2]]
         mean     sd      Min     2.5%     25%     50%    75% 97.5%   Max  nsv
median 0.0538 0.0796 0.00e+00 0.001948 0.00763 0.01598 0.0795 0.272 0.638 1000
mean   0.0544 0.0799 2.37e-05 0.001999 0.00783 0.01639 0.0803 0.276 0.630 1000
2.5%   0.0308 0.0483 0.00e+00 0.000896 0.00411 0.00882 0.0439 0.159 0.429 1000
97.5%  0.0802 0.1120 0.00e+00 0.003280 0.01230 0.02501 0.1220 0.394 0.801 1000
       Na's
median    0
mean      0
2.5%      0
97.5%     0
```

(Do not forget to transfer the number of variates you want in `mcstoc`... (see the definition of `dose`). `mc2d` cannot guess...)

3.3 Multivariate Nodes as a "Third Dimension" for Multiple Vectors/Contaminants

The recycling rules in `mc2d` also allow you to use multivariate nodes as a third dimension for multiple vectors/Contaminants.

Assume in our ground beef example that we have two contaminants: one has a mean concentration that follows an uncertainty distribution $conc \sim N(10, 2)$, the second one follows $conc \sim N(14, 2)$. We can *i*) build a "bivariate" node reflecting these two concentrations[9] ; *ii*) transfer these options into the final dose; *iii*) sum the dose over the variates (using `mcapply`). The behavior of contaminants is transferred in the model.

```
> mconc <- mcdata(c(10, 14), type = "0", nvariates = 2)
> conc <- mcstoc(rnorm, nvariates = 2, type = "U", mean = mconc,
+     sd = 2)
> cook <- mcstoc(rempiricalD, type = "V", values = c(1, 1/5, 1/50),
+     prob = c(0.027, 0.373, 0.6))
> serving <- mcstoc(rgamma, type = "V", shape = 3.93, rate = 0.0806)
> expo <- conc * cook * serving
> dose <- mcstoc(rpois, type = "VU", nvariates = 2, lambda = expo)
> dosetot <- mcapply(dose, margin = "variates", fun = sum)
> r <- mcstoc(runif, type = "U", min = 5e-04, max = 0.0015)
> risk <- 1 - (1 - r)^dosetot
> EC6 <- mc(conc, cook, serving, expo, dose, dosetot, r, risk)
> summary(EC6)
```

[9]Note that we could simulate a correlation between both contaminants using a multivariate normal distribution.

```
conc :
[[1]]
       NoVar
median  9.79
mean    9.77
2.5%    5.96
97.5%  14.83

[[2]]
       NoVar
median  14.0
mean    14.1
2.5%    10.8
97.5%   18.3


cook :
       mean    sd  Min 2.5%  25%  50% 75% 97.5% Max  nsv Na's
NoUnc 0.112 0.169 0.02 0.02 0.02 0.02 0.2     1   1 1000    0

serving :
      mean   sd  Min 2.5%  25%  50%  75% 97.5% Max  nsv Na's
NoUnc   49 24.7 5.58 13.3 30.9 45.5 61.8   108 171 1000    0

expo :
[[1]]
       mean    sd   Min 2.5%   25%  50%   75% 97.5%  Max  nsv Na's
median 55.6  94.2 1.092 2.74  7.76 13.1  77.4   258 1031 1000    0
mean   55.5  93.9 1.090 2.74  7.75 13.1  77.2   257 1028 1000    0
2.5%   33.8  57.3 0.665 1.67  4.72  8.0  47.1   157  627 1000    0
97.5%  84.2 142.6 1.654 4.16 11.76 19.9 117.2   390 1561 1000    0

[[2]]
        mean  sd  Min 2.5%   25%  50%   75% 97.5%  Max  nsv Na's
median  79.4 134 1.56 3.92 11.08 18.8 110.5   368 1471 1000    0
mean    80.0 135 1.57 3.95 11.17 18.9 111.4   371 1483 1000    0
2.5%    61.6 104 1.21 3.04  8.59 14.5  85.7   285 1141 1000    0
97.5%  103.9 176 2.04 5.13 14.51 24.6 144.6   482 1926 1000    0


dose :
[[1]]
       mean    sd   Min 2.5%   25%  50%   75% 97.5%  Max  nsv Na's
median 55.4  94.1 0.000 2.00  7.00 14.0  78.5   262 1038 1000    0
mean   55.5  94.2 0.030 1.76  7.29 14.2  78.5   263 1029 1000    0
2.5%   33.7  57.3 0.000 1.00  4.00  9.0  48.0   158  614 1000    0
97.5%  84.0 142.5 0.525 3.00 11.00 21.0 118.0   400 1539 1000    0

[[2]]
        mean  sd  Min 2.5%  25%  50% 75% 97.5%  Max  nsv Na's
median  79.5 135 0.00 3.00 10.5 20.0 112   372 1478 1000    0
mean    80.1 136 0.23 2.88 10.7 20.0 113   377 1484 1000    0
2.5%    61.8 105 0.00 2.00  8.0 15.7  86   285 1120 1000    0
97.5%  104.3 177 1.00 4.00 14.0 25.3 146   493 1941 1000    0
```

```
dosetot :
       mean  sd  Min 2.5%  25%  50% 75% 97.5%  Max  nsv Na's
median  136 230 1.00 6.00 18.0 33.2 192   635 2491 1000    0
mean    136 230 1.10 5.69 18.3 33.3 191   634 2514 1000    0
2.5%    107 181 0.00 4.00 15.0 27.0 152   510 1972 1000    0
97.5%   164 279 2.52 7.52 23.0 40.0 234   779 3075 1000    0

r :
          NoVar
median 0.001000
mean   0.000994
2.5%   0.000546
97.5%  0.001452

risk :
         mean    sd     Min    2.5%     25%    50%    75% 97.5%   Max  nsv Na's
median 0.1050 0.138 0.00104 0.00564 0.01750 0.0311 0.1647 0.450 0.909 1000    0
mean   0.1076 0.139 0.00110 0.00563 0.01806 0.0326 0.1721 0.459 0.894 1000    0
2.5%   0.0633 0.091 0.00000 0.00292 0.00936 0.0171 0.0954 0.289 0.729 1000    0
97.5%  0.1582 0.188 0.00293 0.00893 0.02943 0.0514 0.2613 0.634 0.981 1000    0
```

As a conclusion, this "third" dimension is highly flexible...

4 Another Example: A QRA of Waterborne Cryptosporidiosis in France

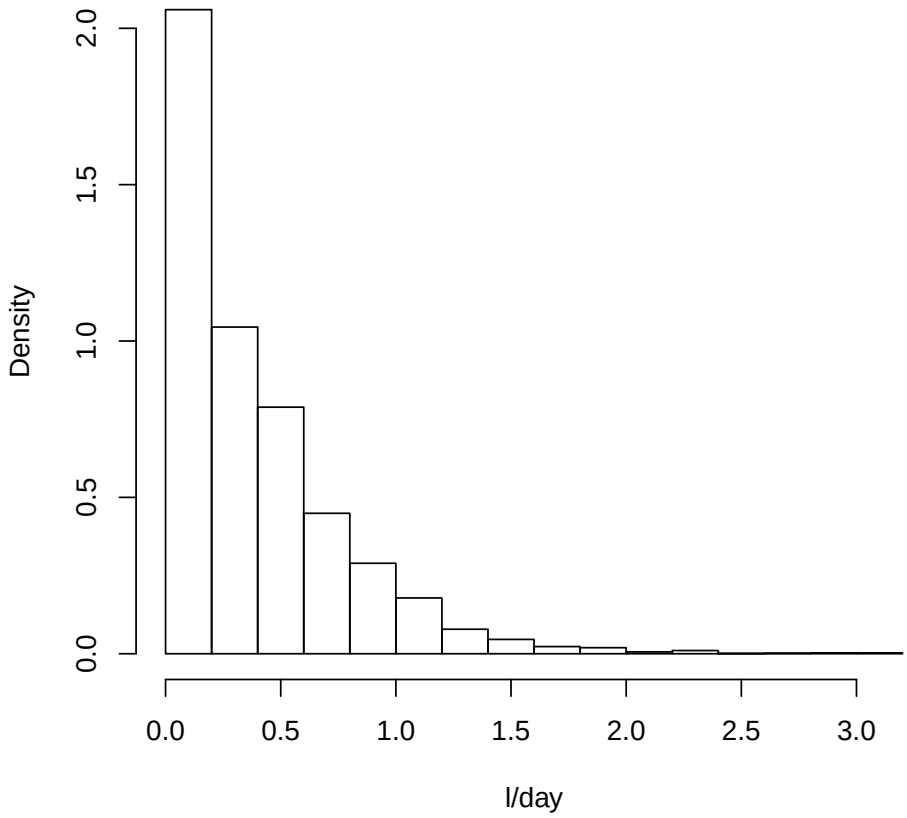
This example is adapted from [4]. The aim is to evaluate the risk of infection with *Cryptosporidium parvum* from consumption of tap water, given that n oocysts /100 l. have been observed in a storage reservoir.

4.1 Tap Water Consumption Model

We have raw data of daily consumption of tap water from 1,180 tap water consumers (var `inca`, see Figure 6). We could choose to use this empirical distribution to evaluate the variability in the tap water consumption:

```
> ndvar(1001)

[1] 1001

> ndunc(1001)

[1] 1001

> mcstoc(rempiricalD, type = "V", values = inca)

  node    mode  nsv nsu nva variate min mean median max Nas type outm
1    x numeric 1001   1   1       1   0 0.41   0.36   3   0    V each
```

Figure 6: Histogram of daily tap water intake



but we will use the "fitdistrplus" library. inca includes a lot of 0 nodes, corresponding to days when individuals do not drink tap water (possibly they drink bottled water on those days). We could try a mixture of distributions, with "0"and "non-0" data.

```
> library(fitdistrplus)
> pzero <- sum(inca == 0)/length(inca)
> inca_non_0 <- inca[inca != 0]
> descdist(inca_non_0)

summary statistics
------
min:  0.0221   max:  3.2
median:  0.48
mean:  0.566
sample sd:  0.385
sample skewness:  1.75
sample kurtosis:  7.98
```

Following the descdist function (See figure 7), let us try the lognormal distribution.

```
> Adj_water <- fitdist(inca_non_0, "lnorm", method = "mle")
> meanlog <- Adj_water$est[1]
> sdlog <- Adj_water$est[2]
> summary(Adj_water)

FITTING OF THE DISTRIBUTION ' lnorm ' BY MAXIMUM LIKELIHOOD
PARAMETERS
        estimate Std. Error
meanlog   -0.784    0.00891
sdlog      0.674    0.00630
Loglikelihood:  -1374
Correlation matrix:
        meanlog sdlog
meanlog       1     0
sdlog         0     1

------
GOODNESS-OF-FIT STATISTICS

_____________ Chi-squared_____________
Chi-squared statistic:  3081
Degree of freedom of the Chi-squared distribution:  23
Chi-squared p-value:  0

!!! For continuous distributions, Kolmogorov-Smirnov and
      Anderson-Darling statistics should be prefered !!!

_____________ Kolmogorov-Smirnov_____________
Kolmogorov-Smirnov statistic:  0.0643
Kolmogorov-Smirnov test:  rejected
!!! The result of this test may be too conservative as it
     assumes that the distribution parameters are known !!!
```

Figure 7: Graph from the `descdist` function.

```
summary statistics
------
min:  0.0221   max:  3.2
median:  0.48
mean:  0.566
sample sd:  0.385
sample skewness:  1.75
sample kurtosis:  7.98
```

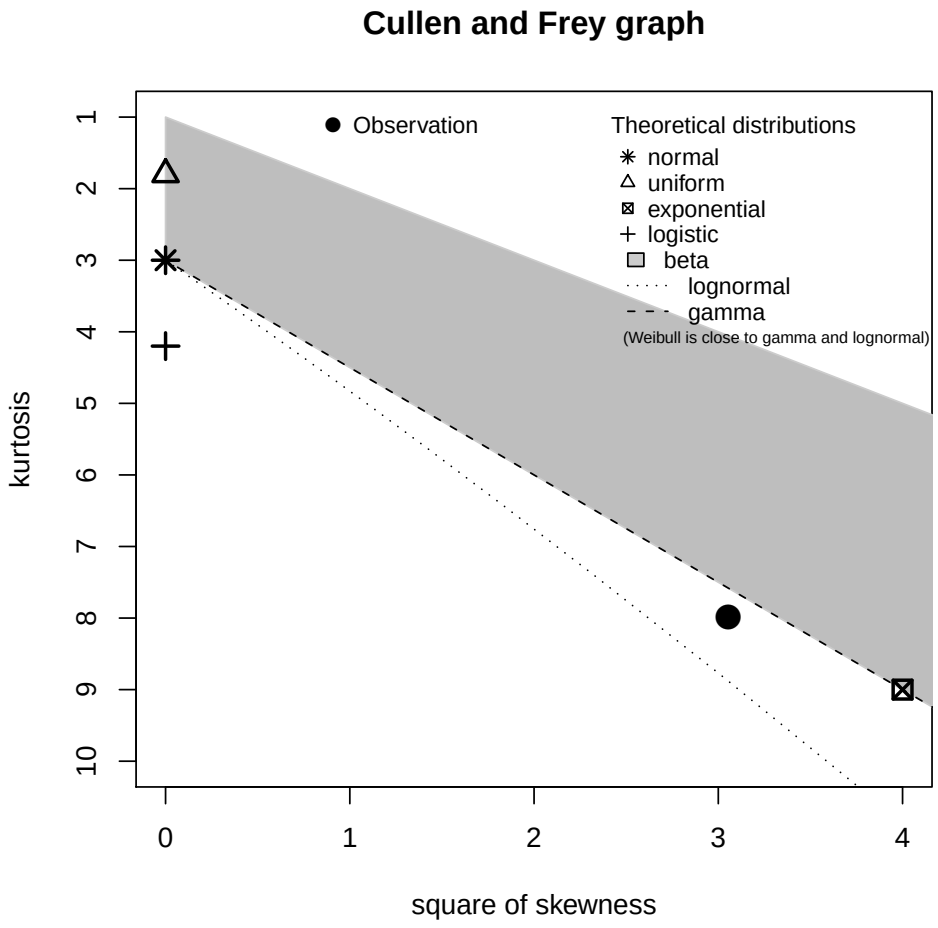
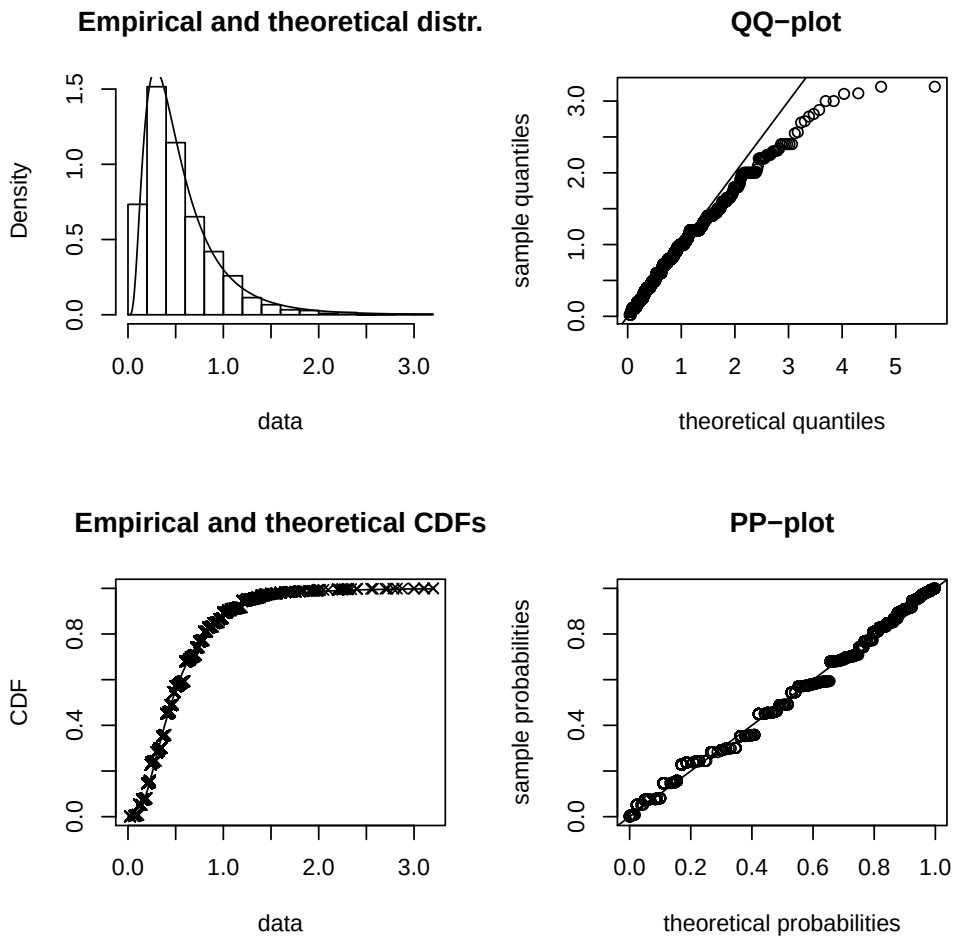


Figure 8: Graph from the `fitdist` function.




```
_____________ Anderson-Darling_____________
Anderson-Darling statistic:  18.8
Anderson-Darling test:  rejected
```

```
> plot(Adj_water)
```

Not so bad (See Figure 8), and better than a gamma distribution (results not shown). We can now rebuild our mixture. We could consider uncertainty around the maximum likelihood estimates using the `bootdist` function of the `fitdistrplus` package, using something like:

```
> Boot <- bootdist(Ajust_lnorm, bootmethod = "param", niter = ndunc())
> Mean_conso <- mcdata(Boot$estim$meanlog, type = "U")
> Sd_conso <- mcdata(Boot$estim$sdlog, type = "U")
> conso1 <- mcstoc(rlnorm, type = "VU", meanlog = Mean_conso, sdlog = Sd_conso)
```

But for simplicity, we will not consider uncertainty around the estimates.

We will use the `mcprobtree` function to construct a mixture of ”0”and ”non-0” distributions:

```
> conso0 <- mcdata(0, type = "V")
> conso1 <- mcstoc(rlnorm, type = "V", meanlog = meanlog, sdlog = sdlog)
> v <- mcprobtree(c(pzero, 1 - pzero), list(`0` = conso0, `1` = conso1),
+     type = "V")
> summary(v)

node :
       mean    sd Min 2.5% 25%  50%   75% 97.5%  Max  nsv Na's
NoUnc 0.418 0.496   0    0   0 0.31 0.624  1.64 7.08 1001    0
```

4.2 The Dose-Response Model

We propose a boostrap from data (`datDR`) derived from [1]. We first define a function "`DR`" with an `n` argument for the size of the sample to draw. This function may then be used in a `mcstoc` function:

```
> datDR <- list(dose = c(30, 100, 300, 500, 1000, 10000, 1e+05,
+     1e+06), pi = c(2, 4, 2, 5, 2, 3, 1, 1), ni = c(5, 8, 3, 6,
+     2, 3, 1, 1))
> estDR <- function(pos, ref) {
+     -glm(cbind(ref$ni - pos, pos) ~ ref$dose + 0, binomial(link = "log"))$coefficients
+ }
> ml <- 1 - exp(-estDR(datDR$pi, datDR) * datDR$dose)
> DR <- function(n) {
+     boot <- matrix(rbinom(length(datDR$dose) * n, datDR$ni, ml),
+         nrow = length(datDR$dose))
+     apply(boot, 2, estDR, ref = datDR)
+ }
> r <- mcstoc(DR, type = "U")
> summary(r)

node :
         NoVar
median 0.00532
mean   0.00571
2.5%   0.00296
97.5%  0.01031
```

4.3 The Model

Deriving the final model is straightforward. We construct the `mcnode` corresponding to the recovery rate (Uncertainty, `Rr`), the probability for an oocyst to be infective (Variability, `w`):

```
> Rr <- mcstoc(rbeta, type = "U", shape1 = 2.65, shape2 = 3.64)
> w <- mcstoc(rbeta, type = "V", shape1 = 2.6, shape2 = 3.4)
```

Given that $O_o = 2$ oocysts are observed in 100 l of water, the expected number of oocysts in the sample is `l`:

```
> Oo <- 2
> l <- (Oo + mcstoc(rnbinom, type = "U", size = Oo + 1, prob = Rr))/100
```

The expected number of oocysts drunk by the individuals is `Or` and the risk ($\times 10000$) is estimated by:

```
> Or <- l * v * w
> P <- 10000 * (1 - exp(-r * Or))
> summary(P)

node :
        mean    sd Min 2.5% 25%    50%   75% 97.5%   Max  nsv Na's
median 0.558 0.787   0    0   0 0.3411 0.789  2.39 12.13 1001    0
mean   0.883 1.244   0    0   0 0.5396 1.248  3.79 19.15 1001    0
2.5%   0.142 0.200   0    0   0 0.0868 0.201  0.61  3.09 1001    0
97.5%  3.349 4.714   0    0   0 2.0463 4.732 14.36 72.54 1001    0
```

This result can be compared (roughly since there is some differences in the modelsvariability) to the results shown in Table 2 in [4].

Improvement: the results for $O_o = \{0, 1, 2, 5, 10, 20, 50, 100, 1000\}$ can be obtained in one step using:

```
> Oo <- mcdata(c(0, 1, 2, 5, 10, 20, 50, 100, 1000), type = "0",
+     nvariates = 9)
```

As a Conclusion

We think and hope that "`mc2d`" could help risk assessors to constuct and analyse their models, and that it may help in developing "two-dimensional" simulations. Nevertheless, "`mc2d`" is currently under development:

CHECK YOUR MODEL CAREFULLY AND EXAMINE RESULTS TO DETECT BUGS

and, if you would like to improve it, join us at

http://riskassessment.r-forge.r-project.org/

Please refer any comments or bugs to `rpouillot@yahoo.fr`.

References

[1] C. L. Chappell, P. C. Okhuysen, C. R. Sterling, and H. L. DuPont. Cryptosporidium parvum: intensity of infection and oocyst excretion patterns in healthy volunteers. *Journal of Infectious Diseases*, 173(1):232–6., 1996.

[2] A.C. Cullen and H.C. Frey. *Probabilistic techniques in Exposure assessment.* Plenum Press, New York, 1999.

[3] R. L. Iman and W. J. Conover. A distribution-free approach to inducing rank correlation among input variables. *Communication in Statistics*, B11(3):311–334, 1982.

[4] R Pouillot, P Beaudeau, J.-B. Denis, F Derouin, and AFSSA Cryptosporidium Study Group. A quantitative risk assessment of waterborne cryptosporidiosis in france using second-order monte carlo simulation. *Risk Anal*, 24(1):1–17, 2004.

[5] R Pouillot, N Miconnet, A.-L. Afchain, M.-L. Delignette-Muller, A Beaufort, L Rosso, J.-B. Denis, and M Cornu. Quantitative risk assessment of listeria monocytogenes in french cold-salmon : I. quantitative exposure assessment. *Risk Analysis*, 27(3):683–700, 2007.

[6] D. Vose. *Risk Analysis, A quantitative guide, 2nd Edition.* Wiley and Sons, Chichester, 2nd edition, 2000.