Runuran

An R Interface to the UNU.RAN Library for Universal Random Variate Generators

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Abstract

Runuran is a wrapper to UNU.RAN (*Universal Non-Uniform RANdom variate generators*), a library for generating random variates for large classes of distributions. It also allows to compute quantiles (inverse cumulative distribution functions) of these distributions efficiently. In order to use UNU.RAN one must supply some data like the denstiy about the target distribution which are then used to draw random samples. Runuran functions provide both a simplified interface to this library for common distributions as well access to the full power of this library.

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0. Introduction

The R package Runuran is a wrapper to UNU.RAN (Universal Non-Uniform RANdom variate generators), a library for generating random variates for large classes of distributions. It also allows to compute quantiles (inverse cumulative distribution functions) of these distributions efficiently. This is in particular a prerequisite for quasi-Monte Carlo integration and copula methods. UNU.RAN implements so called universal (automatic or black-box) generators. In order to use UNU.RAN one must supply some data about the target distribution, usually the density, probability vector or cumulative distribution function and (optinonally) some other information (such as the mode of the distibrubtion). These are then used to draw random samples. Runuran functions provide both a simplified interface to this library for common distributions as well access to the full power of this library.

Runuran functions are alternatives to standard built-in functions in R which are faster or are suitable for particular applications. Runuran is the package you are looking for if you need

- robust and easy-to-use sampling and quantile functions for continuous and discrete distributions (such as Normal, Beta, Gamma, Generalized Hyperbolic, Binomial, . . . distributions);
- to draw samples from truncated distributions;
- random samples for special applications like variate reduction techniques, QMC or copula methods:
- simuilate random variates from some unusual, nameless distribution that you just found in a paper or derived from your statistical model;
- to find out properties of various generation methods (such as speed, quality of generated point set, conservation of structures, ...).

If your aim is just (1) and you are not keen on learning more about universal generators please proceed to Section 1.

Universal algorithms for non-uniform random variate generation work for quite large classes of distributions but require the following three steps:

- (U1) **Information gathering:** The user has to provide some information about the *distribution*. The kind of information depends on the chosen method.
- (U2) Creation of tables: In the *setup* tables are created. These adjust the algorithm for sampling from the target distribution. The table size depends on the chosen method but can be controlled to some extend.
- (U3) Generation of a random sample: These tables are then used to *generate* a random sample.

It is obvious that table size, setup time, and marginal generation time strongly depend on the chosen method. By a rule-of-thumb methods with large tables have very fast marginal generation times that hardly depend on (or are even independent from) the given target distribution. But then they have an expensive setup. Vice versa, when the table is small we have fast setup and slow marginal generation times or the generated points are less accurate in case of approximate methods. Many of the algorithms allow to control the table size to some extend.

The choice of the generation method itself depends on the application for which the random sample is requested. Of course, the target distribution has to satisfy certain conditions for each of these algorithms. We refer the user to our extensive monograph [2] for detailed information about these generation methods. For convenience we have added a (very) short survey on the basic principles of random variate generation in Appendix A (A Short Introduction to Random Variate Generation). Terms and concepts that are used in the description of the methods in this manual are listed in Appendix C (Glossary).

We have compiled a collection of such universal algorithms in UNU.RAN. The source code and a detailed manual can be found in [4]. The library is written in ANSI C and provides an interface to Steps (U1)–(U3) for such universal algorithms. The setup is sometimes quite expensive even if the required table is small, since there are checks whether the conditions for the chosen method (e.g., log-concavity) are satisfied as well as checks for the consistency of the given data for the target distribution. Thus the *setup* and the *generation* are split, such that the former part creates an object that can be used many times for creating random samples.

R package Runuran provides a wrapper to the UNU.RAN library¹. The package implements three sets of functions of increasing power (and thus complexity):

• Runuran – Distribution (Section 1):

These functions provide easy-to-use sampling algorithms for particular distributions. Their syntax is similar to the built-in sampling algorithms (but usually have an additional domain argument). They can be used as replacements for the respective R functions (if the latter exists), e.g., urnorm can be used instead of rnorm for generating normal random variates. These functions also show the interested user how we used the more powerful functions below.

• Runuran – Universal (Section 2):

These functions provide more flexibility. They offer an interface to use a carefully selected collection of UNU.RAN methods with their most important variants. Their arguments allow setting all required data and parameters. Thus they combine Steps (U1) and (U2) in a single function. On the contrary to functions like urnorm, they do not return a random sample but a UNU.RAN generator object that can be used for sampling (Step U3). For example, the function tdr.new creates a generator object that applies the transformed density rejection (TDR) method.

• Runuran – Advanced (Section 3):

These functions implement a wrapper to the UNU.RAN string API and is thus the most powerful interface. Thus more generation methods and more parameters for all UNU.RAN methods are available. Now Steps (U1) and (U2) are split in two different tasks.

Uniform random numbers. All UNU.RAN methods use the R built-in random number generator as the source of (pseudo-) random numbers. Thus the generated samples depend on the state .Random.seed and can be controlled by the R functions RNGkind and set.seed.

¹We first described such a package in [6]. However, the interface has been changed and extended since then.

1. Runuran – Distributions

There are generation functions for approximately 30 standard distributions to facilitate the use of the package. All these functions share a similar syntax and naming scheme (only u is prefixed) with their analogous Rbuilt-in generating functions (if these exist) but have optional domain arguments 1b and ub, i.e., these calls also allow to draw samples from truncated distributions:

```
ur...(n, distribution parameters, lb, ub)
```

Compared to the corresponding R functions these ur... functions have a slightly different behavior.

- For large sample sizes these functions are often much faster (e.g., a factor of about 5 for the t-distribution.
- For small samples they are comparatively slow.
- All ur... functions allow to sample from truncated versions of the original distributions. Therefore the arguments 1b (lower border) and ub (upper border) are available for all ur... functions.
- Almost all ur... functions are based on fast numerical inversion algorithms. This is important for example for generating order statistics or random vectors from copulas.
- All ur... functions do **not** allow vectors as arguments (to be more precise: they only use the first element of the vector).

```
Example

> ## Draw sample of size 10 from standard Gaussian distribution
> urnorm(10)

[1] -0.3340019    0.1467855 -1.8484902 -0.5970556    0.5347111 -0.5765151
[7] -1.6139740 -0.5874209    0.3838749    1.0640604

> ## Draw sample from truncated non-standard Gaussian distribution
> urnorm(10, mean = 1, sd = 0.5, lb = 2, ub = Inf)

[1] 2.246723    2.038957    2.046299    2.355980    2.116156    2.060379    2.224005    2.021544
[9] 2.053674    2.085292
```

The ur... functions can be used as-is. But they also are examples how the more advanced functions in Section 2 and Section 3 can be used. Just type the name of such a function to display its source.

```
prinction (n, mean = 0, sd = 1, lb = -Inf, ub = Inf)
{
    unr <- new("unuran", paste("normal(", mean, ",", sd, "); domain=(", lb, ",", ub, ")"), "HINV")
    unuran.sample(unr, n)
}
<environment: namespace:Runuran>
```

1. Runuran – Distributions

Currently the following distributions are available (see the corresponding help page for details):

Continuous Univariate Distributions (24)

Function Distribution

urburr ... Beta
urburr ... Burr
urcauchy ... Cauchy
urchi ... Chi

urchisq ... Chi-square urexp ... Exponential

urextremeI ... Gumbel (extreme value type I) urextremeII ... Frechet (extreme value type II)

 $\quad \text{urf} \qquad \dots \ F$

urgamma ... Gamma

urgig ... GIG (generalized inverse Gaussian)

urhyperbolic ... Hyperbolic urlaplace ... Laplace urlnorm ... Log-Normal urlogis ... Logistic urlomax ... Lomax

urnorm ... Normal (Gaussian)
urpareto ... Pareto (of first kind)

urplanck ... Planck

urpowerexp ... Powerexponential (Subbotin)

urrayleigh ... Rayleigh
urt ... t (Student)
urtriang ... Triangular
urweibull ... Weibull

Discrete Univariate Distributions (6)

Function Distribution

urbinom ... Binomial

urgeom ... Geometric

urhyper ... Hypergeometric

urlogarithmic ... Logarithmic

urnbinom ... Negative Binomial

urpois ... Poisson

Uniform random numbers. All UNU.RAN methods use the R built-in random number generator as the source of (pseudo-) random numbers. Thus the generated samples depend on the state .Random.seed and can be controlled by the R functions RNGkind and set.seed.

2. Runuran – Universal

The power of UNU.RAN does not lie in a collection of generators for some standard distributions but in a collection of universal generation methods that allow drawing samples of pseudorandom variates for particular purposes. For example, it is possible to generate samples that follow some non-standard distributions for which no special generation methods exist. These black-box methods are also well suited for standard distributions (e.g., some of our methods are much faster when applied to some distributions compared to the corresponding R built-in functions).

Thus we have compiled a set of functions that offer an interface to carefully selected UNU.RAN methods with their most important parameters. Their arguments allow setting all required data about the distribution as well as the parameters of the chosen method. Thus they combine Steps (U1) and (U2) in a single function. These functions return UNU.RAN generator objects that can be used for sampling using ur (Step U3).

```
> ## Use method TDR (Transformed Density Rejection) to
> ## draw a sample of size 10 from a hyperbolic distribution with PDF
> ## f(x) = const * exp(-sqrt(1+x^2)) on domain (-Inf,Inf).
>
> ## We first have to define a function that returns the density.
> pdf <- function (x) { exp(-sqrt(1+x^2)) }
> ## Next create the UNU.RAN object.
> gen <- tdr.new(pdf=pdf, lb=-Inf, ub=Inf)
> ## Now we can use this object to draw the sample.
> ## (Of course we can repeat this step as often as required.)
> x <- ur(gen,10)
> x

[1] -0.6009990  0.1088991  5.8656120 -0.5397085 -1.1834729  2.5366420
[7] -1.7168253 -0.0966564 -0.6989629 -0.9326356
```

UNU.RAN objects provide information about themselves. (Note that the displayed data also give information for advanced uses of Runuran, see Section 3.)

_____ Example ____

```
Object is UNU.RAN object:
    method: tdr
    distr: [S4 class]

generator ID: TDR.003

distribution:
    name = unknown
    type = continuous univariate distribution
    functions = PDF dPDF
    domain = (-inf, inf)
    center = 0 [default]
```

```
method: TDR (Transformed Density Rejection)
  variant = PS (proportional squeeze)
  T_c(x) = -1/sqrt(x) ... c = -1/2

performance characteristics:
  area(hat) = 1.2056
  rejection constant <= 1.00532
  area ratio squeeze/hat = 0.994707
  # intervals = 48</pre>
```

As pointed out, it is possible to sample from quite arbitrary distributions (e.g., truncated distributions). Here is an example using method ARS (Adaptive Rejection Sampling), which is slightly slower but numerically more robust than TDR.

```
Example
> ## Use method ARS (Adaptive Rejection Sampling) to
> ## draw a sample of size 10 from a truncated Gaussian on [100, Inf).
> ## Define a function that returns the log-density.
> 1pdf <- function (x) { -0.5*x^2 }
> ## Create UNU.RAN object.
> gen <- ars.new(logpdf=lpdf, lb=100, ub=Inf)</pre>
> ## Draw sample.
> ur(gen,10)
 [1] 100.0009 100.0028 100.0026 100.0045 100.0241 100.0170 100.0061 100.0131
 [9] 100.0226 100.0186
One also can directly use density functions provided by R.
                                 Example _
> ## Draw a sample from Gaussian distribution with
> ## mean 2 and standard deviation 5.
> ## Create UNU.RAN object.
> ## Use R function 'dnorm(x, mean=2, sd=5, log=TRUE)' as density.
> gen <- ars.new(logpdf=dnorm, lb=-Inf, ub=Inf, mean=2, sd=5, log=TRUE)
> ## Draw sample.
> ur(gen,10)
 [1] 5.530629 0.505376 2.497981 -1.910429 3.585540 3.106492 -2.015426
 [8] -6.739152 8.281584 6.904269
```

Furthermore, an object that implements an inversion method can be used as an argument for the quantile function uq. This is convenient for copula methods or quasi-Monte Carlo methods.

```
Example

> ## Compute quantiles for hyperbolic distribution with PDF
> ## f(x) = const * exp(-sqrt(1+x^2)) on domain (-Inf,Inf).
> ## Thus we need an inversion method. We choose PINV.
>
> ## Create UNU.RAN object.
> pdf <- function (x) { exp(-sqrt(1+x^2)) }
> gen <- pinv.new(pdf=pdf, lb=0, ub=Inf, uresolution=1e-14)
> ## Get some quantiles
> uq(gen, c(0.005, 0.01, 0.025, 0.05, 0.5, 0.95, 0.975, 0.99, 0.995))

[1] 0.008180859 0.016362265 0.040915247 0.081899046 0.924464417 3.386748732
[7] 4.096624431 5.028728582 5.730822726
```

Uniform random numbers. All UNU.RAN methods use the R built-in random number generator as the source of (pseudo-) random numbers. Thus the generated samples depend on the state .Random.seed and can be controlled by the R functions RNGkind and set.seed.

2.1. List of Universal Methods

In the following we give an overview of the available methods. Each of these functions creates a UNU.RAN object that can be used for sampling from the corresponding distribution by means of function ur. Note that methods that implement an *inversion* method can be used for the quantile function uq. For the syntax of these functions see the corresponding help page. For details about the method we refer to our extensive monograph [2].

Most of these sampling methods can be controlled by some additional parameters which are available through the advanced interface unuran.new as described in Section 3. However, these may only be useful in special cases (e.g., distributions with extremal properties).

Warning. It is not possible to save and restore a UNU.RAN object between R sessions, nor to copy such objects to different nodes in a computer cluster. UNU.RAN objects must be created in each session (and in each node) from scratch.

However, generator objects for some generation methods can be "packed" using the command 'unuran.packed(unr)<-TRUE'. Then these objects can be handled like any other R object (and thus saved and restored).

Timing. The *setup time* and *marginal sampling time* given below only give a rough estimate and vary for particular distributions. As a rule-of-thumb the setup time heavily depends on the target distribution. For methods with fast sampling methods the marginal generation times hardly (or even do not) depend on the target distribution. Whereas for slow methods the marginal sampling times depend on the target distribution.

2.1.1. Continuous Univariate Distributions

• ars.new - Adaptive Rejection Sampling (ARS)

2. Runuran – Universal

rejection method type: accuracy exact log-concave PDF required: optional: derivative of log-PDF setup: slow fast sampling: slow fast • itdr.new - Inverse Transformed Density Rejection (ITDR) rejection method type: accuracy exact monotone PDF, derivative of PDF, pole required: setup: slow fast sampling: slow fast • pinv.new - Polynomial interpolation of INVerse CDF (PINV) inversion method type: accuracy numerical approximation required: bounded PDF optional: center, u-resolution setup: slow O sampling: slow fast • srou.new - Simple Ratio-Of-Uniforms method (SROU) type: rejection method exact accuracy $T_{-r/(r+1)}$ -concave PDF, mode, area required: optional: parameter r setup: slow fast sampling: slow fast robust, works for heavy tailed distributions remark: • tdr.new - Transformed Density Rejection (TDR) rejection method type: accuracy exact required: $T_{-1/2}$ -concave PDF derivative of PDF optional: setup: slow fast sampling: slow fast 2.1.2. Discrete Distributions • dari.new - Discrete Automatic Rejection Inversion (DARI) rejection method type: accuracy exact PMF required: optional: center, approximate sum over probabilities slow fast setup: sampling: slow fast

• dau.new - Alias-Urn Method (DAU)

type: patchwork method

accuracy exact

required: (finite) probability vector setup: slow fast sampling: slow fast

• dgt.new - Guide-Table Method for discrete inversion (DGT)

type: inversion method

accuracy exact

required: (finite) probability vector setup: slow fast sampling: slow fast

2.1.3. Multivariate Distributions

• hitro.new - Hit-and-Run algorithm with Ratio-of-Uniforms Method (HITRO)

type: Markov chain sampler (MCMC)

accuracy converging Markov chain

required: PDF

optional: center, mode, thinning factor, burnin

setup: slow fast sampling: slow fast

remark: approximate

• vnrou.new - Multivariate Naive Ratio-Of-Uniforms method (VNROU)

type: Rejection accuracy exact

required: unimodal PDF optional: center, mode

setup: slow fast sampling: slow fast

3. Runuran – Advanced

Using the advanced interface of package Runuran requires three steps:

- (U1) Create a distribution object that contains all required information about the target distribution.
- (U2) Choose a generation method and create a UNU.RAN object.
- (U3) Use this object to draw samples from the target distribution.

In the following we shortly describe the main idea behind. For the syntax and the details of the R function we refer to the corresponding help page. For the UNU.RAN method we refer to its manual [4].

Warning. Both the distribution object and the UNU.RAN generator object contain pointers to external memory. Thus it is not possible to save and restore a UNU.RAN object between R sessions, nor to copy such objects to different nodes in a computer cluster. Distribution and UNU.RAN objects must be created in each session (and each node) from scratch.

However, generator objects for some generation methods can be "packed" using the command 'unuran.packed(unr)<-TRUE'. Then these objects can be handled like any other R object (and thus saved and restored).

3.1. U1 – Create a distribution object

Runuran uses S4 classes to store information about distributions. Thus the following three functions create instances of the corresponding classes (for the syntax and details of these functions we refer to the corresponding help page):

- unuran.cont.new: univariate continuous distributions
- unuran.discr.new: discrete distributions
- unuran.cmv.new: multivariate continuous distributions

Each of these functions allow to set various data about the target distribution. The kind of data depends of course on the type of distribution object. It is the responsibility of the user to supply consistent data. It is not necessary to fill all the "slots" of the objects. It depends on the chosen method which data are essential or used if provided (all other data are simply ignored).

3.2. U2 - Create a UNU.RAN generator object

Runuran uses an S4 class to store information about distributions. It can be created by the following function (for further details we refer to the corresponding help page):

• gen <- unuran.new(distr,method)

where

- distr is an instance of a distribution object created in Step (U1), and
- method is a *string* for the UNU.RAN string API, see Section 3.4 (Method String) in the UNU.RAN manual [4].

The given distribution must contain all data about the target information that are required for the chosen method.

Remark. UNU.RAN also has a string API for distributions, see Section 3.2 (Distribution String) in the UNU.RAN manual [4]. Thus distr can also be such a string. However, besides some special cases the approach described in Section 3.1 above is more flexible inside R.

3.3. U3 – Draw samples

The UNU.RAN object created in Step (U2) can then be used to draw samples from the target distribution. Let gen such a generator object.

- ur(gen,n) draws a pseudo-random sample of size n.
- uq(gen,u) computes quantiles (inverse CDF's) for the *u* values given in vector u. However, this requires that the method (gen) we are using implements an inversion method like PINV or DGT.

In addition it is possible to get some information about the generator object.

- show(gen) (or simply gen) prints some information about the used data of the distribution as well as sampling method and performance characteristics of the generator object on the screen.
- unuran.details(gen) is more verbose and additionally prints parameter settings for the chosen method (including default values) and some hints for changing (improving) its performance.

Uniform random numbers. All UNU.RAN methods use the R built-in random number generator as the source of (pseudo-) random numbers. Thus the generated samples depend on the state .Random.seed and can be controlled by the R functions RNGkind and set.seed.

Example 1: Continuous distribution

```
Example _
> ## Use method TDR (Transformed Density Rejection) to
> ## draw a sample of size 10 from a hyperbolic distribution with PDF
 > ## f(x) = const * exp(-sqrt(1+x^2)) 
> ## restricted to domain [-1,2].
> ## We first have to define functions that return the log-density and
> ## its derivative, respectively. (We also could use the density itself.)
> 1f <- function (x) { -sqrt(1+x^2) }
> dlf \leftarrow function(x) \{ -x/sqrt(1+x^2) \}
> ## Next create the continuous distribution object.
> d <- unuran.cont.new(pdf=lf, dpdf=dlf, islog=TRUE, lb=-1, ub=2,
                       name="hyperbolic")
> ## Create UNU.RAN object. We choose method TDR with
> ## immediate acceptance (IA) and parameter c=0.
> gen <- unuran.new(distr=d, method="tdr; variant_ia; c=0")</pre>
> ## Now we can use this object to draw the sample.
> ## (Of course we can repeat this step as often as required.)
> ur(gen, 10)
     1.6937586 0.6643022 1.0032217 1.1854486 -0.3880564 1.0214270
 [1]
 [7]
     1.2716483
                1.6772524 1.6335524 -0.8110137
```

```
> ## Here is some information about our generator object.
> unuran.details(gen)
Object is UNU.RAN object:
       method: tdr; variant_ia; c=0
        distr:
               [S4 class]
generator ID: TDR.007
distribution:
            = hyperbolic
   name
   type
          = continuous univariate distribution
   functions = PDF dPDF
   domain = (-1, 2)
   center = 0 [default]
[ Hint: You may provide a point near the mode as "center". ]
method: TDR (Transformed Density Rejection)
   variant = IA (immediate acceptance)
   T_c(x) = log(x) \dots c = 0
performance characteristics:
   area(hat) = 0.808085
   rejection constant <= 1.0006
   area ratio squeeze/hat = 0.9994
   # intervals = 32
parameters:
   variant_ia = on
   c = 0
   max_sqhratio = 0.99 [default]
   max_intervals = 100 [default]
[ Hint: You can set "max_sqhratio" closer to 1 to decrease rejection constant. ]
```

Example 2: Discrete distribution with given probability vector (PV)

```
> ## Here is some information about our generator object.
> unuran.details(gen)
Object is UNU.RAN object:
        method: dgt
        distr:
               [S4 class]
generator ID: DGT.008
distribution:
            = binomial(100,0.4)
  name
   type = discrete univariate distribution
   functions = PV [length=101]
   domain = (0, 100)
method: DGT (Guide Table)
performance characteristics:
  E [\#look-ups] = 2
parameters:
   guidefactor = 1 [default]
```

Example 3: Discrete distribution with given probability mass function (PMF)

```
____ Example
> ## Use method DSROU (Discrete Simple Ratio-Of-Uniforms method) to
> ## draw a sample of size 10 from a discrete distribution with
> ## given PMF, mode, and sum.
> ## Define functions that return the PMF.
> f \leftarrow function (x) \{ 0.4 * (1-0.4)^x \}
> ## Create the continuous distribution object.
> d <- unuran.discr.new(pmf=f, lb=0, ub=Inf, mode=0, sum=1)</pre>
> ## Create UNU.RAN object. We choose method DARI with squeezes.
> gen <- unuran.new(distr=d, method="dari; squeeze=on")</pre>
> ## Now we can use this object to draw the sample.
> ur(gen, 10)
 [1] 1 3 0 0 1 0 2 3 0 2
> ## Here is some information about our generator object.
> unuran.details(gen)
Object is UNU.RAN object:
        method: dari; squeeze=on
                [S4 class]
        distr:
generator ID: DARI.009
```

```
distribution:
  name = unknown
          = discrete univariate distribution
   functions = PMF
   domain = (0, 2147483647)
            = 0
   mode
   sum(PMF) = 1
method: DARI (Discrete Automatic Rejection Inversion)
   use table of size 100
   use squeeze
performance characteristics:
   sum(hat) = 1.216
   rejection constant = 1.216
parameters:
  tablesize = 100 [default]
   squeeze = on
```

Example 4: Multivariate distribution

```
_ Example _
> ## Use method VNROU (Multivariate Naive Ratio-Of-Uniforms) to
> ## draw a sample of size 5 from a bivariate distribution
> ## with given PDF, mode and domain.
>
> ## Define functions that return the PDF.
> f \leftarrow function(x) \{ exp(-sum(x^4)) \}
> ## Create the continuous distribution object.
> d < -unuran.cmv.new(dim=2, pdf=f, mode=c(0,0), 11=c(-1,-1), ur=c(1,1),
                      name="bivariate power-exponential")
> ## Create UNU.RAN object. We choose method VNROU with parameter r=0.5.
> gen <- unuran.new(distr=d, method="vnrou; r=0.5")</pre>
> ## Now we can use this object to draw the sample.
> ur(gen,5)
           [,1]
                      [,2]
[1,] -0.2809575 0.3358629
[2,] 0.7675782 -0.7908956
[3,] -0.3913925 -0.8155972
[4,] 0.2203669 -0.1492909
[5,] 0.5602483 -0.7412993
> ## Here is some information about our generator object.
> unuran.details(gen)
Object is UNU.RAN object:
        method: vnrou; r=0.5
        distr: [S4 class]
```

```
generator ID: VNROU.010
distribution:
            = bivariate power-exponential
   name
   type
             = continuous multivariate distribution
   dimension = 2
   functions = PDF
   domain = (-1,1) x (-1,1) [rectangular]
           = (0, 0)
   mode
   center
            = (0, 0) [= mode]
method: VNROU (Naive Ratio-Of-Uniforms)
   r = 0.5
performance characteristics:
   bounding rectangle = (-0.778879, 0.778879) \times (-0.778879, 0.778879) \times (0,1)
   volume(hat) = 2.42661
   rejection constant = 1.69 [approx.]
parameters:
   r = 0.5
   v = 1 [numeric.]
   u = (-0.778879, -0.778879) -- (0.778879, 0.778879) [numeric.]
[ Hint: You can set "v" to avoid numerical estimate. ]
[ Hint: You can set "u" to avoid slow (and inexact) numerical estimates. ]
```

Missing data. If some data are missing then UNU.RAN cannot create a generator object and aborts with an error message.

```
> ## Try to use method TDR with missing data.
> 1f <- function (x) { -sqrt(1+x^2) }
> d <- unuran.cont.new(pdf=lf, 1b=-Inf, ub=Inf, islog=TRUE)
> gen <- unuran.new(distr=d, method="tdr")

[UNU.RAN - error] (distribution) incomplete distribution object, entry missing: derivate [UNU.RAN - error] (parser) invalid parameter: invalid data for method 'tdr'
[UNU.RAN - error] (parser) invalid string: setting method failed
Error: [UNU.RAN - error] cannot create UNU.RAN object
```

Invalid data. UNU.RAN makes some validity checks. If such a check fails the setup aborts with an error message. Such failures can be caused by erroneous data. It also can happen due to serious round-off errors.

```
> d <- unuran.discr.new(pv=c(1,-1,0), lb=1)
> gen <- unuran.new(distr=d, method="dgt")</pre>
```

3. Runuran - Advanced

[UNU.RAN - error] (generator) (possible) invalid data: probability < 0 Error: [UNU.RAN - error] cannot create UNU.RAN object

A. A Short Introduction to Random Variate Generation

Random variate generation is the small field of research that deals with algorithms to generate random variates from various distributions. It is common to assume that a uniform random number generator is available, that is, a program that produces a sequence of independent and identically distributed continuous U(0,1) random variates (i.e., uniform random variates on the interval (0,1)). Of course real world computers can never generate ideal random numbers and they cannot produce numbers of arbitrary precision but state-of-the-art uniform random number generators come close to this aim. Thus random variate generation deals with the problem of transforming such a sequence of uniform random numbers into non-uniform random variates.

In this section we shortly explain the basic ideas of the *inversion*, rejection, and the ratio of uniforms method. How these ideas can be used to design a particular automatic random variate generation algorithms that can be applied to large classes of distributions is shortly explained in the description of the different methods included in this manual.

For a deeper treatment of the ideas presented here, for other basic methods and for automatic generators we refer the interested reader to our book [2].

A.1. The Inversion Method

When the inverse F^{-1} of the cumulative distribution function is known, then random variate generation is easy. We just generate a uniformly U(0,1) distributed random number U and return

$$X = F^{-1}(U) \ .$$

Figure 1 shows how the inversion method works for the exponential distribution.

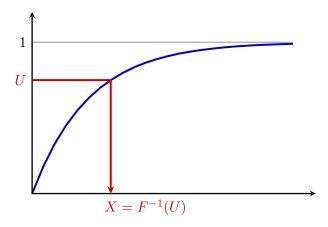


Figure 1: Inversion method for exponential distribution, $X = \log(1 - U)$.

This algorithm is simple so that inversion is certainly the method of choice if the inverse CDF is available in closed form. This is the case, e.g., for the exponential and the Cauchy distribution.

The inversion method also has other special advantages that make it even more attractive for simulation purposes:

• It preserves the structural properties of the underlying uniform pseudo-random number generator.

Consequently,

- it can be used for variance reduction techniques;
- it is easy to sample from truncated distributions;
- it is easy to sample from marginal distributions and thus is suitable for using with copulæ;
- the quality of the generated random variables depends only on the underlying uniform (pseudo-) random number generator.

Another important advantage of the inversion method is that we can easily characterize its performance. To generate one random variate we always need exactly one uniform variate and one evaluation of the inverse CDF. So its speed mainly depends on the costs for evaluating the inverse CDF. Hence inversion is often considered as the method of choice in the simulation literature.

Unfortunately computing the inverse CDF is often comparatively difficult and slow, e.g., for standard distributions like normal, student, gamma, and beta distributions. Often no such routines are available in standard programming libraries. Then numerical methods for inverting the CDF are necessary, e.g., Newton's method or interpolation. Such procedures, however, have the disadvantage that they may be slow or not exact, i.e. they compute approximate values. The methods HINV, HINV and PINV of UNU.RAN are such numerical inversion methods.

A.2. The Acceptance-Rejection Method

The acceptance-rejection method has been suggested by John von Neumann in 1951 [7]. Since then it has proven to be the most flexible and most efficient method to generate variates from continuous distributions.

We explain the rejection principle first for the density $f(x) = \sin(x)/2$ on the interval $(0, \pi)$. To generate random variates from this distribution we also can sample random points that are uniformly distributed in the region between the graph of f(x) and the x-axis, i.e., the shaded region in Figure 2.

In general this is not a trivial task but in this example we can easily use the rejection trick: Sample a random point (X,Y) uniformly in the bounding rectangle $(0,\pi) \times (0,1/2)$. This is easy since each coordinate can be sampled independently from the respective uniform distributions $U(0,\pi)$ and U(0,1/2). Whenever the point falls into the shaded region below the graph (indicated by dots in the figure), i.e., when $Y < \sin(X)/2$, we accept it and return X as a random variate from the distribution with density f(x). Otherwise we have to reject the point (indicated by small circles in the figure), and try again.

It is quite clear that this idea works for every distribution with a bounded density on a bounded domain. Moreover, we can use this procedure with any multiple of the density, i.e., with any positive bounded function with bounded integral and it is not necessary to know the integral of this function. So we use the term density in the sequel for any positive function with bounded integral.

From the figure we can conclude that the performance of a rejection algorithm depends heavily on the area of the enveloping rectangle. Moreover, the method does not work if the target distribution has infinite tails (or is unbounded). Hence non-rectangular shaped regions for the envelopes are important and we have to solve the problem of sampling points uniformly from such domains. Looking again at the example above we notice that the x-coordinate of the random point (X,Y) was sampled by inversion from the uniform distribution on the domain of the given density. This motivates us to replace the density of the uniform distribution by the (multiple of a) density h(x) of some other appropriate distribution. We only have to take care that it is chosen such that it is always an upper bound, i.e., h(x) >= f(x) for all x in the domain of the distribution. To generate the pair (X,Y) we generate X from the

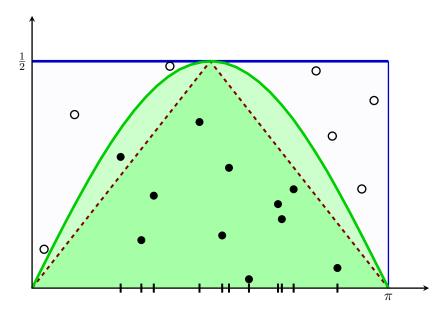


Figure 2: Acceptance-rejection method. Points are drawn randomly in $[0, \pi] \times [0, 1]$. Points above the density (\bullet) are rejected; points below the density (\bullet) are accepted and their x-coordinates are returned. Notice that there is no need to evaluate the density whenever a points falls into the region below the dashed triangle (squeeze).

distribution with density proportional to h(x) and Y uniformly between 0 and h(X). The first step (generate X) is usually done by inversion, see Section A.1.

Thus the general rejection algorithm for a hat h(x) with inverse CDF H^{-1} consists of the following steps:

- 1. Generate a U(0,1) random number U.
- 2. Set $X \leftarrow H^{-1}(U)$.
- 3. Generate a U(0,1) random number V.
- 4. Set $Y \leftarrow V h(X)$.
- 5. If $Y \leq f(X)$ accept and return X.
- 6. Else try again.

If the evaluation of the density f(x) is expensive (i.e., time consuming) it is possible to use a simple lower bound of the density as so called *squeeze function* s(x) (the triangular shaped function in Figure 2 is an example for such a squeeze). We can then accept X when $Y \leq s(X)$ and can thus often save the evaluation of the density.

We have seen so far that the rejection principle leads to short and simple generation algorithms. The main practical problem to apply the rejection algorithm is the search for a good fitting hat function and squeezes. We do not discuss these topics here as they are the heart of the different automatic algorithms implemented in UNU.RAN. Information about the construction of hat and squeeze can therefore be found in the descriptions of the methods.

The performance characteristics of rejection algorithms mainly depend on the fit of the hat and the squeeze. It is not difficult to prove that:

• The expected number of trials to generate one variate is the ratio between the area below the hat and the area below the density.

- The expected number of evaluations of the density necessary to generate one variate is equal to the ratio between the area below the hat and the area below the density, when no squeeze is used. Otherwise, when a squeeze is given it is equal to the ratio between the area between hat and squeeze and the area below the hat.
- The sqhratio (i.e., the ratio between the area below the squeeze and the area below the hat) used in some of the UNU.RAN methods is easy to compute. It is useful as its reciprocal is an upper bound for the expected number of trials of the rejection algoritm. The expected number of evaluations of the density is bounded by (1/sqhratio) 1.

A.3. The Composition Method

The composition method is an important principle to facilitate and speed up random variate generation. The basic idea is simple. To generate random variates with a given density we first split the domain of the density into subintervals. Then we select one of these randomly with probabilities given by the area below the density in the respective subintervals. Finally we generate a random variate from the density of the selected part by inversion and return it as random variate of the full distribution.

Composition can be combined with rejection. Thus it is possible to decompose the domain of the distribution into subintervals and to construct hat and squeeze functions separatly in every subinterval. The area below the hat must be determined in every subinterval. Then the Composition rejection algorithm contains the following steps:

- 1. Generate the index J of the subinterval as the realisation of a discrete random variate with probabilities proportional to the area below the hat.
- 2. Generate a random variate X proportional to the hat in interval J.
- 3. Generate the U(0, f(X)) random number Y.
- 4. If $Y \leq f(X)$ accept and return X.
- 5. Else start again with generating the index J (Step 1).

The first step can be done in constant time (i.e., independent of the number of chosen subintervals) by means of the indexed search method (Section A.7).

It is possible to reduce the number of uniform random numbers required in the above algorithm by recycling the random numbers used in Step 1 and additionally by applying the principle of *immediate acceptance*. For details see [2, Sect. 3.1].

A.4. The Ratio-of-Uniforms Method

The construction of an appropriate hat function for the given density is the crucial step for constructing rejection algorithms. Equivalently we can try to find an appropriate envelope for the region between the graph of the density and the x-axis, such that we can easily sample uniformly distributed random points. This task could become easier if we can find transformations that map the region between the density and the axis into a region of more suitable shape (for example into a bounded region).

As a first example we consider the following simple algorithm for the Cauchy distribution.

- 1. Generate a U(-1,1) random number U and a U(0,1) random number V.
- 2. If $U^2 + V^2 \le 1$ accept and return X = U/V.

3. Else try again.

It is possible to prove that the above algorithm indeed generates Cauchy random variates. The fundamental principle behind this algorithm is the fact that a half-disc in the UV-plane is mapped into the region below the density by the transformation

$$(U, V) \mapsto (X, Y) = (U/V, V^2)$$

in such a way that the ratio between the area of the image to the area of the preimage is constant. This is due to the fact that that the Jacobian of this transformation is constant.

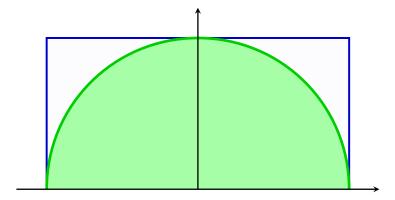


Figure 3: Ratio-of-Uniforms method. The region below the density of the Cauchy distribution is transformed into a half-circle. Points are then sampled uniformly in the bounding rectangle and accepted or rejected.

The above example is a special case of a more general principle, called the *Ratio-of-Uniforms* (RoU) method [3]. It is based on the fact that for a random variable X with density f(x) and some constant μ we can generate X from the desired density by calculating $X = U/V + \mu$ for a pair (U, V) uniformly distributed in the set

$$A_f = \{(u, v): 0 < v \le \sqrt{f(u/v + \mu)}\}$$
.

For most distributions it is best to set the constant μ equal to the mode of the distribution. For sampling random points uniformly distributed in \mathcal{A}_f rejection from a convenient enveloping region is used, usually the minimal bounding rectangle, i.e., the smallest possible rectangle that contains \mathcal{A}_f (see Figure 3). It is given by $(u^-, u^+) \times (0, v^+)$ where

$$v^{+} = \sup_{b_{l} < x < b_{r}} \sqrt{f(x)} ,$$

$$u^{-} = \inf_{b_{l} < x < b_{r}} (x - \mu) \sqrt{f(x)} ,$$

$$u^{+} = \sup_{b_{l} < x < b_{r}} (x - \mu) \sqrt{f(x)} .$$

Then the Ratio-of-Uniforms method consists of the following simple steps:

- 1. Generate a $U(u^-, u^+)$ random number U and a $U(0, v^+)$ random number V.
- 2. Set $X \leftarrow U/V + \mu$.
- 3. If $V^2 \leq f(X)$ accept and return X.

4. Else try again.

To apply the Ratio-of-Uniforms algorithm to a certain density we have to solve the simple optimization problems in the definitions above to obtain the design constants u^- , u^+ , and v^+ . This simple algorithm works for all distributions with bounded densities that have subquadratic tails (i.e., tails like $1/x^2$ or lower). For most standard distributions it has quite good rejection constants (e.g., 1.3688 for the normal and 1.4715 for the exponential distribution).

Nevertheless, we use more sophisticated method that construct better fitting envelopes, like method AROU, or even avoid the computation of these design constants and thus have almost no setup, like method SROU.

A.5. The Generalized Ratio-of-Uniforms Method

The Ratio-of-Uniforms method can be generalized in the following way [5, 8]: If a point (U, V) is uniformly distributed in the set

$$\mathcal{A}_f = \{(u, v) : 0 < v \le (f(u/v^r + \mu))^{1/(r+1)}\}\$$

for some real number r > 0, then $X = U/V^r + \mu$ has the denity f(x). The minimal bounding rectangle of this region is given by $(u^-, u^+) \times (0, v^+)$ where

$$v^{+} = \sup_{b_{l} < x < b_{r}} (f(x))^{1/(r+1)},$$

$$u^{-} = \inf_{b_{l} < x < b_{r}} (x - \mu)(f(x))^{r/(r+1)},$$

$$u^{+} = \sup_{b_{l} < x < b_{r}} (x - \mu)(f(x))^{r/(r+1)}.$$

The above algorithm has then to be adjusted accordingly. Notice that the original Ratio-of-Uniforms method is the special case with r = 1.

A.6. Inversion for Discrete Distributions

We have already presented the idea of the inversion method to generate from continuous random variables (Section A.1). For a discrete random variable X we can write it formally in the same way:

$$X = F^{-1}(U) \;,$$

where F is the CDF of the desired distribution and U is a uniform U(0,1) random number. The difference compared to the continuous case is that F is now a step-function. The following figure illustrates the idea of discrete inversion for a simple distribution.

To realize this idea on a computer we have to use a search algorithm. For the simplest version called $Sequential\ Search$ the CDF is computed on-the-fly as sum of the probabilities p(k), since this is usually much cheaper than computing the CDF directly. It is obvious that the basic form of the search algorithm only works for discrete random variables with probability mass functions p(k) for nonnegative k. The sequential search algorithm consists of the following basic steps:

- 1. Generate a U(0,1) random number U.
- 2. Set $X \leftarrow 0$ and $P \leftarrow p(0)$.
- 3. Do while U > P
- 4. Set $X \leftarrow X + 1$ and $P \leftarrow P + p(X)$.

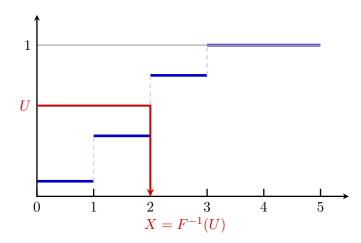


Figure 4: Discrete inversion

5. Return X.

With the exception of some very simple discrete distributions, sequential search algorithms become very slow as the while-loop has to be repeated very often. The expected number of iterations, i.e., the number of comparisons in the while condition, is equal to the expectation of the distribution plus 1. It can therefore become arbitrary large or even infinity if the tail of the distribution is very heavy. Another serious problem can be critical round-off errors due to summing up many probabilities p(k). To speed up the search procedure it is best to use indexed search.

A.7. Indexed Search (Guide Table Method)

The idea to speed up the sequential search algorithm is easy to understand [1]. Instead of starting always at 0 we store a table of size C with starting points for our search. For this table we compute $F^{-1}(U)$ for C equidistributed values of U, i.e., for $u_i = i/C$, i = 0, ..., C-1. Such a table is called *guide table* or *hash table*. Then it is easy to prove that for every U in (0,1) the guide table entry for $k = \lfloor UC \rfloor$ is bounded by $F^{-1}(U)$. This shows that we can start our sequential search procedure from the table entry with index k which can be found quickly by means of the truncation operation.

The two main differences between indexed search and sequential search are that we start searching at the number determined by the guide table, and that we have to compute and store the cumulative probabilities in the setup as we have to know the cumulative probability for the starting point of the search algorithm. The rounding problems that can occur in the sequential search algorithm can occur here as well. Compared to sequential search we have now the obvious drawback of a slow setup. The computation of the cumulative probabilities grows linear with the size of the domain of the distribution L. What we gain is really high speed as the marginal execution time of the sampling algorithm becomes very small. The expected number of comparisons is bounded by 1 + L/C. This shows that there is a trade-off between speed and the size of the guide table. Cache-effects in modern computers will however slow down the speed-up for really large table sizes. Thus we recommend to use a guide table that is about two times larger than the probability vector to obtain optimal speed.

B. Pitfalls

Libraries like Runuran that provide a flexible interface also have the risk of possible traps and pitfalls. Besides the obvious case where the chosen method cannot be used for sampling from the target distribution we observed that users sometimes forget to change the default values of the function arguments, e.g., they do not set the center (a "typical point" of the distribution) when the domain does not contain 0. Then it may happen that the chosen generation method does not work or (the worst case!) does not work as expected.

Check argument defaults whenever you use an Runuran function!

Here is an examples² of possible problems and how to fix these.

Shifted center. Some methods require a "typical" point of the distribution, called **center**. By default this is set to **center=0**. The PDF at the center must not be too small. Thus if pdf(center) returns 0 the chosen method does not work.

```
___ Example
> pdf <- function (x) { x^2 / (1+x^2)^2 }
> gen <- pinv.new(pdf=pdf,lb=0,ub=Inf)</pre>
 [UNU.RAN - error] (generator) condition for method violated: PDF(center) <= 0.
Error: [UNU.RAN - error] cannot create UNU.RAN object
Solution: Set center to (a point near) the mode of the distribution.
                                ___ Example _
> pdf <- function (x) { x^2 / (1+x^2)^2 }
> gen <- pinv.new(pdf=pdf,lb=0,ub=Inf, center=1 )</pre>
                                                        ## Add 'center'
> x <- ur(gen, 10)
 > x
  [1]
       0.5882186 4.2182782 0.4753110 2.4816067
                                                     1.4573010 19.5895715
       1.2625293 5.5915360 64.3125652
  [7]
                                         2.8971545
```

Broken Runuran objects. Runuran objects contain pointers to external objects. Consequently, it is not possible to save and restore an Runuran object between R sessions, nor to copy such objects to different nodes in a computer cluster. Runuran objects must be newly created in each session (and in each node) from scratch. Otherwise, the object is broken and ur and ur refuse do not work.

However, *generator objects* for *some* generation methods can be *packed*. Then these objects can be handled like any other R object (and thus saved and restored).

Here is an example how a generator object can be packed.

 $^{^2\}mathrm{Please}$ sent us examples where you had problems with the concept of Runuran.

B. Pitfalls

```
Example _
 > ## create a unuran object using method 'PINV'
 > gen <- pinv.new(dnorm,1b=0,ub=Inf)</pre>
 > ## such an object can be packed
> unuran.packed(gen) <- TRUE</pre>
 > ## it can be still used to draw a random sample
 > x \leftarrow ur(gen, 10)
 > x
  [1] 0.3362478 0.7919103 1.3401460 0.5111629 0.3278236 0.8362710 0.9197225
  [8] 0.5737696 1.0033686 1.5771101
 > ## we also can check whether a unuran object is packed
 > unuran.packed(gen)
 [1] TRUE
 Now can save or R session and start a new one with the previously saved workspace restored.
Then we can reuse object gen (after loading library Runuran).
 Withour packing gen, it would be broken after restoring the saved workspace.
                             _____ Example _
 [Previously saved workspace restored]
 > library(Runuran)
 > ur(gen, 10)
Error in ur(gen, 10): [UNU.RAN - error] broken UNU.RAN object
```

C. Glossary

CDF – cumulative distribution function.

center – "typical point" of distribution ("near the mode").

HR – hazard rate (or failure rate).

inverse local concavity – local concavity of inverse PDF $f^{-1}(y)$ expressed in term of $x = f^{-1}(y)$. Is is given by

$$ilc_f(x) = 1 + x f''(x)/f'(x)$$
.

mode – maximum of PDF.

local concavity – maximum value of c such that PDF f(x) is T_c -concave. Is is given by

$$lc_f(x) = 1 - f''(x) f(x)/f'(x)^2$$
.

log-concave – a PDF f(x) (and hence the corresponding distribution) is called log-concave if $\log(f(x))$ is concave, i.e., if $(\log(f(x))'' \le 0$. See also T_0 -concave.

For discrete distributions, a PMF p is log-concave if and only if

$$p_i \ge \sqrt{p_{i-1} p_{i+1}}$$
 for all i .

PDF – probability density function.

PMF – probability mass function.

PV – (finite) probability vector.

URNG – uniform random number generator.

U(a,b) – continuous uniform distribution on the interval (a,b).

 T_c -concave – a PDF f(x) is called T-concave if the transformed function T(f(x)) is concave. We only deal with transformations T_c , where

In particular, a PDF f(x) is T_c -concave when its local concavity is less than c, i.e., $lc_f(x) \leq c$.

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