Universal Algorithms as an Alternative for Generating Non-Uniform Continuous Random Variates

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ABSTRACT: This paper presents an overview of the most powerful universal methods. These are based on acceptance/rejection techniques where hat and squeezes are constructed automatically. Although originally motivated to sample from non-standard distributions these methods have advantages that make them attractive even for sampling from standard distributions and thus are an alternative to special generators tailored for particular distributions. Most important are: the marginal generation time is fast and does not depend on the distribution. They can be used for variance reduction techniques, and they produce random numbers of predictable quality. These algorithms are implemented in a library, called UNURAN, which is available by anonymous ftp.

1 INTRODUCTION

There exists a vast literature on generation methods for continuous standard distributions; see, for example, Devroye (1986), Dagpunar (1988) or Gentle (1998). These algorithms are often especially designed for a particular distribution and tailored to the features of each probability density function. The designing goals for these methods are fast generators and/or simple code. However in many simulation situations the application of standard distributions is not adequate. Thus during the last decade so called universal (or black box) algorithms have been developed to avoid the design of special algorithms for these cases.

Black box methods work for large classes of distributions and require the knowledge of some data about the desired distribution. Often no more than (a multiple of) the probability density function is necessary. Depending on the chosen method additional information like the (approximate) mode of the distribution, (approximate) regions of monotonicity or log-concavity of the density function are required or useful. Obviously these universal methods need some setup step, in opposition to special generators, e.g., to the Box-Muller method (Box & Muller 1958). However we always can select between a fast setup step and slow marginal generation times or (very) fast marginal generation times at the expense of a time consuming setup step. Some of the algorithms can be adjusted by a single parameter to the needs of the current situation.

1.1 *The inversion method*

The *inversion method* is the most general method for generating non-uniform random variates. It works for all distributions provided that the cumulative distribution function F is given. Let U be a uniform $(0,1)$ random number. Then

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

has the target distribution. This method preserves the structural properties of the underlying uniform pseudo-random number generator. Consequently it can be used for variance reduction techniques, see, e.g., Bratley, Fox, & Schrage (1983), and it is easy to sample from truncated distributions. Moreover the quality of the generated random numbers depends only on the underlying uniform random number generator. Thus it would be the method of choice.

However the inverse of a c.d.f. is not given in a simple form for many distributions. Methods based on numerical inversion (e.g., Newton-Raphson method) are rather slow and can only be speeded up by the usage of (large) tables; see, e.g., Devroye (1984a) or Ahrens & Kohrt (1981). Additionally these numerical methods are not exact, i.e., they produce random numbers which are only approximately distributed as the given distribution.

1.2 *Acceptance/Rejection Methods*

Let f denote the probability density function. The *acceptance/rejection method* is based on the following (well-known) proposition.

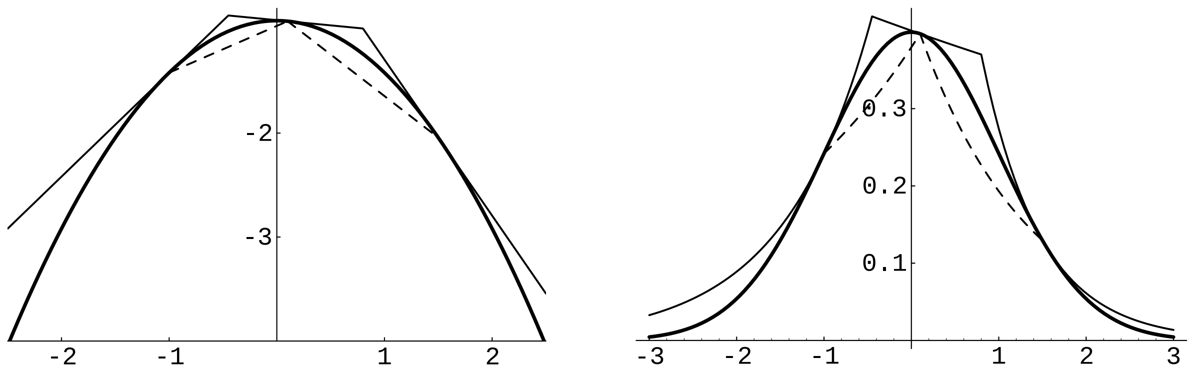

Figure 1. Construction of a hat function for the normal density utilizing transformed density rejection. The left hand side shows the transformed density with three tangents. The right hand side shows the density function with the resulting hat. Squeezes are drawn as dashed lines.

THEOREM 1 *If a random vector* (X, U) *is uniformly distributed on*

$$\mathcal{G} = \{(x, y)\colon 0 < y \le c\, f(x)\} \qquad (2)$$

then X *has density function* f *for every constant* $c > 0$. *Vice versa, for a uniform* $(0, 1)$ *random number,* $(X, U\, c\, f(X))$ *is uniformly distributed on* $\mathcal{G}$.

Thus utilizing this theorem we need a *majorizing* or *hat* function $c\,h(x) \ge f(x)$, where h is a p.d.f., such that it is easy to generate from this distribution (e.g., by inversion). Then generate X with p.d.f. h and a $(0, 1)$ random number U. If $U\,c\,h(X) \le f(X)$ return X, otherwise reject and try again. c is called the *rejection constant* and gives the expected number of interations to get one random variate. Simple lower bounds $s(x) \le f(x)$, called *squeezes*, can be used to reduce the number of (expensive) evaluations of f.

The most efficient algorithms based on this method compute hat and squeezes automatically. These algorithms are very flexible in their applications. In this paper we consider the following three methods: *transformed density rejection (TDR)*, a *table method (TABL)* introduced in (Ahrens 1993), and a version of the *ratio-of-uniforms method (AROU)*. We have implemented various versions of these (and some other methods) in ANSI C. Our main goal was to get a portable, flexible and robust program. The resulting library is called UNURAN and is available via ftp (see Leydold & Hörmann (2000)).

2 UNIVERSAL METHODS

2.1 *Transformed density rejection*

TDR ist the most flexible method. It has been introduced in Devroye (1986) and under a different name in Gilks & Wild (1992), and generalized in Hörmann (1995). It is based on the idea that the given density f is transformed by a strictly montonically increasing differential transformation $T\colon (0, \infty) \to \mathbb{R}$ such that $T(f(x))$ is concave. We then say that f is *T-concave*; log-concave densities are an example with $T(x) = \log(x)$.

By the concavity of $T(f(x))$ it is easy to construct a majorizing function for the transformed density as the minimum of several tangents. Transforming this function back into the original scale we get a hat function $h(x)$ for the density f. By using secants between the touching points of the tangents of the transformed density we analogously can construct squeezes (details can be found in Hörmann (1995) or Evans & Swartz (1998)). Figure 1 illustrates the situation for the standard normal distribution and $T(x) = \log(x)$. Evans & Swartz (1998) have shown that this technique is even suitable for arbitrary densities provided that the inflection points of the transformed density are known. It should be noted here that the tangent on the transformed density can be replaced by secants through two points that are close together, shifted away from the mode by the distance of these two points. Thus no derivatives are required.

Algorithm `tdr` applies this idea for a black box algorithm. The I_j are the intervals where the hat h is given by the tangent with touching point c_j.

Step 5 is executed in constant time by means of *indexed search* (Chen & Asau 1974). Notice that the random variate X is generated by inversion, when random numbers are *recycled* (Devroye 1986, §II.3, p.58) and the algorithm is implemented properly. Therefore we do not recommend the alias method by Walker (1974).

It is obvious that the transformation T must have the property that the area below the hat is finite, and that generating a random variable with density proportional to the hat function by inversion must be easy (and fast). Thus we have to choose the transforma-

Algorithm 1 `tdr`

Require: density $f(x)$; transformation $T(x)$, construction points $c_1, \ldots, c_n$.

/* Setup */
- Construct hat $h(x)$ and squeeze $s(x)$.
- Compute intervals $I_1, \ldots, I_n$.
- Compute areas H_j below the hat for each I_j.

/* Generator */
- **loop**
  - Generate I with probability vector proportional to $(H_1, \ldots, H_n)$.
  - Generate X with density proportional to $h|_I$ (by inversion).
  - Generate $U \sim U(0,1)$.
  - **if** $U\,h(X) \leq s(X)$ **then** /* evaluate squeeze */
    - **return** X.
  - **if** $U\,h(X) \leq f(X)$ **then** /* evaluate density */
    - **return** X.

tions T carefully. Hörmann (1995) suggests the family T_c of transformations, where

$$T_0(x) = \log(x) \quad \text{and} \quad T_c(x) = \operatorname{sign}(c)\,x^c. \qquad (3)$$

($\operatorname{sign}(c)$ makes T_c increasing for all c.) For densities with unbounded domain we must have $c \in (-1, 0]$. For the choice of c it is important to note that the area below the hat increases when c decreases. Moreover we find

THEOREM 2 (Hörmann 1995) *If f is T_c-concave, then f is $T_{c'}$-concave for every $c' \leq c$.*

Because of computational reasons, the choice of $c = -1/2$ (if possible) is suggested. As a corollary of the above theorem algorithm `tdr` then can generate random variate of (at least) all log-concave distributions. Table 1 give examples of $T_{-1/2}$-concave distributions.

2.2 *A table method*

Ahrens (1993) introduces the *table method* (TABL) that uses piecewise constant hat and squeezes. (Ahrens (1995) gives a modified version.) It can be seen as the special case of the transformed density rejection with $c \to -\infty$. It works for all monotone distributions and consequently for all unimodal distributions when the mode is known. (If the mode is not known Zaman (1996) describes a methods that uses upper bounds on the mode.) Figure 2 illustrates the situation for the exponential distribution. Notice that we have to cut off the unbounded tail of the distribution to get a hat with finite integral. We have to take care that the truncated part is not of "computational relevance". Alternatively we can combine this table method with TDR for the tail of the distribution. It is obvious that generating from the hat distribution is

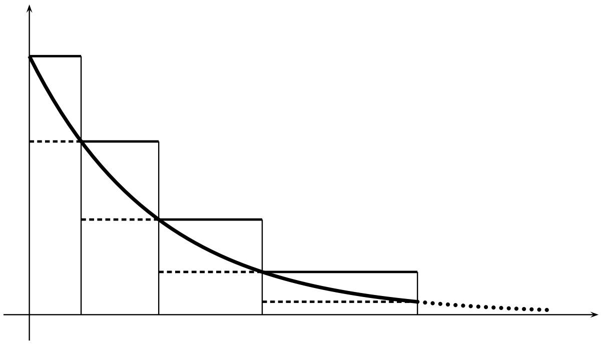

Figure 2. Piecewise constant hat and squeeze (dashed lines) for the exponential distribution. The tail of the distribution has to be cut off (dotted line).

very fast. Moreover we have a region of "immediate acceptance" below the squeeze, where no second uniform random number is required. I.e., we have a mixture of two distribution with p.d.f. proportional to squeeze $s(x)$ and $h(x) - s(x)$, respectively. We first use a uniform random number to decide whether we are below the squeeze or above. In the first case simply return the appropriate uniform random variate. In the latter case, use the acceptance/rejection method.

Remark. This technique of splitting the area below the hat could also be used for TDR. However the region between hat and squeeze is much more complicated and requires additional work, see Leydold (2000b) for an example.

2.3 *Ratio-of-uniforms*

The *ratio-of-uniforms* method (AROU) has been introduced in Kinderman & Monahan (1977). It is a very flexible method that can be adjusted to a large variety of distributions. It has become a popular transformation method since it usually results in exact, efficient, fast and easy to implement algorithms (see, e.g., Barabesi (1993)). It is based on the following theorem.

THEOREM 3 (Kinderman & Monahan 1977) *If (V, U) is uniformly distributed in*

$$\mathcal{A} = \{(v, u) \colon 0 < u \leq \sqrt{f(v/u)}\}, \qquad (4)$$

then the ratio V/U has density function f.

This theorem (as well as the theorem 4 below) is proved by means of a map $\mathcal{A} \to \mathcal{G}$ with constant Jacobian between the regions in (4) and (2).

For sampling random points uniformly distributed in $\mathcal{A}$ rejection from a convenient enveloping region is used; usually a minimal bounding rectangle. For a large class of distributions, however, $\mathcal{A}$ is convex. Hence it is possible to construct an enveloping polygon and squeezes automatically. For computing the tangent lines at the boundary of $\mathcal{A}$ the total differential of $u^2 - f(v/u)$ is used. Figure 3 illustrates the

Distribution	Density	Support	$T_{-1/2}$-concave for
Normal	$e^{-x^2/2}$	$\mathbb{R}$	
Log-normal	$1/x \exp(-\ln(x-\mu)^2/(2\sigma^2))$	$[0,\infty)$	$\sigma \le \sqrt{2}$
Exponential	$\lambda\, e^{-\lambda x}$	$[0,\infty)$	$\lambda > 0$
Gamma	$x^{a-1}\, e^{-b x}$	$[0,\infty)$	$a \ge 1,\, b > 0$
Beta	$x^{a-1}\,(1-x)^{b-1}$	$[0,1]$	$a, b \ge 1$
Weibull	$x^{a-1} \exp(-x^a)$	$[0,\infty)$	$a \ge 1$
Perks	$1/(e^x + e^{-x} + a)$	$\mathbb{R}$	$a \ge -2$
Gen. inv. Gaussian	$x^{a-1} \exp(-bx - b^*/x)$	$[0,\infty)$	$a \ge 1,\, b, b^* > 0$
Student's t	$(1 + (x^2/a))^{-(a+1)/2}$	$\mathbb{R}$	$a \ge 1$
Pearson VI	$x^{a-1}/(1+x)^{a+b}$	$\mathbb{R}$	$a, b \ge 1$
Cauchy	$1/(1+x^2)$	$\mathbb{R}$	
Planck	$x^a/(e^x - 1)$	$[0,\infty)$	$a \ge 1$
Burr	$x^{a-1}/(1+x^a)^b$	$[0,\infty)$	$a \ge 1,\, b \ge 2$
Snedecor's F	$x^{m/2-1}/(1+m/n\, x)^{(m+n)/2}$	$[0,\infty)$	$m, n \ge 2$

Table 1. $T_{-1/2}$-concave densities (normalization constants omitted).

situation for the standard normal distribution. Notice that we have a natural triangulation of the enveloping region, the squeeze region, and the region between squeeze and envelope. For sampling from a triangle the simple algorithm by Devroye (1986, p.570) can be used.

Again we have a region of immediate acceptance as for method TABL. Notice that inside this region only the ratio $x = v/u$ is of interest. Thus it suffices to generate a point uniformly distributed on the boundary of the squeeze region (the dashed line in figure 3). As a consequence sampling points in the squeeze region can be seen as sampling from the corresponding distribution by means of the inversion method. We refer to Leydold (2000a) for details and for a comprehensive description of the resulting algorithm.

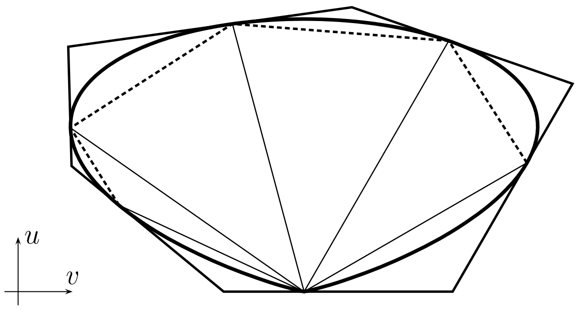

Figure 3. Enveloping polygon and squeeze polygon (dashed line) of $\mathcal{A}$ for the standard normal distribution and its "natural" triangulation.

Stadlober (1989) and Dieter (1989) have clarified the relationship of the ratio-of-uniforms method to the ordinary acceptance/rejection method. But there is also a deeper connection to the transformed density rejection, that gives us a useful characterization for densities with convex region $\mathcal{A}$.

THEOREM 4 (Leydold 2000a) *$\mathcal{A}$ is convex if and only if $f(x)$ is T-concave with transformation $T(x) = -1/\sqrt{x}$.*

3 CONSTRUCTION POINTS

The above algorithms work well when the ratio

$$\varrho = \int h / \int s = \text{area below hat/area below squeeze} \tag{5}$$

is close to one. (For AROU the definition of ϱ has to be changed accordingly.) Thus we have to find construction points, such that ϱ is small.

3.1 *Adaptive rejection sampling*

For the problem of finding appropriate construction points for the hat function Gilks & Wild (1992) introduce the ingenious concept of *adaptive rejection sampling*. For TDR it works in the following way:

Start with (at least) two points on either side of the mode and sample points x from the hat distribution. Add a new construction point at x whenever we have to evaluate the p.d.f. $f(x)$, i.e., when $s(X) < U\, h(X)$, until a certain stopping criterion is fulfilled, e.g., the maximal number of construction points or the aimed ratio ϱ is reached. Obviously the ratio ϱ is a random variable that converges to 1 almost surely when the number n of construction points tends to infinity. This technique works analogously for AROU.

For method TABL the construction points are simply the points of discontinuity (see figure 2). However in simulation experiments the choice of the rejected point x was not optimal. The convergence has been improved for some heavy tail distributions when $\bar{x} = \tan((\arctan(c_i) + \arctan(c_{i+1}))/2)$ was used instead. $\bar{x}$ can be seen as a mixture of the arithmetic mean and the harmonic mean of c_i and c_{i+1} (which denote the boundary points of the interval that contains x.)

3.2 *Equidistributed points*

Figure 3 suggests the usage of the following construction points:

$$c_i = \tan(-\pi/2 + i\pi/(n+1)), \quad i = 1, \ldots, n. \quad (6)$$

If the mode m of the distribution is known, the points $c_i + m$ should be used. Numerical simulations with several density functions have shown that this heuristic rule gives an acceptable good choice for construction points when the ratio of length and width of the minimal bounding rectangle of $\mathcal{A}$ is not too far from one. For this case it can be shown that $\varrho < 1 + O(n^{-1})$ (Leydold 2000a). These points are at least very good starting points for adaptive rejection sampling. Due to theorem 4 the points c_i can equally well be used for methods TDR and AROU.

3.3 *Optimal construction points*

There exists methods for finding construction points for TDR such that ϱ is minimized for given number of construction points, transformation and distribution. By a simple consideration we find for the optimal choice of construction points $\varrho = 1 + O(n^{-2})$ when $c > -1$ (Leydold & Hörmann 1998). Hörmann (1995) describes a method how three optimal construction points can be found. If more points are required, Derflinger & Hörmann (1998) describe a very efficient method. The latter works for TDR, TABL and AROU.

Ahrens (1993) notices that there exists a method for finding optimal construction points for TABL. However it is rather expensive and thus the usage of the "equal-area rule" (i.e., the area below the hat is the same for each interval) is suggested and a heuristic rule for further improvements is presented. For TABL we have $\varrho = 1 + O(n^{-1})$.

4 PROPERTIES

4.1 *Flexible and almost inversion*

The performance of these three methods can be controlled by a single parameter, the ratio ϱ. Notice that $\varrho - 1$ is the expected number of evaluation of the density function f. Moreover ϱ is an upper bound for the rejection constant. Thus for decreasing ϱ the algorithm works faster and the performance becomes more predictable. Moreover this makes these algorithms very flexible. If only a few random variates are required, we can have a cheap setup step (use only some construction points) at the expense of a high ratio ϱ, i.e., slower marginal generation times. (Devroye (1984b) and Leydold (2000c) give algorithms that have almost no setup step.)

If we want ϱ to be close to 1 (say 1.01) then a more expensive setup step and/or adaptive steps are necessary. But then the marginal generation time does not depend on the particular distribution. In fact they are fast and have competitive speed even for the normal distribution (e.g., it is faster than the algorithm by Leva (1992) that has been proposed as "fast"). Moreover the algorithm is then close to the inversion method and consequently shares its properties (at least approximately). For example it can be used for correlation induction by means of the technique suggested by Schmeiser & Kachitvichyanukul (1986, 1990) for the acceptance/rejection method. For $\varrho \approx 1$ we have almost optimal correlation (Hörmann & Derflinger 1994).

What we consider most important is the fact that these universal methods almost preserve the structural properties of the underlying uniform pseudo-random number generator. Thus it generates random variates of predictable quality provided that those of the underlying pseudo-random number generator is known. This aspect of non-uniform random variate generation is almost neglected in literature in contrast to the literature on uniform random number generation, where this is a prominent point of research. Leydold, Leeb, & Hörmann (2000) give a short survey and some empirical results. The quality of non-uniform pseudo-random variates generated by other methods has less correlation to the quality of the underlying uniform generator and is thus "unpredictable".

These properties make the discussed methods attractive even for standard distributions and hence they provide an alternative to special generators tailored for particular distributions.

4.2 *Computational experiences*

Of course there are differences between these methods. We have implemented various versions of TDR, TABL and AROU (and some other methods) in ANSI C. Our main goal was to get a portable, flexible and robust program. Using this library first a generator object has to be created that then can be used to sample from the given distribution. Thus it is easy to exchanged distributions in simulations. Moreover each generator object may have its own pseudo-random number generator or share one with other generators. The resulting library is called UNURAN and is available via ftp (see Leydold & Hörmann (2000)).

We have run numerical experiments with several distributions. The timings have been performed on a PC running Linux. For comparison the marginal generation times for the Box-Muller method and the algorithm by Leva (1992) are given which have also been implemented in UNURAN. For the underlying pseudorandom number generator we have used gen-

	TDR	TABL	AROU
Required	p.d.f. f, (f')	p.d.f. f, mode	p.d.f. f, f'
Distributions	T_c-concave	unimodal	$T_{-1/2}$-concave
# uniform random numbers	2ϱ	ϱ	ϱ
30 construction points (heuristic rule):			
setup time	250–310 μs	90–130 μs	180–240 μs
rejection constant	1.03–1.14	1.26–5.23	1.03–1.14
marginal generation time	1.53–1.68 μs	1.03–3.74 μs	0.77–0.92 μs
adaptive rejection sampling until $\varrho < 1.01$:			
# construction points	35–57	540–1600	35–57
marginal generation time	1.51 μs	0.80 μs	0.76 μs

Table 2. Comparison of the three methods. TDR for $c \leq -1$ and TABL can only be used when the tail of the distribution is cut off. The computational experiments have been made with UNURAN using the normal, Student's t, Cauchy, gamma(10) and beta(10,20) distributions. We have started with 30 construction points using the equidistribution rule and equiarea rule, respectively. Then adaptive rejection sampling has been used to get $\varrho < 1.01$ (thus the union of 90%-percentiles at sample sizes of 10^5 are given). The marginal generation time for the Box-Muller method within UNURAN is 0.83 μs, for Leva's algorithm we have found 1.28 μs.

erator `CMRG` from the library prng-2.2 (Lendl 1997). This is a combined multiple recursive random number generator by L'Ecuyer (1996) with a long period (generation time 0.31 μs).

The results are sumerized in table 2. TABL is the method that is applicable to every unimodal distribution restricted to a bounded interval. It is the most simple one and very fast but requires (much) more construction points than the other two methods. If we want to use it for heavy tail distributions (e.g., Cauchy) we have problems with cutting off the tails and need a lot of construction points. TDR needs more uniform random variates but can be adjusted to a given distribution in a better way than TABL. AROU is very fast and does not need more construction points than TDR or more uniform random numbers than TABL. However it is restricted to $T_{-1/2}$-concave distributions.

5 AUTOMATIC CODE GENERATION

Implementing the above methods results in a rather long computer program for two reasons: (1) A hat function and squeezes have to be constructed in a setup step and improved in possible adaptive steps. (2) The given distribution has to fulfill the assumption of the choosen method or transformation T_c. This has to be tested in the setup step. However the actual sampling routines consist only of a few lines of code. Thus the same methods can be used to produce a single piece of (C, C++, Fortran, ...) code for a fast generator of a particular distribution given by a user who needs no experience in random number generation. This program then produces random variates at a known speed and of predictable quality.

6 CONCLUSIONS

We have given a survey about three efficient universal algorithms for non-uniform random variate generation. Although originally motivated to generate from non-standard distributions these universal methods have advantages which makes their usage attractive even for standard distributions:

- Only one piece of code, well implemented and debugged only once, is required.
- By a simple parameter ϱ it is possible to choose between fast setup with slow marginal generation time and vice versa.
- It can sample from truncated distributions.
- The algorithms can be made as close to inversion as requested. Then:
- The marginal generation time does not depend on the density function and is faster than many of the specialized generators (even for the normal distribution).
- It can be used for variance reduction techniques.
- The quality of the generated random numbers only depends on the underlying uniform random number generator.

Moreover these methods can be used to automatically produce a computer program for a given distribution that produces random variates at a known speed and of predictable quality.

The only task that is done really better by standard generators is the problem of generating random variates for a distribution family (e.g., Gamma or Beta) where the shape parameters of the distribution are changing very frequently or even after every call. There are automatic methods specially designed for this case (e.g., Devroye (1984b)) but they are still much slower than algorithms tailored to the standard distribution.

The algorithms have been implemented in C by the authors in a library called UNURAN which is available via anonymous ftp (Leydold & Hörmann 2000).

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