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Working Paper

Original Citation:
Leydold, Josef (1999) Automatic Sampling with the Ratio-of-uniforms Method. *Preprint Series / Department of Applied Statistics and Data Processing*, 26. Department of Statistics and Mathematics, Abt. f. Angewandte Statistik u. Datenverarbeitung, WU Vienna University of Economics and Business, Vienna.

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Automatic Sampling with the Ratio-of-uniforms Method

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Preprint Series

Preprint 26
June 1999

http://statmath.wu-wien.ac.at/

Automatic Sampling with the Ratio-of-Uniforms Method

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Applying the ratio-of-uniforms method for generating random variates results in very efficient, fast and easy to implement algorithms. However parameters for every particular type of density must be precalculated analytically. In this paper we show, that the ratio-of-uniforms method is also useful for the design of a black-box algorithm suitable for a large class of distributions, including all with log-concave densities. Using polygonal envelopes and squeezes results in an algorithm that is extremely fast. In opposition to any other ratio-of-uniforms algorithm the expected number of uniform random numbers is less than two. Furthermore we show that this method is in some sense equivalent to transformed density rejection.

Categories and Subject Descriptors: G.3 [**Probability and Statistics**]: Random number generation

General Terms: Algorithms

Additional Key Words and Phrases: random number generation, non-uniform, rejection method, ratio of uniforms, log-concave, T-concave, adaptive method, universal method

1. INTRODUCTION

There exists a large literature on generation methods for standard continuous distributions; see, for example, Devroye [1986]. These algorithms are often especially designed for a particular distribution and tailored to the features of each density. However in many situations the application of standard distributions is not adequate for a Monte-Carlo simulation. Besides sheer brute force inversion (that is, tabulate the distribution function at many points), several universal methods for large classes of distributions have been developed to avoid the design of special algorithms for these cases. Some of these methods are either very slow (e.g. Devroye [1984]) or need a slow set-up step and large tables (e.g. Ahrens and Kohrt [1981],

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Marsaglia and Tsang [1984], and Devroye [1986, chap. VII]).

Recently two more efficient methods have been proposed. The *transformed density rejection* by Gilks and Wild [1992] and Hörmann [1995] is an acceptance/rejection technique that uses the concavity of the transformed density to generate a hat function automatically. The user only needs to provide the probability density function and perhaps the (approximate) location of the mode. A *table method* by Ahrens [1993] also is an acceptance/rejection method, but uses a piecewise constant hat. A region of immediate acceptance makes the algorithm fast when a large number of constant pieces is used. The tail region of the distribution is treated separately. In Ahrens [1995] the algorithm is modified to use a piecewise constant hat such that the area below each piece is the same. Thus generation is simplified but the algorithm requires more adjustments for the setup for each distribution.

The ratio-of-uniforms method introduced by Kinderman and Monahan [1977] is another flexible method that can be adjusted to a large variety of distributions. It has become a popular transformation method to generate non-uniform random variates, since it results in exact, efficient, fast and easy to implement algorithms. Typically these algorithms have only a few lines of code (e.g. Barabesi [1993] gives a survey and examples of FORTRAN codes for several standard distributions). It is based on the following theorem.

THEOREM 1 (KINDERMAN AND MONAHAN 1977). *Let X be a random variable with density function $f(x) = g(x)/\int g(x)dx$, where $g(x)$ is a positive integrable function with support (x_0, x_1) not necessarily finite. If (V,U) is uniformly distributed in*

$$\mathcal{A} = \mathcal{A}_g = \{(v,u)\colon 0 < u \leq \sqrt{g(v/u)},\, x_0 < v/u < x_1\}, \tag{1}$$

then $X = V/U$ has probability density function $f(x)$.

For sampling random points uniformly distributed in $\mathcal{A}_g$ rejection from a convenient enveloping region $\mathcal{R}_g$ is used. The basic form of the ratio-of-uniforms method is given by algorithm `rou`.

Algorithm `rou`

Require: function $g(x)$ (prop. to density $f(x)$); enveloping region $\mathcal{R}$

1: **repeat**
2: Generate random point (V,U) uniformly distributed in $\mathcal{R}$.
3: $X \leftarrow V/U$.
4: **until** $U^2 \leq g(X)$.
5: **return** X.

Usually the input in `rou` is prepared by the designer of the algorithm for each particular distribution. To reduce the number of evaluations of the density function in step 4, squeezes are used. It is obvious that the performance of this simple algorithm depends on the *rejection constant*, i.e. on the ratio $|\mathcal{R}|/|\mathcal{A}|$, where $|\mathcal{R}|$ denotes the area of region $\mathcal{R}$. Kinderman and Monahan [1977] and others use rejection from the *minimal bounding rectangle*, i.e. the smallest possible rectangle $\{(v,u)\colon 0 \leq u \leq u^*,\, v_* \leq v \leq v^*\}$. This basic algorithm has been improved in several ways[1]: A tighter fitting enclosing region decreases the rejection constant. Possible choices are parallelograms (e.g. Cheng and Feast [1979]) or quadratic bounding curves (e.g. Leva [1992]). Often it is convenient to decompose $\mathcal{A}$ into a countable set of non-overlapping subregions (*"composite ratio-of-uniforms method"*, Robertson and Walls [1980] give a simple example). Dagpunar [1988, p. 65] considers the possibility of an enclosing polygon.

In this paper we develop a new algorithm that uses polygonal envelopes and squeezes. Random variates inside the squeeze are generated by mere inversion and therefore in opposition to any other ratio-of-uniforms method the expected number of uniform random numbers is less than two. For a large class of distributions, including all log-concave distributions, it is possible to construct envelope and squeeze automatically. Moreover we show that the new algorithm is in some sense equivalent to transformed density rejection.

The new method has several advantages:

—Envelopes and squeezes are constructed automatically. Only the probability density function is necessary.

—The expected number of uniform random numbers is $1 + \varrho$, where $\varrho > 0$ can be made arbitrarily small.

—For small ϱ the method is close to inversion and thus the resulting random variates can be used for variance reduction techniques. Moreover the structure of the resulting random variates is similar to that of the underlying uniform random number generator. Hence the non-uniform random variates inherit its quality properties.

—It avoids some possible defects in the quality of the resulting pseudo-random variates that have been reported for the ratio-of-uniforms method [Hörmann 1994a; Hörmann 1994b].

—It is the first ratio-of-uniforms method and the first implementation of transformed density rejection where the expected number of uniform random numbers is less than two.

In section 2 we give an outline of this new approach and in section 4 we discuss the problem of getting a proper envelope for the region $\mathcal{R}$. Section 5 describes the algorithm in detail and section 6 reports the computational experiences we have had with the new algorithm and compare these with other algorithms. Section 3 shows that this algorithm is applicable for all T-concave densities, with $T(x) = -1/\sqrt{x}$. Remarks on the quality of random numbers generated with the new algorithm are given in section 7.

[1]Moreover the method has been extended: Wakefield, Gelfand, and Smith [1991] replaces the function $q(u) = u^2$ by a more general strictly increasing differentiable function $q(u)$.
Stadlober [1989, 1990] gives a modification for discrete distributions.
Jones and Lunn [1996] embeds this method into a "general random variate generation framework".
Wakefield et al. [1991] and Stefănescu and Văduva [1987] apply this method to the generation of multivariate distributions.

2. THE METHOD

Enveloping polygons

We are given a distribution with probability density function $f(x) = g(x)/\int g(x)dx$ with convex set $\mathcal{A}_g$. Notice that g must be continuous and bounded since otherwise $\mathcal{A}_g$ would not be convex. To simplify the development of our method we first assume unbounded support for g. (This restriction will be dropped later.)

For such a distribution it is easy to make an enveloping polygon: Select a couple of points $\mathbf{c}_i$, $i = 0, \ldots, n$, on the boundary of $\mathcal{A}$ and use the tangents at these points as edges of the enclosing polygon P^e (see figure 1). We denote the vertices of P^e by

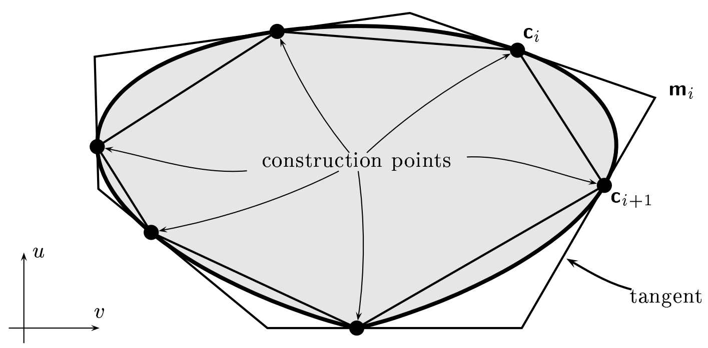


Fig. 1. Polygonal envelope and squeeze for convex set A_g.

$\mathbf{m}_i$. These are simply the intersection points of the tangents. Obviously our choice of the construction points of the tangents has to result in a bounded polygon P^e. The procedure even works if the tangents are not unique for a point (v, u), i.e. if $g(x)$ is not differentiable in $x = v/u$. Furthermore it is very simple to construct squeezes: Take the inside of the polygon P^s with vertices $\mathbf{c}_i$.

Sampling from the enveloping polygon

Notice that the origin $(0, 0)$ is always contained in the polygon P^e. Moreover every straight line through the origin corresponds to an $x = v/u$ and thus its intersection with $\mathcal{A}$ is always connected. Therefore we use $\mathbf{c}_0 = (0, 0)$ for the first construction point and the v-axis as its tangent. To sample uniformly from the enclosing polygon we triangulate P^e and P^s by making segments S_i, $i = 0, \ldots, n$, at vertex $\mathbf{c}_0$. Figure 2 illustrates the situation. Segment S_i has the vertices $\mathbf{c}_0$, $\mathbf{c}_i$, $\mathbf{m}_i$ and $\mathbf{c}_{i+1}$, where $\mathbf{c}_{n+1} = \mathbf{c}_0$ for the last segment. Each segment is divided into the triangle S_i^s inside the squeeze (dark shaded) and a triangle S_i^o outside (light shaded). Notice that the segments S_0 and S_n have only three vertices and no triangles S_0^s and S_n^s.

To generate a random point uniformly distributed in P^e, we first have to sample from the discrete distribution with probability vector proportional to $(|S_0|, |S_1|, \ldots, |S_n|)$,

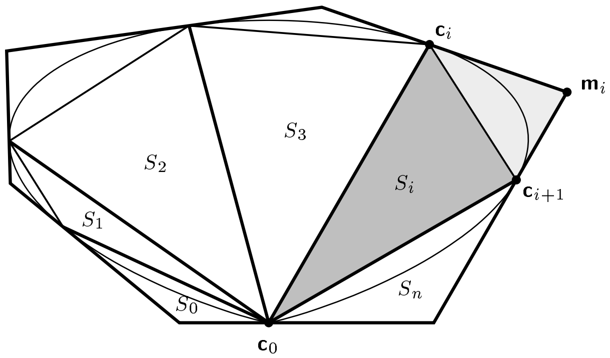


Fig. 2. Triangulation of enveloping polygon

to select a segment and further a triangle S_i^o or S_i^s. This can be done by inversion:

Algorithm `get_segment`

Require: list of segments
1: Generate $R \sim U(0,1)$.
2: Find the smallest k, such that $\sum_{i \le k} |S_i| \ge |P^e|\, R$.
3: **if** $\sum_{i \le k} |S_i| - |P^e|\, R \le |S_k^s|$ **then**
4: **return** triangle S_k^s.
5: **else**
6: **return** triangle S_k^o.

For step 2 *indexed search* (or *guide tables*) is an appropriate method (Chen and Asau [1974], see also Devroye [1986, §III.2.4]).

Uniformly distributed points in a triangle $(\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2)$ can be generated by the following simple algorithm [Devroye 1986, p. 570]:

Algorithm `triangle`

Require: triangle $(\mathbf{v}_0, \mathbf{v}_1, \mathbf{v}_2)$
1: Generate $R_1, R_2 \sim U(0,1)$.
2: **if** $R_1 < R_2$ **then** swap R_1 and R_2.
3: **return** $(1 - R_1)\mathbf{v}_0 + (R_1 - R_2)\mathbf{v}_1 + R_2\mathbf{v}_2$.

For sampling from S_i^s this algorithm can be much improved. Every point in such a triangle can immediately be accepted without evaluating the probability density function and thus we are only interested in the ratio of the components. Since the triangle S_i^s has vertex $\mathbf{c}_0 = (0,0)$, we arrive at

$$x = \frac{v}{u} = \frac{(R_1 - R_2)\, c_{i,1} + R_2\, c_{i+1,1}}{(R_1 - R_2)\, c_{i,2} + R_2\, c_{i+1,2}} = \frac{c_{i,1} + R\,(c_{i+1,1} - c_{i,1})}{c_{i,2} + R\,(c_{i+1,2} - c_{i,2})} \tag{2}$$

where $c_{i,j}$ is the j-th component of vertex $\mathbf{c}_i$, and $R = R_2/R_1$ again is a $(0,1)$-uniform random variate by the ratio-of-uniforms theorem, since $0 \leq R_2 \leq R_1 \leq 1$ [Kinderman and Monahan 1977]. Notice that we save one uniform random number in the domain P^s by this method. Furthermore we can reuse the random number R from routine `get_segment` by $R' = (\sum_{i\leq k} |S_i| - |P^e|\, R)/|S^s_k|$ without risk. We find

$$x = \frac{v}{u} = \frac{|S^s_k|\, c_{i,1} + (\sum_{i\leq k} |S_i| - |P^e|\, R)(c_{i+1,1} - c_{i,1})}{|S^s_k|\, c_{i,2} + (\sum_{i\leq k} |S_i| - |P^e|\, R)(c_{i+1,2} - c_{i,2})} \tag{3}$$

Sampling from P^s can then be seen as inversion from the cumulative distribution function defined by the boundary of the squeeze polygon. Thus for a ratio $|P^s|/|P^e|$ close to 1 we have almost inversion for generating random variates. The inversion method has two advantages and is thus favored by the simulation community (see Bratley, Fox, and Schrage [1983]): (1) The structure of the generator is simple and can easily be investigated (see section 7). (2) These random variates can be used for variance reduction techniques.

Expected number of uniform random numbers

Let $\varrho = |P^e \setminus P^s|/|P^e| = 1 - |P^s|/|P^e|$. Then the expected number of uniform random numbers for generating one ratio v/u is given by $(1-\varrho)+2\varrho = 1+\varrho$. Since we have to reject this ratio if $(v,u) \notin \mathcal{A}$ and $\mathcal{A} \supseteq P^s$ we find for the expected number of uniform random numbers per generated non-uniform variate $E \leq (1+\varrho)/(1-\varrho)$. Notice that by a proper choice of the construction points, ϱ can be made arbitrarily small.

Bounded domain for g

If $x_0 > -\infty$ or $x_1 < \infty$ than the situation is nearly the same. We have to distinguish between two cases:

(1) $f(x_i) > 0$ and $f'(x_i)$ exists for the limit point x_i. We then use x_i as construction point and the respective triangular segment S_0 or S_n is not necessary.

(2) Otherwise we can restrict the triangular segment S_0 or S_n, i.e. we use the tangent line $v - x_i\, u = 0$ at vertex $\mathbf{c}_0 = (0,0)$, instead of the v-axis. Notice that we then have different tangent lines at $\mathbf{c}_0$ for S_0 and S_n.

Adding a construction point

To add a new point for a given ratio $x = v/u$ we need (c_v, c_u) on the "outer boundary" of $\mathcal{A}$ and the tangent line of $\mathcal{A}$ at this point. These are given by the positive root of $u^2 = g(x)$ and the total differential of $u^2 - g(v/u)$, hence

$$\begin{aligned} \text{boundary: } & c_u = \sqrt{g(x)}, \quad c_v = x\, c_u; \\ \text{tangent: } & a_v\, v + a_u\, u = a_c = a_v\, c_v + a_u\, c_u, \\ \text{where } & a_u = 2\,u + g'(x)\, x/u \quad \text{and} \quad a_v = -g'(x)/u \end{aligned} \tag{4}$$

3. RATIO-OF-UNIFORMS AND TRANSFORMED DENSITY REJECTION

Transformed density rejection

One of the most efficient universal methods is *transformed density rejection*, introduced in Devroye [1986] and under a different name in Gilks and Wild [1992], and generalized in Hörmann [1995]. This acceptance/rejection technique uses the concavity of the transformed density to generate a hat function and squeezes automatically by means of tangents and secants. The user only needs to provide the density function and perhaps the (approximate) location of the mode. It can be utilized for any density f where a strictly increasing, differentiable transformation T exists, such that $T(f(x))$ is concave (see Hörmann [1995] for details). Such a density is called *T-concave*; log-concave densities are an example with $T(x) = \log(x)$. Figure 3 illustrates the situation for the standard normal distribution and the transformation $T(x) = \log(x)$. 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. Evans and Swartz [1998] have shown that this technique is even suitable for arbitrary densities provided that the inflection points of the transformed density are known.

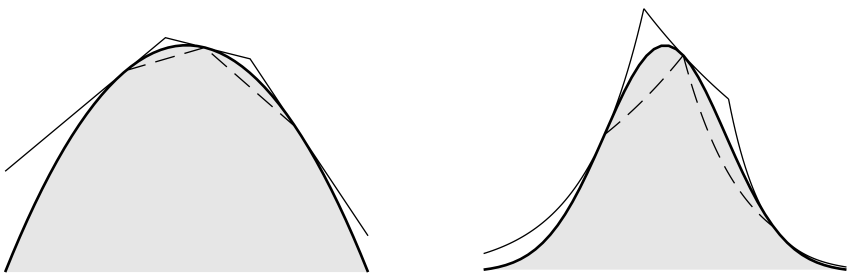


Fig. 3. Construction of a hat function for the normal density utilizing transformed density rejection.

Densities with convex region $\mathcal{A}$

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 $\mathcal{A}_g$. We first provide a proof of theorem 1.

Proof of theorem 1. Consider the transformation

$$\mathbb{R} \times (0, \infty) \to \mathbb{R} \times (0, \infty), \quad (V, U) \mapsto (X, Y) = (V/U, U^2). \tag{5}$$

Since the Jacobian of this transformation is 2, the joint density probability function of X and Y is given by $w(x, y) = 1/(2\,|\mathcal{A}|)$, if $0 < y \le g(x)$, and $w(x, y) = 0$ otherwise. Thus X has marginal density $w_1(x) = \int_0^{g(x)} 1/(2\,|\mathcal{A}|)\, dy = g(x)/(2\,|\mathcal{A}|)$. Consequently $|\mathcal{A}| = 1/2 \int g(x) dx$ and $w_1(x) = f(x)$. Therefore $X = V/U$ has probability density function $f(x)$. □

Transformation (5) maps $\mathcal{A}_g$ one-to-one onto $\mathcal{B}_g = \{(x, y) : 0 < y \le g(x),\ x_0 < x < x_1\}$, i.e. the set of points between the graph of $g(x)$ and the x-axis. Moreover the "outer boundary" of $\mathcal{A}_g$, $\{(v,u): u^2 = g(v/u), u > 0, x_0 < v/u < x_1\}$, is mapped onto the graph of $g(x)$.

THEOREM 2. *$\mathcal{A}_g$ is convex if and only if $g(x)$ is T-concave with transformation $T(x) = -1/\sqrt{x}$.*

PROOF. Since $T(x) = -1/\sqrt{x}$ is strictly monotonically increasing, the transformation $(X,Y) \mapsto (X, T(Y))$ maps $\mathcal{B}_g$ one-to-one onto $\mathcal{C}_g = \{(x,y): y \le T(g(x)), x_0 < x < x_1\}$, i.e. the region below the transformed density. Hence by $T(u^2) = -1/u$,

$$\mathbb{R} \times (0,\infty) \to \mathbb{R} \times (-\infty,0), \quad (V,U) \mapsto (X,Y) = (V/U, -1/U). \tag{6}$$

maps $\mathcal{A}_g$ one-to-one onto $\mathcal{C}_g$. Notice that g is T-concave if and only if $\mathcal{C}_g$ is convex. Thus it remains to show that $\mathcal{A}_g$ is convex if and only if $\mathcal{C}_g$ is convex, and consequently that straight lines remain straight lines under transformation (6).

Let $a\,x + b\,y = d$ be a straight line in $\mathcal{C}_g$. Then $a\,(v/u) - b/u = d$ and $a\,v - d\,u = b$, i.e. a straight line in $\mathcal{A}_g$. Analogously we find for a straight line $a\,v + b\,u = d$ in $\mathcal{A}_g$ the line $a\,x + d\,y = -b$ in $\mathcal{C}_g$. □

Remark 1. By theorem 2 the new universal ratio-of-uniforms method is in some sense equivalent to transformed density rejection. It is a different method to generate points uniformly distributed in the region below the hat function. But in opposition to the new method transformed density rejection always needs at least two uniform random numbers. A similar approach for the transform density rejection, i.e. decomposing the hat function into the squeeze (region of immediate acceptance) and the region between squeeze and hat, does not work well. Sampling from the second part is very awkward and prone to numerical errors [Hörmann 1999].

Since every log-concave density is T-concave with $T(x) = -1/\sqrt{x}$ [Hörmann 1995], our algorithm can be applied to a large class of distributions. Examples are given in table 1. The given conditions on the parameters imply T-concavity on the support of the densities. However the densities are T-concave for a wider range of their parameters on a subset of their support. E.g. the density of the gamma distribution with $b = 1$ is T-concave for all $a > 0$ and $x \ge -1 + \sqrt{2-2a} + a \le 1/2$.

4. CONSTRUCTION POINTS

The performance of the new algorithm depends on a small ratio of $\varrho = |P^e \setminus P^s|/|P^e|$, and thus on the choice of the constructions points for the tangents of the enveloping polygon. There are three possible solutions: (1) simply choose equidistributed points, (2) use an adaptive method, or (3) use optimal points. It is obvious that setup time is increasing and marginal generation time is decreasing from (1) to (3) for a given number of construction points.

Equidistributed points

The simplest method is to choose points $x_1, \ldots, x_n$ with equidistributed angles:

$$x_i = \tan(-\pi/2 + i\,\pi/(n+1)) \qquad i = 1, \ldots, n. \tag{7}$$

If the density function has bounded domain, (7) has to be modified to

$$x_i = \tan(\theta_l + i\,(\theta_r - \theta_l)/(n+1)) \qquad i = 1, \ldots, n \tag{8}$$

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

Table 1. T-concave densities (normalization constants omitted)

where $\tan(\theta_l)$ and $\tan(\theta_r)$ are the left and right boundary of the domain (see also section 2). If the distribution has a mode $m \neq 0$ use the points $x_i + m$ (and shift the domain of the density function by $-m$). For x_i close to 0 a point is approximately the arithmetic mean of its neighbors; for very large points a point is approximately the harmonic mean of its neighbors. Numerical simulations with several density functions have shown that this is an acceptable good choice for construction points for several distributions where the ratio of length and width of the minimal bounding rectangle is not too far from one.

To get an idea about the relationship between ϱ_n and the number of construction points n, we look at the following special case: Assume 0 is the mode of a T-concave monotonically decreasing density f with domain $[0,\infty)$. Let (a,b) be the right upper vertex of its minimal bounding rectangle $\mathcal{R}$, i.e., $a = \sup_{x\geq 0} x\sqrt{f(x)}$ and $b = f(0) = \max_{x\geq 0} f(x)$. Furthermore assume that $x_0 = 0$ and that the slope of the tangent line at the mode is 0 (such a tangent always exists). The region between enveloping polygon and squeeze consists of n triangles, each of which with base line c_i (consisting of an edge of the squeezing polygon) and base angles α_i and β_i, respectively. Due to the convexity of the region $\mathcal{A}$ we find $\sum c_i \leq 2a + b$, $\sum(\alpha_i + \beta_i) \leq \pi$ and $\alpha_i + \beta_i < \pi$. Moreover there is at most one triangle not completely inside $\mathcal{R}$. For the areas of these triangles we find

$$A_i = \frac{c_i^2}{2} \cdot \frac{\tan\alpha_i\ \tan\beta_i}{\tan\alpha_i + \tan\beta_i}, \qquad \text{for } \alpha_i, \beta_i \notin \{0, \pi/2\}. \tag{9}$$

The total sum of areas will become as large as possible, when the base angles in all but one triangles become zero, i.e., the areas become zero. Figure 4 shows the limit case. Using (9) we find

$$\rho_n < \frac{a^2 + b^2}{a\, b}\, \frac{\tan(\frac{\pi}{n})}{1 + \frac{a}{b}\tan(\frac{\pi}{n})} \approx \frac{a^2+b^2}{a\, b}\left(\frac{\pi}{n} - \frac{a}{b}\left(\frac{\pi}{n}\right)^2 + O(n^{-3})\right) \tag{10}$$

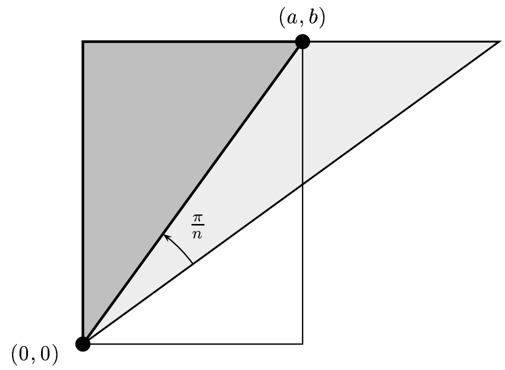


Fig. 4. Worst case for ratio ϱ_n for given n

Adaptive rejection sampling

Gilks and Wild [1992] introduces the ingenious concept of *adaptive rejection sampling* for the problem of finding appropriate construction points for the tangents for the transformed density rejection method. Adopted to our situation it works in the following way: Start with (at least) two points on both sides of the mode and sample points from the enveloping polygon P^e. Add a new construction point at $x = v/u$ whenever a point (v, u) falls into $P^e \setminus P^s$ until a certain stopping criterion is fulfilled, e.g. the maximal number of construction points or the aimed ratio $|P^s|/|P^e|$ is reached. To ensure that the starting polygon P^e is bounded, a construction point at (or at least close to) the mode should be used as a third starting point.

Sampling a point in the domain $P^e \setminus P^s$ is much more expensive than sampling from the squeeze region. Firstly the generation of a random point requires more random numbers and multiplications; secondly we have to evaluate the density and check the acceptance condition. Thus we have to minimize the ratio $\varrho = |P^e \setminus P^s|/|P^e|$ which is done perfectly well by adaptive rejection sample, since by this method the region $\mathcal{A}$ is automatically approximated by envelope and squeeze polygon. The probability for adding a new point in a segment S_i depends on the ratio $|S_i^o|/|P^e|$, i.e. from the probability to fall into S_i^o. Hence the adaptive algorithm tends to insert a new construction point where it is "more necessary".

Obviously the ratio ϱ_n is a random variable that converges to 0 almost surely when the number construction points n tends to infinity. A simple consideration gives $\varrho_n = O(n^{-2})$ [Leydold and Hörmann 1998]. Figure 5 shows the result of a simulation for the standard normal distribution with (non optimal) starting points at $x = \pm 0.4$ (50 000 samples). ϱ_n is plotted against the number n of construction points. The range of ϱ_n is given by the light shaded area, 90%- and 50%-percentiles are given by dark shaded areas, median by the solid line.

We have run simulations with other distributions and starting values and have made the observation that convergence is even faster for other (non-normal) distri-

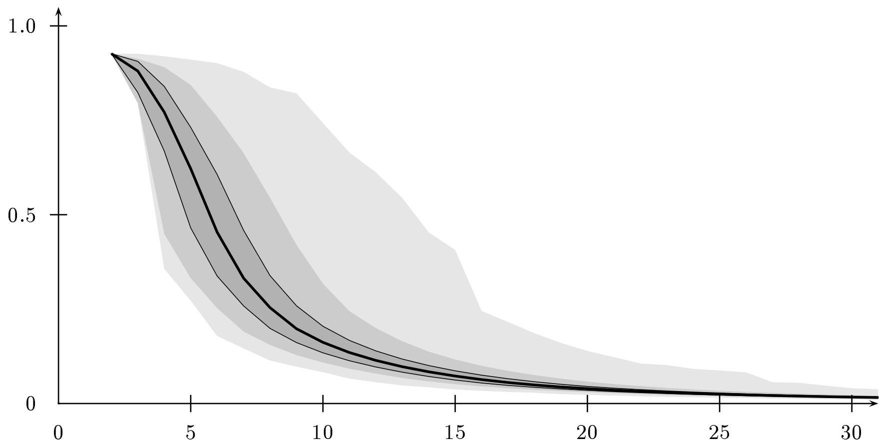


Fig. 5. Convergence of the ratio $\varrho_n = |P^e \setminus P^s|/|P^e|$ for the standard normal distribution with starting points at $x = \pm 0.4$. (50 000 samples)

butions. However analytical investigations are interesting. Upper bounds for the expected value of ϱ_n are an open problem.

Optimal construction points

By theorem 2 the area between hat and squeeze of the transformed density rejection method is mapped one-to-one and onto the region $P^e \setminus P^s$. Thus we can use methods for computing optimal construction points for transformed density rejection for finding optimal envelopes for the new algorithm. If only three construction points are used, see Hörmann [1995]. If more points are required, Derflinger and Hörmann [1998] describe a very efficient method. However some modification are necessary. Improvements over adaptive rejection sampling are rather small and can be seen in figure 5 (The lower boundary of the range gives a good estimate for the optimal choice of construction points.).

5. THE ALGORITHM

Algorithm `arou` consists of three main parts:

(1) Construct the starting enveloping polygon P^e and squeeze polygon P^s in routine `arou_start`. Here we have to take care about a possibly bounded domain and the two cases described in section 2. The starting points must be provided (e.g. by using equidistributed points as describes in section 4).

(2) Sample from the given distribution in routine `arou_sample`.

(3) Add a new construction point with routine `arou_add` whenever we fall into $P^e \setminus P^s$.

We store the envelope into a list of segments (table 2). When using this algorithm we first have to initialize the generator by calling `arou_start`. Then sampling can be done by calling `arou_sample`.

PARAMETER	VARIABLE	DEFINITION / REMARK
left construction point	$\mathbf{c}_i$	
right construction point	$\mathbf{c}_{i+1}$	pointer, stored in next segment
tangent at left point	$\mathbf{a}_i$	(a_v, a_u, a_c), see (4)
tangent at right point	$\mathbf{a}_{i+1}$	pointer, stored in next segment
intersection point	$\mathbf{m}_i$	
area inside/outside squeeze	A_i^{in}, A_i^{out}	$\lvert S_i^s\rvert$, $\lvert S_i^o\rvert$
accumulated area	A_i^{cum}	$\sum_{j\leq i} \lvert S_j\rvert$, for fast inversion

Table 2. object segment

Algorithm `arou_start`

Require: density $f(x)$, derivative $f'(x)$;
domain (x_0, x_k), construction points $x_1, \ldots, x_{k-1}$.

$\mathbf{c}_0 \leftarrow (0,0)$; $\mathbf{c}_{k+1} \leftarrow (0,0)$; /* origin */
$\mathbf{a}_0 \leftarrow (\cos(\arctan(x_0)), -\sin(\arctan(x_0)), 0)$. /* tangent line for S_o */
$\mathbf{a}_{k+1} \leftarrow (\cos(\arctan(x_k)), -\sin(\arctan(x_k)), 0)$. /* tangent line for S_k */
for $i = 1, \ldots, k$ **do** /* all construction points x_i */
  if $f(x_i) > 0$ and $\exists f'(x_i)$ **then**
    $c_{i,2} \leftarrow \sqrt{f(x_i)}$; $c_{i,1} \leftarrow x_i\, c_{i,2}$.
    $a_{i,v} \leftarrow -f'(x_i)/c_{i,2}$; $a_{i,u} \leftarrow 2\,c_{i,2} + x_i\, f'(x_i)/c_{i,2}$; $a_{i,c} \leftarrow c_{i,1}\, a_{i,v} + c_{i,2}\, a_{i,u}$.
    add S_i to list of segments.
  /* else x_i cannot be used as construction point */
for all segments S_i **do**
  insert $\mathbf{c}_{i+1}$ and $\mathbf{a}_{i+1}$. /* already stored in next segment in list */
  compute $\mathbf{m}_i$.
  compute A_i^{in}, A_i^{out} and A_i^{cum}.
check if polygon P^e is bounded.
return list of segments.

Algorithm `arou_sample`

Require: density $f(x)$, list of segments S_i.

loop
  generate $R \sim U(0,1)$.
  find smallest i such that $A_i^{\text{cum}} \geq |P^e|\, R$. /* use guide table */
  $R \leftarrow A_i^{\text{cum}} - |P^e|\, R$.
  if $R \leq A_i^{\text{in}}$ **then** /* inside squeeze, S_i^s */
    return $(A_i^{\text{in}}\, c_{i,1} + R\,(c_{i+1,1} - c_{i,1}))/(A_i^{\text{in}}\, c_{i,2} + R\,(c_{i+1,2} - c_{i,2}))$. /* eq. (3) */
  else /* outside squeeze, S_i^o */
    $R_1 \leftarrow (R - A_i^{\text{in}})/A_i^{\text{out}}$.
    generate $R_2 \sim U(0,1)$.
    if $R_1 > R_2$ **then swap** R_1, R_2.
    $R_3 \leftarrow 1 - R_2$, $R_2 \leftarrow R_2 - R_1$.
    $U \leftarrow c_{i,2}\, R_1 + c_{i+1,2}\, R_2 + m_{i,2}\, R_3$.
    $X \leftarrow (c_{i,1}\, R_1 + c_{i+1,1}\, R_2 + m_{i,1}\, R_3)/U$.
    if number of segments < maximum **then**
      call `arou_add` **with** X, S_i.

if $U^2 \leq f(X)$ **then**
  return X.

Algorithm arou_add

Require: density $f(x)$, derivative $f'(x)$; new construction point x_n; segment S_r.

if $f(x_n) = 0$ or $\nexists f'(x_n)$ **then** /* cannot add this point */
  return
$c_{n,2} \leftarrow \sqrt{f(x_n)}$; $c_{n,1} \leftarrow x_n\, c_{n,2}$.
$a_{n,v} \leftarrow -f'(x_n)/c_{n,2}$; $a_{n,u} \leftarrow 2{*}c_{n,2}{+}x_n\, f'(x_n)/c_{n,2}$; $a_{n,c} \leftarrow c_{n,1}\, a_{n,v}{+}c_{n,2}\, a_{n,u}$.
insert S_n into list of segments. /* Take care about $\mathbf{c}_{i+1}$ and $\mathbf{a}_{i+1}$ */
remove old segment S_r from list.
compute $\mathbf{m}_n$.
compute A_n^{in} and A_n^{out}.
for all segments S_i **do**
  compute A_i^{cum}.
return new list of segments.

To implement this algorithm, a linked list of segments is necessary. Whenever A_i^{cum} are (re-)calculated, a guide table has to be made. Using linear search might be a good method for finding S_i when only a few random variates are sampled.

Special care is necessary when $\mathbf{m}_i$ is computed in `arou_start` and `arou_add`. There are three possible cases for numerical problems when solving the corresponding linear equation:

(1) The vertices $\mathbf{c}_i$ and $\mathbf{c}_{i+1}$ are very close and (consequently) $|S_i|$ is very small. Here we simply reject $\mathbf{c}_{i+1}$ as new construction point.
(2) $\mathbf{c}_i$ and $\mathbf{c}_{i+1}$ are very close to $\mathbf{c}_0 = (0,0)$. Again $|S_i|$ is very small.
(3) The boundary of $\mathcal{A}$ between $\mathbf{c}_i$ and $\mathbf{c}_{i+1}$ is almost a straight line and A_i^{out} is (almost) 0. In this case we set $\mathbf{m}_i = 1/2\,(\mathbf{c}_i + \mathbf{c}_{i+1})$.

A possible way to define "very small" is to compare such numbers with the smallest positive ε with $(M + \varepsilon) \neq M$ in the used programming language. M denotes the magnitude of the maximum of the density function. (In ANSI C for $M = 1$, ε is defined by the macro `DBL_EPSILON`.)

It is important to check whether $\mathbf{m}_i$ is on the outer side of the secant through $\mathbf{c}_i$ and $\mathbf{c}_{i+1}$. This condition is violated in `arou_start` when the polygon P^e is unbounded. It may be violated in `arou_start` and `arou_add` when $\mathcal{A}$ is not convex.

6. COMPUTATIONAL EXPERIENCES

A version of algorithm `arou` is coded in C and available by email request from the author. We have compared it to two other universal methods: transformed density rejection with $T(x) = -1/\sqrt{x}$ (`tdr`) and the table method (`tabl`) by Ahrens [1993] (However we have modified split B by replacing the recursive search by $\bar{x} = \tan((\arctan(x_1) + \arctan(x_2))/2)$, a mean value similar to eq. (8).) Notice that this method is only applicable for densities with bounded support. Thus we have to cut unbounded domains (we used -10^{50} and 10^{50}, respectively). The main goal for the implementations of all three algorithms is to get a flexible and robust program. Moreover, for small ρ, generation should be close to inversion. Thus linked lists of structures have been used. Constructions like storing all data in a single array and using sophisticated indices to find these again (as described in Ahrens [1993]) have been avoided. For the underlying uniform random number generator we have used the library prng-2.2 [Lendl 1997]. We used generator `CMRG` by L'Ecuyer [1996], a combined multiple recursive random number generator with a long period (generation time 0.31 μs).

The timings have been performed on a PC (AMD K2 400 MHz, Linux 2.0.36, gcc version 2.95.1). We started with 30 construction points, using the "equidistribution rule" for `arou` and `tdr`, and "equiarea rule with splitting" for `tabl` (see Ahrens [1993] for details). Tables 3 and 4 show the result for some distributions. We then continued with adaptive rejection sampling to get more construction points until $\varrho \leq 0.01$ (Zaman [1996] has suggested this procedure for the table method). Table 5 shows the number of the resulting segments and intervals, respectively, and the marginal generation times for the generator, when no more construction points are added.

	`arou`		`tdr`		`tabl`	
	ϱ	#urn	ϱ	#urn	ϱ	#urn
Normal	0.021	1.029	0.021	2.014	0.192	1.334
Student(2)	0.022	1.028	0.022	2.013	0.561	2.475
Cauchy	0.067	1.068	0.067	2.002	0.788	5.231
Gamma(10)	0.094	1.137	0.094	2.079	0.207	1.362
Beta(10,20)	0.022	1.029	0.022	2.016	0.160	1.265

Table 3. ϱ and average number of uniform random numbers for 30 fixed construction points using "equidistribution rule" (`arou`, `tdr`) and "equiarea rule with splitting" (`tabl`), respectively.

	`arou`		`tdr`		`tabl`	
	t_s (μs)	t_g (μs)	t_s (μs)	t_g (μs)	t_s (μs)	t_g (μs)
Normal	182	0.77	261	1.53	110	1.03
Student(2)	230	0.79	303	1.55	124	2.52
Cauchy	178	0.81	251	1.55	91	3.74
Gamma(10)	220	0.92	295	1.68	127	1.16
Beta(10,20)	235	0.78	312	1.54	130	1.10

Table 4. Setup time (t_s) and average marginal generation time (t_g) (sample size 10^6) for 30 construction points (see table 3).

As expected, tables 3 and 4 show that method `arou` is superior to `tdr`. It requires fewer uniform random numbers. Moreover since it requires less computations its setup time is shorter and the marginal generation is much faster. Table 4 demonstrates the advantage of the better fitting hat of method `arou` compared to `tabl`. A considerably lower number of segments is required. This results in a faster set-up step for a fixed small ϱ. This observation is supported by the theoretical result that

	arou		tdr		tabl	
	t_g (μs)	segments	t_g (μs)	intervals	t_g (μs)	intervals
Normal	0.75	(40,46)	1.51	(41,48)	0.78	(573, 598)
Student(2)	0.76	(37,44)	1.52	(38,46)	0.80	(1057,1093)
Cauchy	0.75	(34,40)	1.52	(35,43)	0.81	(1559,1601)
Gamma(10)	0.76	(49,56)	1.50	(49,57)	0.79	(562, 587)
Beta(10,20)	0.76	(44,50)	1.50	(45,52)	0.79	(540, 564)

Table 5. Adding construction points by adaptive rejection sampling until $\rho \leq 0.01$. Average marginal generation time (when $\rho = 0.01$) and 90%-percentile for respective number of segments and intervals (sample size 10^5).

ϱ is $O(1/n^2)$ for `arou` and `tdr` but $O(1/n)$ for `tabl`. The average generation times that include setup time and rebuilding the guide tables for sample size 10^5 have been found about the same as the marginal generation time for `arou` and `tdr`, but are considerable larger for `tabl` (more than 100% larger for Cauchy distribution).

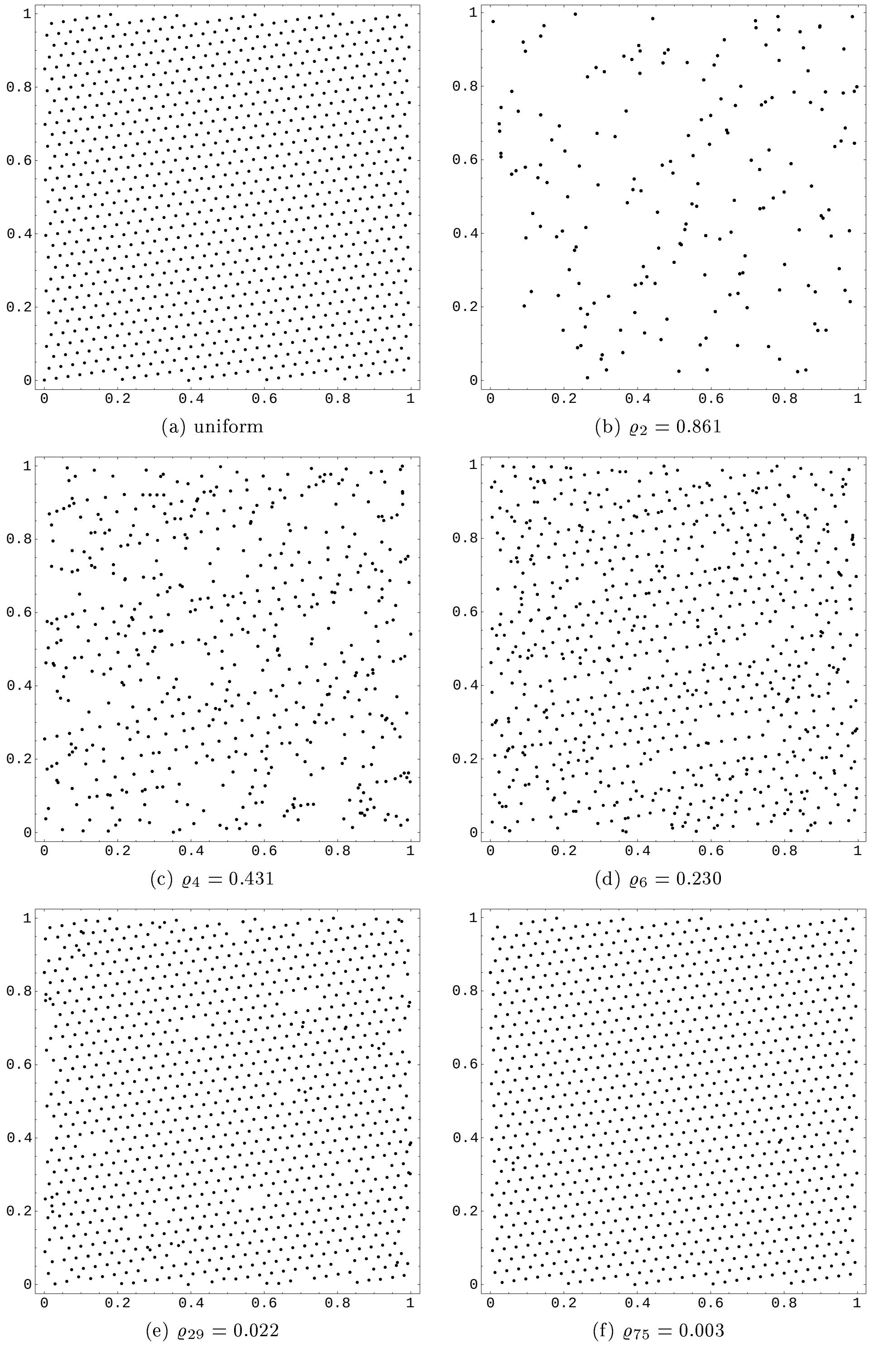
7. A NOTE ON THE QUALITY OF RANDOM NUMBERS

The new algorithm is a composition method, similar to the acceptance-complement method (see Devroye [1986, § II.5]). We have $f(x) = (1 - \varrho)\, g_s(x) + \varrho\, g_o(x)$, where $g_s(x)$ is the distribution defined by the squeeze region and $g_o(x) = f(x) - g_s(x)$. By theorem 1 the algorithm is exact, i.e. the generated random variates have the required distribution. However defects in underlying uniform random number generators may result in poor quality of the non-uniform random variate. Moreover the transformation into the non-uniform random variate itself may cause further deficiencies.

Although there is only little literature on this topic, the ratio-of-uniforms method in combination with any linear congruental generator (LCG) was reported to have defects [Hörmann 1994a; Hörmann 1994b]. Due to the lattice structure of random pairs generated by an LCG there is always a hole without a point with probability of order $1/\sqrt{M}$, where M is the modulus of the LCG.

Random variates generated by the inversion inherit the structure of the underlying uniform random numbers and consequently their quality. We consider this as a great advantage of this method, since *generators whose structural properties are well understood and precisely described may look less random, but those that are more complicated and less understood are not necessarily better. They may hide strong correlations or other important defects. ... One should avoid generators without convincing theoretical support.* This statement by L'Ecuyer [1998] on building uniform random number generator is also valid for non-uniform distributions. Other methods *may* have some hidden inferences, which make a prediction of the quality of the resulting non-uniform random numbers impossible [Leydold et al. 2000].

Notice that a random variate with density $g_s(x)$ is generated by inversion. Thus as ratio ϱ tends to 0, most of the random variates are generated by inversion by the new algorithm. As an immediate consequence for small ϱ the new generator avoids the defects of the basic ratio-of-uniforms method. Figure 6 shows scatter plots of all overlapping tuples $(u_0, u_1), (u_1, u_2), (u_2, u_3), \ldots$ using the "baby" generator $u_{n+1} = 869\, u_n + 1 \bmod 1024$. (a) shows the underlying generator. (b)–(f) show



(a) uniform
(b) $\varrho_2 = 0.861$
(c) $\varrho_4 = 0.431$
(d) $\varrho_6 = 0.230$
(e) $\varrho_{29} = 0.022$
(f) $\varrho_{75} = 0.003$

Fig. 6. Scatter plots of "baby" generator $u_{n+1} = 869\, u_n + 1 \bmod 1024$ (a) and of normal variates using algorithm `arou` with 2, 4, 6, 29 and 75 equidistributed construction points (b–f).

the tuples $(\Phi(u_0), \Phi(u_1))$, $(\Phi(u_1), \Phi(u_2))$, $(\Phi(u_2), \Phi(u_3))$, ... for different number of construction points using the equidistribution method (Φ denotes the cumulative distribution function of the standard normal distribution).

We have made an empirical investigation using M-tuple tests [Good 1953; Marsaglia 1985] in the setup of Leydold, Leeb, and Hörmann [2000] with the standard normal distribution and various numbers of construction points. We have used a linear congruential generator `fish` by Fishman and Moore [1986], an explicit inversive congruential generator [Eichenauer-Herrmann 1993], and a twisted GFSR generator (`tt800` by Matsumoto and Kurita [1994]); at last the infamous `randu` (again an LCG) as an example of a generator with bad lattice structure (see Park and Miller [1988]). These tests have demonstrated that for small ratio ϱ, the quality of the normal generators are strongly correlated with the quality of the underlying uniform random number generator. Especially, using `randu` results in normal generator of bad quality. Notice however that this correlation does not exist, if ϱ is not close to 0. Indeed, using only 2 or 4 construction points results in a normal generator which might be better (e.g. `fish` in our tests) or worse (e.g. `randu`) than the underlying generator.

8. POSSIBLE VARIANTS

Non-convex region

The algorithm can be modified to work with non-convex region $\mathcal{A}_f$. Adapting the idea of Evans and Swartz [1998] we have to partition $\mathcal{A}_f$ into segments using the inflection points of the transformed density with transformation $T(x) = -1/\sqrt{x}$. In each segment of $\mathcal{A}_f$ where $T(f(x))$ is not concave but convex, we have to use secants for the boundary of the enveloping polygon P^e and tangents for the squeeze P^s (see figure 7). Notice that the squeeze region in such a segment is a quadrangle $\mathbf{c}_0\mathbf{c}_i\mathbf{m}_i\mathbf{c}_{i+1}$ and has to be triangulated. The changes of algorithm `arou` are straight forward: (1) Include $A_i^{\text{in},l}$ and $A_i^{\text{in},r}$ into object 2; (2) compute $A_i^{\text{in},l}$ and $A_i^{\text{in},r}$ instead of A_i^{in} for all non-convex segments of $\mathcal{A}$; (3) in `arou_sample`, when we generate a point inside the squeeze polygon of a non-convex segment, we first have to decide by means of $A_i^{\text{in},l}$ and $A_i^{\text{in},r}$ which triangle (left of right) has to be used.

Multivariate distributions

Wakefield, Gelfand, and Smith [1991] and Stefănescu and Văduva [1987] have generalized the ratio-of-uniforms method to multivariate distributions. Both use rejection from an enclosing multidimensional rectangle. However the acceptance probability decreases very fast for higher dimension. For multivariate normal distribution in four dimension it is below 1%. Using polyhedral envelopes similar to Leydold and Hörmann [1998] or Leydold [1998] is possible and increases the acceptance probability. However this requires some additional research.

ACKNOWLEDGMENTS

The author wishes to thank Hannes Leeb for helpful discussions on the quality of random number generators.

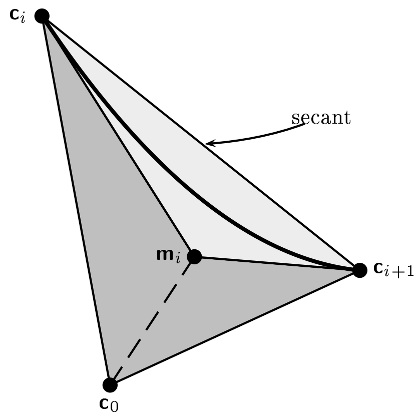


Fig. 7. Non-convex set A_g. The squeeze polygon (dark shaded area) has to be divided into two triangles.

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