Automatic generation of non-uniform random variates for arbitrary pointwise computable probability densities by tiling

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Abstract

We present a rejection method based on recursive covering of the probability density function with equal tiles. The concept works for any probability density function that is pointwise computable or representable by tabular data. By the implicit construction of piecewise constant majorizing and minorizing functions that are arbitrarily close to the density function the production of random variates is arbitrarily independent of the computation of the density function and extremely fast. The method works unattended for probability densities with discontinuities (jumps and poles). The setup time is short, marginally independent of the shape of the probability density and linear in table size. Recently formulated requirements to a general and automatic non-uniform random number generator are topped. We give benchmarks together with a similar rejection method and with a transformation method.

1 Introduction and background

This article introduces a setup method for a rejection algorithm for the production of random numbers with an arbitrary probability density functions (PDF) with finite support and that is at least pointwise computable. The key feature is fast production of random variates in computational applications and simple applicability to any probability density with any number of modes. The principle consists of covering the surface under the PDF with equal tiles for which no a priori information is required. The speed of random number production is arbitrarily independent of the shape and computational cost to evaluate the PDF. Prior to the introduction of the method we give a brief review of the subject, some existing methods and terminology.
The two topics of uniform and non-uniform random number generators (RNG) are rather disjoint, with little overlap in the literature and the associated communities. This is not surprising as the respective problems are quite distinct and can be considered as subsequent tasks. A non-uniform RNG requires a uniform one, usually employed as a black box, and the quality of the former depends on the quality of the latter. Contrary to what one might have expected, the past 15 years have seen a considerable development of uniform RNGs (URNGs). For almost half a century since the beginning of the age of computing in the 1950s, uniform random numbers have been produced with linear congruential generators, which are based on the recurrence relation \( I_{j+1} = aI_j + c \mod m \). After shortcomings began to be noticed in the 1960s, much effort went into reducing them by tuning the parameters, especially \( a \) and \( m \). However it took decades until alternative algorithms were discovered, and then over a dozen appeared within a short time, with the possibility of improving the quality by combining different methods: the XOR shift URNG [28], the multiply with carry URNG, the linear feedback shift register URNG, etc. For reviews, see Refs. [7, 14, 16, 17, 39].

Fast generation of non-uniform random numbers is important in e.g. Monte Carlo simulations [1, 7, 11, 13, 17, 22, 23, 31]. Statistical theory shows how one can produce random variates for any meaningful distribution. Nevertheless, intelligent mathematical but also purely computational methodology was developed to achieve speed for well known analytical and invertible distributions, for non-analytic but transformable distributions and also for empirical PDFs that only exist as tabular data. In the earlier days of computing any progress was taken very seriously [26, 27, 29, 30] in applied mathematics but also more recently new perspectives on seemingly converged methodology on, for example, Gaussian distributed random numbers can be found [19, 40, 42].

A plethora of mathematically involved publications was inspired by the practitioner’s need to increase the speed and quality of non-uniform random number production in applications of statistical computing. Another big driving force is simplicity of application. Special requirements of initialisation for example are a nuisance. Each context and application provides different and often opposite challenges. For example the famous Ziggurat method by Marsaglia [31] and its implementation by Marsaglia and Tsang [32] is a non-truncating method within the narrow class of symmetric, strictly decreasing, analytic and invertible densities. Other algorithms existed long before, but the method’s appeal is that the specific implementation is even faster than any other that is specialized entirely on exponential or normal distributed numbers. The required initial data structure setup depends on parameters that so far have been published only for the exponential and normal distributions [32] and are difficult to derive automatically [10]. A more general approach is taken by Ahrens [1]. This well-known method is able to process any tabular data that fulfills few restrictions on smoothness, but the setup and production of random numbers is slower. The latter two methods are related to more general strip or slice methods — already existing for a long time [7, 29, 30, 35, 38] — but are of much higher importance in computational applications. It should be kept in mind that information on the speed of a method is only meaningful with respect to a particular implementation and hardware. Some famous methods are actually specialized implementations that rely on the cache memory of contemporary processors.
There are many collections of specialized non-uniform random number generators, usually more than one for a particular class of PDFs, each of them consisting of tailored code. The generators can be categorized into two classes:
a) A setup of some data structure is carried out before the first random variate is drawn, and 
b) a setup is not needed, e.g. with PDFs for which inversion methods exist. Clearly, any “universal” method will need a setup, as explained well for instance in Ref. [24].

In statistical computing the user taps from these collections of software choosing a particular generator. Ideally one can also choose gradually between large setup time and fast generation of random numbers or fast setup and slow generation. The drawbacks of such collections can be huge codes, each bug prone, and the increasingly intractable specialties of the requirements for the setup. Furthermore, the classes of available distributions are limited in the end. The ultimate goal is a universal, easy to use and also fast black box generator [24].

The definition and limitations of a universal random number generator, however, is often imprecise in many publications. For example, it does not have any built-in knowledge of the PDF, except that a meaningful PDF can be known only in as much as the number of modes is not infinite [2] and that the modes are not infinitely thin, i.e. meaningless delta-like functions. For universal applicability all transformation methods drop out because they cannot be found automatically by a general algorithm. Therefore, in the general case only some approximation like pointwise data will be available to represent the PDF, implying that the support of the distribution cannot be infinite either. Any computational approach subdues to this restriction. If the PDF can only be evaluated at horrendous costs and no inversion method exists, then no procedure will be able to produce usefully random numbers. Thus, we can assume that the evaluation cost of the PDF for the appropriate number of points is within a similar order of magnitude as the overall task within which the random numbers are used, e.g. a Monte Carlo calculation.

In some cases of PDFs with infinite support truncation of the probability density can be justified with statistical negligibility of the tails. In few cases of distributions with infinite support and where the PDF is at best pointwise computable as with the Lévy distribution [36, 37], which we use as a benchmark, transformation methods that do sample the infinite range were found [6], at least within overflow limitations. Such heavy-tailed distributions deserve attention if truncated early unless justified (or required) by the application [4, 5, 25]; however, this aspect is largely left undiscussed in the literature. State of the art methods, e.g. Refs. [7, 11, 13, 17, 22, 23], construct in the setup phase a majorizing (or envelope or comparison) function and usually also a minorizing (or squeeze) function (see Sec. 2.2 for an introduction) with secants or other segmentations to be used within a rejection technique with look-up tables. In addition to truncation, in many methods it is often also required to know the approximate or even exact location of the mode (of which mostly only one is allowed), while the method is still declared to be suitable for “arbitrary PDFs” [9, 20]. More limitations to “general methods” are explained in Ref. [9], where it is argued that the modes of the PDF must be known beforehand for certain techniques to be suitable for “arbitrary densities”. The same authors also construct “general algorithms” that depend on concavity properties and analyticity of the density. It is common in several methods, e.g. adaptive procedures for log-concave distributions to use the value of maximum density explicitly in the setup of the approximation of the comparison function [7]. Another example
is the transformed density method \cite{21}, that employs a strictly monotonically increasing differentiable transform such that the transformed PDF is concave. This method is also considered universal. In the improved ratio of uniforms method \cite{20} the setup is restricted to certain classes of distributions if the required transform of variables must yield a region that can be sampled efficiently. In some cases one often resorts to a rejection technique and the concept of squeeze functions, as also employed in this paper, to improve the situation. Yet another general and adaptive approach constructs a polynomial approximation of the inverse distribution function in \( X = F^{-1}(U) \) that is stored in tables to be used for interpolation during production \cite{12}. For the class of log-concave distributions Ref. \cite{10} introduces piecewise exponentials for the approximation of the majorizing and minorizing functions using previously sampled points of the density function. This method however is dedicated to the context of Gibbs sampling where each variate is usually drawn from different densities. Finally, closing the topic of piecewise approximation, we mention the approximation of arbitrary densities via a mixture of simpler densities. An interesting example is the triangular approximation giving a piecewise linear approximation of the target density via many overlapping triangle densities, which recently was also implemented in hardware \cite{41}. The most generally applicable method published so far that is also fast is due to Ahrens \cite{1,2}. It can deal with more than one mode without a priori information on the modes.

Overall we find inevitably that methods titled “universal”, “automatic”, “black box”, “out of the box” and combinations thereof clearly cannot sample an infinite support of the PDF, are restricted to certain classes of density functions or are not automatic out of the box. But this verdict is much less restrictive in realistic applications of statistical computing where the requested distributions can always be represented for example in terms of (interpolated) pointwise data or other approximations to any computationally sensible accuracy and finite support limits. We stress that approximations of the density function via previous sampling of points or the approximation of the inverse distribution function \( F^{-1} \) as mentioned above are like other similar concepts a common approach in the field of non-uniform random numbers \cite{7,12}. It is accepted to truncate the originally infinite support, if statistically justified. Moreover, if the PDF is given as an arbitrarily accurate approximation, the location of extrema can always be determined within any required accuracy in finite time. Our method is applicable in this context and belongs to the type of rejection and segmentation methods as the ones by Ahrens \cite{11} and Marsaglia \cite{32}. In this context and for our claim we can therefore continue to speak of arbitrary PDFs since this nomenclature is widely accepted within the literature. Therefore, in the quest for a universal random number generator, a method can be called universal if it can process arbitrary finite density function data without any further information. Techniques that take finite samples of the desired distribution and then try to match this distribution \cite{20} are not discussed here.

Lately easy applicability has become more important. The initial motivation for this work was to overcome the setup difficulty of the Ziggurat method for the general symmetric monotonic decreasing case. Eventually, we developed a simpler method for a significantly more general class of PDFs, at the cost of a moderate performance penalty due to larger memory requirement as compared to the original Ziggurat implementation of Ref. \cite{32} and to specialized transformation methods, were available.
With the intention to provide a quintessence of recent research and demands of statistical computing a wish-list of requirements to a universal random number generator was presented in Ref. [24], which we quote here:

1. Only one piece of code, debugged only once.
2. By a simple parameter choose between fast setup and slow generation or long setup time and fast generation.
3. It can sample from truncated distributions.
4. The rejection rate can be made as close to zero as desired, i.e. as close to inversion as one wants.
5. The setup time is independent of the density function and is faster than many specialized generators.
6. The quality of the non-uniform random numbers is as good as the underlying uniform random numbers.

Point 5 should be made more precise. It refers to the independence of the shape of the density function, but a density with complicated shape usually requires more information, in particular in regions of high curvature. If the input size increases, the setup time is indeed allowed to grow. There is no obvious universal measure that gives the minimum input size required for the suitable representation of a function. This is responsibility of the scientist. Several of the methods mentioned in the above overview are considered to meet these requirements. This is also the case with the method presented here plus additional relaxations with respect to the properties of the PDF.

In Sec. 2 the tiling is introduced along with some numerical considerations, an explanation of the role of the squeeze function, and a proof of correctness. Sec. 3 shows that the tiling procedure is capable of dealing unattended with poles and other discontinuities. Sec. 4 gives benchmarks of typical and a-typical situations. Sec. 5 summarizes and provides a short discussion. We chose for comparison well-known methods for specialized distributions (Gaussian and exponential) but also a difficult non-analytic distribution (Appendix) for which a transformation method is available. We explain computational issues that are usually ignored but are decisive for performance. This serves in placing the tiling method into the right context among other methods with respect to speed and applicability.

2 The tiling and numerical considerations

2.1 The tiling procedure

For any computational task a PDF with finite support, even one with a non-invertible distribution for which no specialized method exists, can be represented either as a) a sufficiently good approximation that can be evaluated sufficiently fast, e.g. by series expansion or polynomials, or b) as tabular data for interpolation. Any feature of a meaningful PDF $f(x)$ can be represented in the latter case by varying the sampling density of the tabular data that represents the PDF in the form $(x_1, f(x_1)), (x_2, f(x_2)), \ldots$. However, since the tiling is completely
independent of such considerations, we will simply speak of “evaluating \( f(x) \)”. Furthermore, it can safely be assumed that the PDF can be evaluated in a finite time comparable to the duration of the application within which the random variates are to be used. With these prerequisites the determination of local extrema is achievable in \( O(N) \) where \( N \) is the number of data points.

For the following considerations the integral over the density function is required only up to a constant factor \( C = \int_a^b f(x)dx \). The rejection method does not require \( C = 1 \). The tiling concept is simple, see Fig. 1. The area under the PDF \( f(x) \), \( x \in [a, b] \), is covered with rectangular tiles of equal area. The procedure starts from one single tile \( b-a \) wide and \( \max(f(x)) \) high. Choosing an initial tile larger than required by the support and the maximum did not show significant influence on the outcome in all cases we tested. The initial tile is split into four equal tiles, and so on recursively. At each refinement cycle all tiles are split. Those that lie entirely above the PDF are discarded in each cycle. The splitting can be stopped once a given accuracy of the covering is reached; Sec. 2.2 explains the details of the calculation of this condition. Fig. 1 shows a truncated asymmetric Lévy PDF with parameters \( \alpha = 1, \beta = 0.7, \gamma = 1, \delta = 0 \) according to the \( S_0 \)-parametrization convention \[36, 37\]. We use this distribution as an arbitrary example for comparisons that provides fat tails and for which a fast transformation method is available; for details see Sec. 6. The support is chosen small to produce deliberately a visible truncation. Fig. 2 shows the tiling of a bimodal PDF. The above recursive procedure may be considered the most elegant and simple way to construct the tiling. For the subsequent production stage it is irrelevant however if the tiling was constructed, for example, by plastering, i.e. starting from a small initial tile somewhere within the support.

Thus, the tiling constructs a piecewise constant majorizing function \( g(x) \) of the PDF \( f(x) \), with \( g(x) \geq f(x) \forall x \in [a, b] \). The closer \( g(x) \) to \( f(x) \), the better. The universal von Neumann rejection method has two main steps:

a) Generate a random \( X \in [a, b] \sim g(x) \) and a random uniform \( Y \in [0, g(X)] \).

b) Accept \( X \) if \( Y < f(X) \), otherwise reject it and repeat the procedure.

The rejection rate is given by the ratio \( R \) of the areas under the PDF and the comparison function:

\[
R = 1 - \frac{\int_a^b f(x)dx}{\int_a^b g(x)dx} = 1 - \frac{1}{NS} \int_a^b f(x)dx.
\] (1)

The denominators correspond to the sum over all \( N \) tile surfaces \( S \) which are equal.

At this point one could think that an adaptive scheme would be more appropriate, e.g. only tiles intersected by the PDF are split or even deformed to fit the boundary better, or tiles lying below the PDF are merged. Indeed this is common practice in computer graphics and some approximation methods. However, this measure to save memory is not recommended here; actually, it is to be avoided for the sake of simplicity and speed. In the production stage the probability of random selection of a tile would have to be proportional to its area to guarantee uniform probing. This is more complicated and slower especially if the area ratios are not integer. Moreover, a uniform random coordinate
is more expensive to produce in shapes other than rectangles. Additional details to why the segmentation into equal areas is crucial are given in numerous publications [11 17 31 32]. Instead of using strips of different height and width or even different shape as in other methods, here we suggest equal tiles as the clearly simplest and fastest approach. This is the key idea in this work.

Now the von Neumann rejection can be implemented with a modified first step:

a) Generate a random tile index \( i = 1, \ldots, N \); generate a random coordinate \((X,Y)\) within tile \( i \).

b) Accept \( X \) if \( Y < f(X) \), otherwise reject it and repeat the procedure.

This way we are able to sample efficiently the majorizing function \( g(x) \). Moreover, the evaluation of the condition in b) is hugely sped up using the implicitly constructed minorizing function as explained in more detail in the following Sec. 2.2.

Although the sampling with tiles seems sufficiently intuitive and equivalent to analogous methods of this kind [31 32] we give nevertheless a reasoning on the correctness.

**Theorem** The introduced sampling of the comparison function is equivalent to the standard von Neumann sampling, i.e. \( g(x) \) is sampled uniformly within all tiles generated on the support \( x \in [a,b] \).

**Proof** Define \( I = \{i_1, i_2, i_3, \ldots, i_N\} \) the set of tile indices and \( I_j \subset I \) the subset of all indices \( i_1^j, i_2^j, \ldots \) corresponding to a particular tile column \( j \) with width \( \Delta x = (b-a)/r \), where \( r \) is the number of columns. Thus \( \bigcup_j I_j = I \). Construct an bijective mapping \( i_k^j \rightarrow n_l^j \) with \( n_l < n_{l+1} \). The mapping is purely a renaming of indices in column \( j \). So we have \( n_l^j = 1, \ldots, n_{\text{max}}^j \). Let \( n_{\text{max}}^j = g(x)/\Delta y \) where \( \Delta y \) is the height of the tile. Note that within column \( j \) the

![Figure 1: For the intuitive introduction of the tiling procedure the plot shows an early refinement stage in the tiling of a truncated asymmetric Lévy PDF with parameters used as an arbitrary example.](image)
Figure 2: Tiling of a bimodal probability density function. $f(x)$ is composed of two Lévy density functions with parameters $\alpha = 1$, $\beta = 0.7$, $\gamma = 1$ (left part) and $\alpha = 2$, $\beta = 1$, $\gamma = 1$ (right part); the heights are adjusted to fit the curves seamlessly at $x = 10$.

function $g(x)$ is constant. Now define a random number $Y_j = n^j_l \Delta y$ with uniform random $u \in [0,1)$. The index $n^j_l$ is random by the random choice of $i^j_k$ and the subsequent mapping. Then $Y_j \in [0,g(x))$ is a uniform random number in column $j$ and we arrive at the standard situation of the rejection method for the interval $x \in \Delta x_j$: Generate a uniform coordinate $(X_j,Y_j)$ with uniform $X_j \in \Delta x_j$ and reject $X_j$ if $Y_j > f(x)$. The sampling of $j$ is implicitly proportional to the size of $I_j$, i.e. the height of column $j$, due to the uniform sampling of tile indices $i \in I$ and $\bigcup_j I_j = I$. Therefore $X_j$ is sampled as desired according to $g(x)$ and the sampling of pairs $(X,Y)$ is achieved with $X \in \bigcup_j \{X_j\} \sim g(x)$. □

The correctness of the standard rejection method can be taken for granted since the seminal paper by John von Neumann [43].

2.2 Implicit squeeze function

The tiling also constructs implicitly a so-called squeeze function $q(x)$ that fulfills the condition $q(x) \leq f(x) \leq g(x)$ within the required interval $[a,b]$. This is the usual definition of the squeeze and comparison functions, see for example Ref. [17]. $q(x)$ is the upper edge of the top tiles lying completely underneath $f(x)$, or equivalently the bottom edge of the tiles intersected by $f(x)$. The role of the squeeze function is to reduce the number of evaluations of $f(x)$ if $q(x)$ can be evaluated faster: In the setup all tiles below $f(x)$ are labeled and the test $Y \leq q(X)$ involves no computation — just one label look-up. Actually $Y$ must not be generated at all for tiles that are not intersected by $f(x)$. The latter is the key advantage of the squeeze function. Thus the following modified steps
implement the von Neumann rejection:

a) Generate a random tile with index $i = 1, \ldots, N$; generate a random $X$ within tile $i$.

b) Look up if tile $i$ is labeled as “$< f(x)$”. If yes, accept $X$. Otherwise generate $Y$ within tile $i$ and compare $Y < f(X)$. If yes, accept $X$. Otherwise reject it and repeat the procedure.

With dense tiling most $X$ are accepted in b) by one table look-up only without the generation of a second real coordinate $Y$. The PDF itself is hardly ever evaluated. The relative number of evaluations of $f(x)$ per non-uniform variate is given by

$$E = 1 - \frac{1}{NS} \int_a^b q(x)dx.$$  

(2)

The integral over the squeeze function is given by the sum of all tile surfaces not intersected by $f(x)$. Thus, the number of evaluations of $f(x)$ can be greatly reduced and is equal to the area fraction of the border tiles. Both numbers $R$ and $E$ are cheaply calculated on the fly, so that the resulting rejection rate can be pre-imposed as a condition for the tile refinement. The latter results will be reconsidered in Sec. 2.3 on the distribution cutoff.

To have a better measure of the “quality” of $g(x)$ and $q(x)$ we estimate an upper limit for the probability density $p_E$ that $f(x)$ must be evaluated for one non-uniform random number. Define $\Delta x := (b - a)/n$ where $n$ is the number of columns, so $\Delta x$ is simply the final width of the tiles. For $\Delta x \ll b - a$, i.e $n$ sufficiently high, $f(x)$ can be assumed linear in the interval $\Delta x$. Then

$$p_E(x, \Delta x) \propto \frac{b - a}{r} \frac{d \log f(x)}{dx}.$$  

(3)

This expression is deduced from the ratio of areas contained in a tile column corresponding to $Y \leq q(x)$ and $q(x) < Y \leq g(x)$ respectively.

2.3 Distribution cutoffs

In the introduction and thereafter we explained that all procedures that are not specialized to particular analytic and thus invertible distributions will never sample an infinite support. Considerations on the appropriate cutoff apply only to special distributions [7]. If the support of the PDF $f(x)$ is infinite, a general algorithm will inevitably reduce it to a reasonable finite interval $x \in [a,b]$. It is the scientist’s responsibility to control appropriately these support limits.

However, the period length $L$ of the $[0,1]$-uniform generator used in the sampling along the abscissa must satisfy the condition $f(x) < 1/L$ at both limits $a,b$ [2]. This situation appears for example in the standard rejection method or the Ziggurat method. In the latter, the $[0,1]$-uniform generator must sample the whole bottom strip. The sampling procedure in our method lifts this limitation by the number of columns $n = 2^{r-1}$, where $r = 1, 2, \ldots$ is the refinement level: A random integer is generated to sample a tile and a subsequent uniform $X$ is generated within the tile. In practically relevant cases the number of tiles will always be exceedingly smaller than the period length of any sensible random integer generator. Fat (or somehow long) tailed distributions deserve attention for the above reason.
3 Discontinuous probability densities

The literature also considers density functions which contain a pole (which numerically is indistinguishable from a cusp) [2], i.e. \( f(x) \to \infty \) as \( x \to c^+ \) or \( x \to c^- \) in the range of interest \([a,b]\). Within the standard von Neumann rejection method [43] a pole is dealt with as follows: Choose \( \epsilon \ll 1 \) and assign the cumulative probability

\[
P_c = \int_{c-\epsilon}^{c+\epsilon} f(x) \, dx
\]

(4)
to the interval \([c-\epsilon, c+\epsilon]\), a so-called mass point. If the \([0,1]\)-uniform deviate is smaller than \( P_c \) return \( c \). Otherwise sample from \([a,b]\) \( \setminus [c-\epsilon, c+\epsilon] \). If \( c \) and \( c \pm \epsilon \) have the same numerical representation then no better method exists to sample from \( f(x) \). Usually this situation must be treated computationally as a special case in the setup and production phases.

The tiling procedure and subsequent production works unchanged with an appropriately approximated (or modified) density function as follows. Fig. 3 shows the situation of a density function with a pole at \( x = c \). Figure dimensions, especially the vertical scale, are exaggerated to convey intuitively the geometry. Choose \([c-\epsilon, c+\epsilon]\) and modify \( f(x) \) yielding \( \bar{f}(x) \) such that the cumulative probability \( P_c \) according to Eq. (4) is preserved (hatched area in Fig. 3):

\[
\int_{c-\epsilon}^{c+\epsilon} f(x) \, dx = \int_{c-\epsilon}^{c+\epsilon} \bar{f}(x) \, dx
\]

(5)

which gives the implicit condition for \( \max(\bar{f}(x)) \):

\[
\max(\bar{f}(x)) = \frac{1}{2\epsilon} \int_{c-\epsilon}^{c+\epsilon} f(x) \, dx.
\]

(6)

This is the minimum value of the height of the initial tile. If \( \epsilon \) is chosen sufficiently small with numerical or/and statistical reasoning, the result will be identical to the procedure in the standard von Neumann rejection described above.

One has to be aware that the choice of \( \epsilon \) as the smallest representable “distance” from the position of the pole is unnecessarily restrictive. Any statistical verification requires a significant number of deviates to fall in the region of the pole to reveal a possibly too large value for \( \epsilon \). Depending on the error norm and test method it is likely to turn out that \( \epsilon \) can safely be chosen magnitudes larger than the initial numerical consideration. The statistical needs of the application must be considered in any case. Thus, there is no generally obvious upper limit for \( \epsilon \).

An example application is the scaled symmetric modified Bessel function of the second kind \( K_0(|x|)/\pi \), which is the density of the product \( XY \), where \( X \) and \( Y \) are independent normal distributed random numbers. \( K_0(|x|) \) diverges at \( x = 0 \). A possible setting could be the following. Restricting the support to \( x \in [-15, 15] \) accounts for over 99.99999% of all mass. With \( \epsilon = 0.00001 \) we get a fraction of \( 8.03978 \times 10^{-5} \) of the mass contained in the interval \([0-\epsilon, 0+\epsilon] \). The number of recursive refinements is given by \( \lceil \log_2(30/(2\epsilon)) \rceil = 21 \). About 235 000 tiles are retained to cover the density function, corresponding to two megabytes of memory in our data format. Benchmarks for the setup are presented in
Figure 3: Probability density containing a pole at $x = c$ (schematic). The returned deviates are numerically correct if the modified density function $\tilde{f}(x)$ fulfills the condition of equal area (hatched region) for $x \in [c - \epsilon, c + \epsilon]$ and $\epsilon \ll 1$ sufficiently small. The initial tile is chosen $\max(\tilde{f}(x))$ high. The true or modified PDF can be approximated via data points as shown or by any other method that implements this condition. The mathematical jumps in the modified PDF can be modeled numerically via two very close consecutive data points along $x$.

4 Measurements and comparisons

In general, speed comparisons are not obvious to do and interpret and only meaningful with respect to a particular software and hardware implementation. With increasing optimization of code, the mathematical description of a method and its implementation become inseparable. We must stress this and point to technical aspects that are responsible for a speed difference of two orders of magnitude, even though the mathematical/algorithmic description is identical.
The issue of this paper is not pure speed, but portability and easy applicability in compromise with speed.

All measurements were performed on a desktop PC with a 2.4 GHz Intel Pentium 4 processor using the GNU C++ compiler version 3.2.2 on Red Hat Linux. We explain below the importance of using a multi-tasking operating system in its standard operation mode with a typical process time slice during the measurements. This will almost always be the case with applications in statistical computing.

4.1 Memory requirements

At the start the graph of the PDF is embedded in one tile. The memory requirements for a Gaussian-like density function and rejection rate below 0.02 [32] is never more than a few megabytes. For details on a uni-modal example as in Fig. 1 see Tab. 1 for the bimodal case in Fig. 2 see Tab. 2. Only obnoxious density functions with fat tails and many sharp peaks require more memory. In the tested variations of such extreme cases using multiple peaks and the support truncated very far out the memory needed to achieve a rejection rate below 0.02 did not exceed 10 megabytes (about one million tiles). This happens using two numbers to store the coordinates of one tile and is more than acceptable for contemporary desktop computers. We skipped entirely memory optimization and removal of redundancy since we preferred a clear class structure and simple data management. Setup time can be reduced via speed optimized data structures, but that typically increases computation time and storage. Just a decade ago the above memory requirements were large for a standard desktop computer with a few megabytes memory. This may explain why this fairly straightforward method has not been proposed before.

4.2 Speed of random variate production

With the SHR3 uniform RNG [32] on the above mentioned configuration our method produces 2.6 million non-uniform random numbers per second independently of all tested PDFs. In the following we discuss a few pitfalls of speed measurement and code execution, and we compare to other methods. The benchmarks refer to methods and implementations that appear most similar or useful in judging the tiling method. In any case, the comparisons cannot be entirely fair since each method has different specialities.

In rejection methods the speed of random variate production is arbitrarily independent of the PDF and its representation, whether by data points or a closed formula. The speed depends only on the properties of the comparison and squeeze functions. In all our tested examples with tabular data or simple explicit density functions the evaluations representing \( f(x) \) are negligible at a rejection rate below 0.02. Since interpolation or evaluation of density functions is not the topic of this paper, we only give as a rule of thumb that evaluations for 1% of the produced random numbers is sufficiently low for almost all practically relevant densities. The production of one random variate with the desired distribution requires at least two uniform random variates as in most methods. Recently a method was published that can provide non-uniform variates with \( 1 + s, s \in [0, 1] \), uniform variates where \( s \) can be made arbitrarily small [24]. However, it turns out that in almost all applications the generation of uniform random...
Table 1: Number of tiles, rejection rate and evaluation rate for the uni-modal PDF shown in Fig. 1 but with a larger cutoff at $x = \pm 64$. Refinement level 5 is shown in Fig. 1. The memory needed to store 49,685 tiles (refinement level 10) is ca. 0.4 megabytes. The evaluation rate tells how often $f(x)$ must be evaluated per non-uniform random number.

| Refinement level $r$ | Number of tiles $N$ | Rejection rate $R$ | Evaluation rate $E$ |
|----------------------|---------------------|--------------------|--------------------|
| 1                    | 1                   | 0.813              | 1                  |
| 2                    | 3                   | 0.750              | 1                  |
| 3                    | 8                   | 0.627              | 1                  |
| 4                    | 24                  | 0.502              | 0.910              |
| 5                    | 70                  | 0.317              | 0.650              |
| 6                    | 238                 | 0.196              | 0.390              |
| 7                    | 857                 | 0.108              | 0.220              |
| 8                    | 3,246               | 0.058              | 0.110              |
| 9                    | 12,609              | 0.029              | 0.058              |
| 10                   | 49,685              | 0.015              | 0.029              |
| 11                   | 197,233             | 0.007              | 0.013              |
| 12                   | 785,936             | 0.002              | 0.005              |

numbers is not the major sink of computer time. It is up to the scientist to evaluate the trade-off between a few percent gain in overall speed and quality of the obtained variates. The use of less than two uniform random variates per non-uniform variates in the context of a rejection technique but also the importance of uniform random number quality, in particular in the Ziggurat implementation by Marsaglia and Tsang, is commented in Refs. [3, 8, 18, 38]. Some constructive remarks on the Ziggurat implementation in Ref. [32] can be found in Ref. [34].

We chose as one of the benchmarks the symmetric Lévy $\alpha$-stable distribution. It is a generalization of the Gaussian distribution, that is recovered for $\alpha = 2$; see Appendix. The transformation method by Chambers et al. [6] is the contemporary method of choice. As opposed to other published methods it has no accuracy deficiency, it does not truncate the support and is sufficiently fast for most applications. Moreover, it is applicable to asymmetric Lévy $\alpha$-stable deviates too. We use an implementation in C++ for the purpose of this comparison. It is about 3 times faster than our method on the above mentioned test configuration.

We also compared to the most efficient implementation of the Ziggurat method [32] for $\exp(-x)$ and $\exp(-x^2)$ distributed variates. This implementation is considered the fastest for these two distributions. The exponential and normal densities could be wired into the code exploiting their mathematical properties and using inline coding. In the limit of a negligible rejection rate, this Ziggurat implementation could produce 232 million variates per second. This means one variate per 10 CPU clock cycles! It is important to note that this number could only be achieved if executed alone without any other code, for example within a Monte Carlo application. This speed may be surprising...
Table 2: Statistics for the bimodal PDF shown in Fig. 2, where refinement level 6 is plotted. The memory needed to store 151 068 tiles for refinement level 11 is ca. 1.2 megabytes.

| Refinement level $r$ | Number of tiles $N$ | Rejection rate $R$ | Evaluation rate $E$ |
|----------------------|---------------------|-------------------|--------------------|
| 1                    | 1 0.858             | 1                 |                    |
| 2                    | 4 0.858             | 1                 |                    |
| 3                    | 9 0.747             | 1                 |                    |
| 4                    | 23 0.605            | 0.956             |                    |
| 5                    | 70 0.481            | 0.871             |                    |
| 6                    | 213 0.317           | 0.582             |                    |
| 7                    | 718 0.189           | 0.356             |                    |
| 8                    | 2 602 0.106         | 0.195             |                    |
| 9                    | 9 859 0.056         | 0.104             |                    |
| 10                   | 38 324 0.029        | 0.053             |                    |
| 11                   | 151 068 0.014       | 0.025             |                    |
| 12                   | 599 819 0.007       | 0.011             |                    |

at first sight since the rejection principle is quite similar to the tiling method. Actually there are profound differences. First and most obviously, the number of tiles is not a power of two. Choosing randomly between exactly $2^8$ or $2^7$ objects is faster if one uses 8 bits of the 32 bit XOR shift RNG as in Ref. [32]. Secondly, it is stated self-evidently in Ref. [32] that small code is important. This purely technical issue is hardly ever explained in the literature on random numbers despite being highly technical on several occasions. Numerical literature [39, Chap. 7] finally picks up this issue and also more recently in Ref. [40], but only briefly say why small code is important. We outline the situation.

CPUs use hierarchical memory to speed up computation. The access to the internal cache memory is magnitudes faster than to the external main memory. However, the code and data fitting into this cache is not the only condition for faster execution. An algorithm hard-wired in the CPU transfers repeatedly and frequently used sections of memory into the cache and also considers the size and distribution of the data over the memory banks. A good implementation (and compiler) therefore tries to minimize cache misses by arranging data of subsequent memory accesses into the same cache line. The latter are sequences of bytes transferred into the cache with each memory access. This statistics is disrupted by cache misses that are also provoked by a process switch of the operating system at built-in time intervals or other events. Small code might therefore end up in the cache for a significant time. Very large code that accesses its data in random fashion as it is the case in the sampling with tiles will not be able to exploit properly cache memory. We can therefore say that the execution of code is subject to decisive factors of hardware, compilation and operating system that can usually not be controlled entirely. It is also known that CPU-specific compilers are able to produce code that can be several times faster than a more generic compiler.

On our typical configuration of operating system and compiler the execution
of the Ziggurat code \cite{32} is the fastest by far. The speed factor of ca. 100 to
our code is in fact consistent to the latency of low-level memory as compared to
second-level cache of contemporary hardware. This speed difference is leveled
out considerably if the code and tables of the Ziggurat implementation is forced
to leave the cache by executing some arbitrary and larger code alternatingly
with calls to the Ziggurat generator. This measure creates a more realistic use
case and reduces the execution speed of the Ziggurat code by a factor of ca.
50. A more rigorous analysis of code and hardware interplay would require the
exact reproduction of the original test environment which is not readily available
anymore.

Finally we make a few more technical remarks and comparisons. The im-
plementation of the tiling method is only moderately optimized, but completely
portable and uses throughout Standard Template Library arrays. The period of
the XOR shift RNG is considered short with 32 bit arithmetic but modification
to higher models is possible. Following the results in Refs. \cite{3, 8, 18, 34, 38} on quality,
resolution and portability we recommend a slower and also portable uniform
RNG. Refs \cite{3, 8, 18, 34, 38} also comment other problems of the XOR shift
RNG in conjunction with the Ziggurat method. The Ziggurat method requires
for the decision whether to evaluate the density function one coordinate com-
parison for each attempt to draw a non-uniform number. Our method requires
one table look-up only. But this advantage is not enough to compensate the
disadvantage of a large table and resulting slow memory access.

For accelerated production of random variates to make sense, their part
must take up a significant proportion of the overall CPU time. But there is
hardly anything do-able within the order of 10 clock cycles. Moreover, fast
production of variates imply that enormous amounts are required. This poses
very high demands on their quality. The findings above as well as the critical
publications on the Ziggurat implementation Ref. \cite{32} encourage to analyse
the appropriateness of extremely fast but medium quality variates. A detailed
analysis of this issue can be found in Ref. \cite{42}.

4.3 Speed measurements of the setup

The setup part in our implementation is not speed-optimized but turned out
to be sufficiently fast for the production of ca. one million variates and above.
This includes the extreme examples with more than one mode and a very large
support. To provide a meaningful time measurement for the setup we subtract
the cumulative time for the evaluations of $f(x)$. For the presented examples
we used a standard polynomial interpolation with 7 data points. The setup for
a typical uni-modal PDF (Gaussian or Lévy, the latter with sufficiently wide
support) with $2^{15}$ data points takes ca. 0.2 seconds plus cumulative 2.1 seconds
for all evaluations of $f(x)$. The calculation time of the Lévy PDF via fast
Fourier transform for $2^{15}$ points is negligible with only 0.2 seconds. Thus, as a
rule of thumb, the overall total speed of the setup depends almost entirely on
the number of evaluations of $f(x)$. With a constant number of data points the
total speed of the setup increases noticeably only for very unusual multi-modal
PDFs with many sharp peaks and long tails.

The setup of the Ziggurat for general symmetric, strictly decreasing, non-
analytic and safely truncatable PDFs was attempted in Ref. \cite{15}. This setup,
our C++ version of the Matlab code from Ref. \cite{15} as well as our own generalized
iterative C++ code along the original Ziggurat setup formula \[32\] is sensitive and computationally expensive. For example, a numerical error in the flat regions of the tail or in the inversion of the PDF can cause a disturbance which often causes a breakdown of the procedure. Precautions to mend this are possible but complicate the code further and do not guarantee unattended functionality. The empirical parameters needed for the setup of the Ziggurat method are an additional difficulty for making the method truly automatic. The setup time depends strongly on the given data and the above mentioned empirical parameters, and is at least one order of magnitude slower than the tiling.

5 Discussion and conclusion

We presented a fast method for automatic generation of random variates with arbitrary probability density functions independent of symmetry, number of modes, and discontinuities. The only prerequisites are pointwise computability and finite support. We also explained that the most general thinkable or universal method will require no less but also no more than these two requirements. In the introductory overview on some representative methods it is shown that many less powerful methods exist that truncate the infinite support for analytic density functions with only one mode. The accuracy of our method is exact up to the computation of the probability density function and meets any numerical demand which includes density functions with poles or cusps without additional attention.

The generation of one non-uniform random variate requires only one random integer, one random uniform real, two additions, one multiplication and one table look-up (no float comparison) most of the time. This is close to the minimum of principally required operations, so that additional speed can only come from hardware exploitation or specialized methods. Even for complicated density functions the memory requirements are suitable for any contemporary desktop computer.

These properties are not available in other methods of this kind. We can extend the wish list from Sec. 2 to a random number generator by additional items:

8. No need for a priori knowledge about the location of any number of modes or discontinuities within the density function.

9. Only pointwise computability and representability of the density function is necessary.

10. Fast setup time and fast generation of random variates.

11. The discretization and therefore sampling efficiency is asymptotically exact and can be pre-imposed.

An extension to the multivariate case is simple in principle. It means to substitute a two-dimensional tile with a cube or hypercube. The required storage for data however increases with a power of the dimension.
6 Appendix: Lévy density function

The generation of the pointwise density function of the Lévy \( \alpha \)-stable distribution and numbers is a technicality that we report for completeness. Any density would suffice for purpose of proving correctness numerically and there are certainly more cumbersome densities in statistical computing but we prefer also to have inversion methods at hand to produce random numbers. We choose the formula by Chambers et al., 1976 [6]:

\[
\xi = \gamma \left( \frac{-\log u_1 \cos \phi}{\cos((1-\alpha)\phi)} \right)^{1-\frac{1}{\alpha}} \frac{\sin(\alpha \phi)}{\cos \phi},
\]

where \( \phi = \pi(u_2 - 1/2); \ u_1, \ u_2 \in (0, 1) \) are uniformly distributed random numbers, \( \gamma \) is the scaling parameter, and \( \xi \) is a Lévy distributed random number. This expression, however, requires different representations for certain ranges of \( \alpha \) to reduce numerical error. Direct coding is possible but not recommended.

The pointwise calculation of the PDF is more difficult. It requires the calculation of a very slowly converging integral \([36, 37]\). In the symmetric case the Lévy distribution can be defined by

\[
L(z; \alpha, \gamma) = \frac{1}{\pi} \int_0^{\infty} \exp(-\gamma q^\alpha) \cos(qz) \ dq .
\]

This is a parade example of a non-analytic density function. It does not possess any moments other than the first for \( \alpha \in (1, 2] \) due to the divergence of the respective integrals except for \( \alpha = 2 \) which is the Gaussian limit. Values for \( L(z) \), Eq. (8), can be computed directly \([36, 37]\) or by carrying out the Fourier Transform \([33]\).

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