J. Statist. Comput. Simul., 1982, Vol. 14, pp. 149–158
0094-9655/82/1402-0149 $06.50/0

A Note on Approximations in Random Variate Generation

LUC DEVROYE†
McGill University

(*Received December 1, 1980*)

If random variates with density f are needed in simulations, but random variates with density g (close to f) are used instead, how does one measure the error committed? The usefulness of the total variation criterion is pointed out, and some examples are given.

When the total variation is hard to compute, good upper bounds can be used in its place. Some inequalities are reviewed that link the total variation to other quantities such as the rejection and composition constants, the uniform deviation, the divergence and so forth.

1. INTRODUCTION

Consider the situation where one needs random variates with distribution function F on R^d, but uses random variates with distribution function G instead. The reasons for this replacement are sometimes economical (random variates from G are obtainable in less time or with less space) and sometimes practical (for the particular application a good approximation of F is all that is needed). Sometimes one just doesn't want to spend a lot of time writing a complicated program for the generation of random variates from F. Whatever the reason of the replacement may be, it is necessary to have a good understanding of the consequences of the replacement. How should one measure the goodness of the approximation for simulation purposes?

One of the classical criteria,

$$\Delta_1 = \sup_x |F(x) - G(x)|$$

†The author is with the School of Computer Science, McGill University, 805 Sherbrooke Street West, Montreal, Canada H3A 2K6. Research of the author was partially supported by National Research Council of Canada Grant No. A3456.

has the disadvantage that it is not sensitive to local discrepancies between the distributions. For example, if F puts all its mass uniformly on $[0,1]$, $[2,3],\ldots,[2n-2,2n-1]$, and G puts all its mass uniformly on $[1,2]$, $[3,4],\ldots,[2n-1,2n]$, then $\Delta_1=1/n$. For large n this is quite small, although it is clear that one would be reluctant to replace F by G in any simulation.

If F and G are continuous and U is a uniform $(0,1)$ random variable, then $F^{-1}(U)$ and $G^{-1}(U)$ are random variables with distribution functions F and G respectively. This fact is of course at the basis of the *inversion method* in random variate generation. Thus,

$$\Delta_2=\sup_{0<u<1}|F^{-1}(u)-G^{-1}(u)|$$

would be a very good measure of the goodness of the replacement were it not for its overemphasis on the tails and other low-probability areas of the space. For example, if F has infinite support and G has compact support, then $\Delta_2=\infty$.

In this paper we would like to point out the usefulness of the *total variation criterion*

$$\Delta=\sup_{A\in\mathscr{A}}\left|\int_A dF-\int_A dG\right| \quad (\mathscr{A}=\text{class of all Borel sets of } R^d)$$

as a measure of the goodness of the approximation for simulation purposes. If F and G have densities f and g, then it is easy to see that

$$\Delta=\frac{1}{2}\int|f(x)-g(x)|dx=\int_{f>g}(f(x)-g(x))dx=\int_{f<g}(g(x)-f(x))dx.$$

Also, if F and G are both discrete with probability vectors $p_1,p_2,\ldots$ and $q_1,q_2,\ldots$ on the integers, then

$$\Delta=\frac{1}{2}\sum_i|p_i-q_i|=\sum_{p_i>q_i}(p_i-q_i)=\sum_{p_i<q_i}(q_i-p_i).$$

The total variation criterion has a clear physical meaning: if X and Y are random variables with distribution functions F and G respectively, then no matter how we choose a set A from the class of Borel sets, we are guaranteed that

$$|P(X\in A)-P(Y\in A)|\leq\Delta.$$

Thus, the absolute error of all probability assignments is bounded. Notice here also that Δ generalizes Δ_1 since Δ_1 is also a supremum of the same kind as Δ, except that the class $\mathscr{A}$ is the class of all sets of the form $(-\infty,x_1]x\ldots x(-\infty,x_d]$. In any case, $\Delta_1\leq\Delta$.

If random variates are required for the purpose of the Monte Carlo evaluation of a functional $\int h dF$ (with $h\geq 0$), then

$$\left|\int h dF-\int h dG\right|$$

$$=\left|\int_0^\infty\int_{h(x)\geq t}dF(x)\,dt-\int_0^\infty\int_{h(x)\geq t}dG(x)\,dt\right|$$

$$\leq\int_0^\infty\left|\int_{h(x)\geq t}dF(x)-\int_{h(x)\geq t}dG(x)\right|dt\leq\Delta\sup_x h(x).$$

Hence, for bounded functions h, we have a clear upper bound on the error committed if a perfect evaluation of $\int h dG$ were possible. For unbounded functions h, Δ may be very small and the difference $|\int h dF-\int h dG|$ may be arbitrarily large. For example, if F is Cauchy and G is Cauchy truncated at $[-n,n]$, and if $h(x)=|x|$, then $\Delta\to 0$ as $n\to\infty$, while $\int h dF-\int h dG=\infty$ for all n.

Often the quantity Δ can be determined without much effort, but in some cases it is very hard to compute. In Section 2, we give several inequalities that may help in the determination of upper bounds for Δ. In Section 3, we introduce and discuss a relative error criterion, and in Sections 4 and 5 we briefly comment on two popular replacements: the normal and the Poisson replacements.

2. PRACTICAL INEQUALITIES FOR Δ

Let f and g be densities on R^d, and let us define the following constants:

$$\alpha=\alpha(f,g)=\inf_x\frac{g(x)}{f(x)} \quad (\text{inf is taken over all } x \text{ with } f(x)>0);$$

$$\beta=\beta(f,g)=\inf_x\frac{f(x)}{g(x)} \quad (\text{inf is taken over all } x \text{ with } g(x)>0).$$

These constants are often easier to determine than $\int|f-g|$. It is clear that $f\leq g/\alpha$ and that $f\geq\beta g$. Thus, if α is close to 1, then g/α would be a candidate the choice of the dominating curve if the *rejection method* is considered for the generation of random variates with density f. Similarly, if β is close to 1, then βg would be a prime candidate for the principal component in the *composition (mixture) method*. If we do not use the rejection method or the composition method, but merely replace f by g, then we commit an error. This error is related to α and β in the following way.

Inequality 1 Let F and G have densities f and g on R^d. Then

$$\Delta \le \min(1-\alpha, 1-\beta).$$

Proof Notice that

$$\Delta = \int_{f>g} (f(x)-g(x))dx = \int_{f>g} f(x)\left(1-\frac{g(x)}{f(x)}\right)dx \le 1-\alpha.$$

Inequality 1 now follows by symmetry.

Another quantity that is often easily computed is

$$\Delta_\infty = \sup_x |f(x)-g(x)|$$

although it has no obvious physical interpretation for simulation purposes. We just mention the following simple inequalities relating Δ to Δ_∞:

Inequality 2 (Serfling, 1979) Let F and G have densities f and g on R^d.
Let

$$c_{f,\infty} = \inf(t: \int_{\|x\| \le t} f(x)\,dx = 1);$$

$$c_{f,r} = \sup_t t^r \int_{\|x\|>t} f(x)\,dx \;(\le \int \|x\|^r f(x)\,dx)\; (r>0)$$

and

$$v_d = \pi^{d/2}\Gamma\left(\frac{d}{2}+1\right).$$

Then

i) $\Delta \le v_d c^d_{f,\infty} \Delta_\infty$

and

ii) $\Delta \le 2 c_{(f,r)}^{d/(r+d)} (v_d \Delta_\infty)^{r/(r+d)}$.

In the inequalities, $c_{f,\infty}$ and $c_{f,r}$ may be replaced by $c_{g,\infty}$ and $c_{g,r}$.

Proof

$$\Delta = \int_{f>g} (f(x)-g(x))dx = \int_{\substack{\|x\|\le t\\ f>g}} (f(x)-g(x))dx$$

$$+ \int_{\substack{\|x\|>t\\ f>g}} (f(x)-g(x))dx \le v_d t^d \Delta_\infty + c_{f,r} t^{-r}.$$

The terms on the right-hand side are equal if $t^{r+d} = c_{f,r}/(v_d \Delta_\infty)$. Resubstitution gives (ii). Also, when $f=0$ outside the set $\{\|x\| \le t\}$, then $\Delta \le v_d t^d \Delta_\infty$, which proves (i).

Let us mention another inequality that has proven useful in information theory, and might be of some use here.

Inequality 3 (Kullback (1967), Csiszar (1969), Kemperman (1969)). Let F and G have densities f and g on R^d. Then

$$\Delta \le \left[\frac{1}{2}\int f(x)\log\frac{f(x)}{g(x)}dx\right]^{1/2}.$$

It should be noted that since $1-x < \log 1/x$, we always have

$$\Delta = \int_{f>g} f(x)\left(1-\frac{g(x)}{f(x)}\right)dx \le \int_{f>g} f(x)\log\frac{f(x)}{g(x)}dx.$$

Finally, since an L_2 norm is often easier to handle than an L_1 norm, we cite

Inequality 4 Let F and G have densities f and g on R^d. Then

$$\Delta \le \frac{1}{2}\left[\int \frac{g^2(x)}{f(x)}dx - 1\right]^{1/2}.$$

Proof When $p, q > 1$ and $p^{-1} + q^{-1} = 1$, then, by Holder's inequality,

$$\int|f-g| = \int \frac{|f-g|}{f^{1/p}} f^{1/p} \leq \left[\int \frac{|f-g|^q}{f^{q/p}}\right]^{1/q} [\int f]^{1/p}$$

$$= \left[\int \frac{|f-g|^q}{f^{q/p}}\right]^{1/q}$$

Inequality 4 follows if we let $p = q = 2$.

3. A RELATIVE ERROR CRITERION

For "unlikely" sets A, the knowledge that $|\int_A f - \int_A g| < \Delta$ is not very helpful. We recall here that g is absolutely continuous with respect to f if whenever $\int_A f = 0$, we have $\int_A g = 0$. For such densities g we define the relative error Δ_{rel} by

$$\Delta_{rel} = \sup_A \left|\int_A f(x)dx - \int_A g(x)dx\right| / \int_A f(x)dx$$

$$= \sup_{A: \int_A f > 0} \left|1 - \int_A g(x)dx / \int_A f(x)dx\right|$$

$$\leq \max\left(1 - \alpha, \frac{1}{\beta} - 1\right). \qquad (1)$$

When g is not absolutely continuous with respect to f, then $\Delta_{rel} = \infty$. In any case, we have that $\Delta \leq \Delta_{rel}$. For any Borel set A we are guaranteed that

$$(1 - \Delta_{rel}) \int_A f(x)dx \leq \int_A g(x)dx \leq (1 + \Delta_{rel}) \int_A f(x)dx.$$

When Δ_{rel} is small, we therefore know that f and g have quite similar tails.

Example Let (X, Y) be a random vector uniformly distributed in the unit circle, and let (U, V) be a random vector uniformly distributed in $[-1, 1]^2$. It is known that X/Y has density $f(x) = \pi^{-1}(1 + x^2)^{-1}$, and that U/V has density $g(x) = \max(\frac{1}{4}, 1/4x^2$. It is clear that $\alpha = \pi/4$, $\beta = 2/\pi$. Also, $\Delta_{rel} = \max(1 - \alpha, 1/\beta - 1) = \pi/2 - 1 \simeq 0.6$. Clearly, the replacement of f, by g for simulation purposes is outrageous, but nevertheless, the fact that $\Delta_{rel} \simeq 0.6$ indicates that both densities must have similar tails.

Remark By taking sets A that are spheres centered at x with radius $r > 0$, we note that for almost all x (with respect to f)

$$\int_A g(x)dx / \int_A f(x)dx \to \frac{g(x)}{f(x)} \text{ as } r \to 0 \qquad (2)$$

(this is known as the Lebesgue density theorem; see Wheeden and Zygmund, 1977). Let L be the set of all x with $f(x) > 0$, and for which (2) is valid. Define further

$$\alpha' = \inf_{x \in L} \frac{g(x)}{f(x)}, \quad \beta'^{-1} = \sup_{x \in L} \frac{g(x)}{f(x)}.$$

Clearly,

$$\Delta_{rel} \geq \max\left(1 - \alpha', \frac{1}{\beta'} - 1\right).$$

When f and g are both continuous and strictly positive on R^d, then $\alpha = \alpha'$ and $\beta = \beta'$. Thus, in that case, (1) is valid with equality. In other words, (1) cannot be improved upon except possibly in some uninteresting cases.

Optimization It happens sometimes that one can choose the approximating density g from a family of densities g_θ where θ is a parameter. In view of the fact that α and β are simple functions of θ only, we may try to minimize

$$\min\left(1 - \alpha, \frac{1}{\beta} - 1\right)$$

(which would minimize the upper bound for Δ; see inequality 1). In some cases, we may try to minimize

$$\max\left(1 - \alpha, \frac{1}{\beta} - 1\right)$$

(which would minimize Δ_{rel} in most cases; see the previous remark).

4. THE NORMAL APPROXIMATION

Scheffe's theorem (1947) states that if g_n is a sequence of densities on R^d with $g_n(x) \to f(x)$ as $n \to \infty$ for almost all x, then $\int|g_n(x) - f(x)|dx \to 0$ as $n \to \infty$. This property is valid for all densities f. Unfortunately, no rate of convergence can be derived from this theorem, and one usually falls back on the inequalities of Section 2. In addition to these, there are some known results that are valid for certain special sequences g_n. Some are mentioned here.

If $X_1, \ldots, X_n$ are i.i.d. zero mean random variables with variance σ^2, then the density g_n of the normalized sum

$$S_n = \frac{X_1 + \ldots + X_n}{\sigma\sqrt{n}}$$

satisfies $\Delta_n = \sup_x |g_n(x) - f(x)| \to 0$ where f is the standard normal density if and only if g_n is bounded for some $n \geq 1$ (Gnedenko, 1954; Petrov, 1956; Petrov, 1975, pp. 198). By inequality 2 this would also imply the convergence to 0 of Δ. In particular, if we assume that the variance is 1 and that $E(|X_1|^3) = c_3 < \infty$, then there is a universal constant a such that

$$\Delta_n \leq a c_3 \max(1, \sup_x g_1^3(x))/\sqrt{n}$$

and

$$\Delta \leq \pi a c_3^4 \max(1, \sup_x g_1^3(x))/\sqrt{n}$$

(Sahaidarova, 1966). In fact, for asymmetrical distributions for X_1, the rate $n^{-1/2}$ is optimal because

$$\Delta = \frac{|E(X_1^3)|}{6\sqrt{2\pi n}}(1 + 4e^{-3/2}) + o(n^{-1/2})$$

(Sirazdinov and Mamatov, 1962). Only for symmetric random variables can we hope to do better: for example, if g_1 is the uniform density on $(-\sqrt{3}, \sqrt{3})$, then $\Delta = O(1/n)$.

Most of the previous results carry over to the discrete case. Perhaps the most famous result here is due to Prohorov (1961). Let p_i be the i-th probability of the binomial (n, p) distribution ($0 < p < 1$ is fixed), let f be the normal density and let q_i be the integral of f between $(i - np)/\sigma$ and $(i + 1 - np)/\sigma$ where $\sigma^2 = np(1-p)$, then

$$\Delta = \frac{1}{2}\sum_i |p_i - q_i| = \frac{c|1 - 2p|}{\sqrt{np(1-p)}} + O\left(\frac{1}{np(1-p)}\right)$$

where

$$c = \frac{1}{6\sqrt{2\pi}}(1 + 4e^{-3/2}) \simeq 0.126.$$

We should point out here that for the computer generation of binomial (n, p) random variables when n is large, the normal approximation is now obsolete and almost always inadmissible in view of the constant average time procedures of Ahrens and Dieter (1980) and Devroye (1980a, 1980b).

5. THE POISSON APPROXIMATION

If p_i is the i-th binomial (n, p) probability and q_i is the i-th Poisson (np) probability, then

$$\Delta = \frac{1}{2}\sum_i |p_i - q_i| \leq \frac{1}{2}\frac{p}{\sqrt{1-p}}$$

for all n (Romanowska, 1979). Thus, the binomial distribution is close to the Poisson distribution for small p. However, no approximation of the binomial by the Poisson distribution or vice versa is necessary in view of the uniformly fast algorithms known for both distributions (Ahrens and Dieter, 1980b; Atkinson, 1979; Schmeiser, 1980; Devroye, 1981). However, there are situations where the Poisson approximation may be helpful, for example, for the computer generation of

$$X = \sum_{i=1}^{n} X_i$$

where n is large and $X_1, \ldots, X_n$ are independent $\{0, 1\}$-valued random variables with $P(X_i = 1) = z_i$. Indeed, if Y is a Poisson $(\sum_{i=1}^{n} z_i)$ random variable, then it is known that

$$\Delta = \frac{1}{2}\sum_i |P(X = i) - P(Y = i)| \leq \sum_{i=1}^{n} z_i^2$$

(LeCam, 1960). For example, when $z_i = \varepsilon/i^2$, $i > 0$, and $X = \sum_i X_i$ $(n = \infty)$, and when X is approximated by a Poisson $(\varepsilon\pi^2/6)$ random variable Y, then

$$\Delta \leq \varepsilon^2 \sum_{i=1}^{\infty} i^{-4} = \frac{\varepsilon^2\pi^4}{90}.$$

When $\varepsilon \simeq 10^{-3}$, then $\Delta \simeq 10^{-6}$, and the Poisson approximation seems quite acceptable.

References

Ahrens, J. H. and Dieter, U. (1974). Computer methods for sampling from gamma, beta, Poisson and binomial distributions. *Computing* **12**, 223–246.

Ahrens, J. H. and Dieter, U. (1980a). Sampling from binomial and Poisson distributions: a method with bounded computation times. *Computing*, to appear.

Ahrens, J. H. and Dieter, U. (1980b). Computer generation of Poisson deviates from modified normal distributions, manuscript.

Atkinson, A. C. (1979). The computer generation of Poisson random variables. *Applied Statistics* **28**, 29–35.

Csiszar, I. (1967). Information-type measures of difference of probability distributions and indirect observations. *Studia Scientiarum Mathematicarum Hungarica* **2**, 299–318.

Devroye, L. (1980a). The computer generation of binomial random variables when $p = 1/2$, manuscript, McGill University.

Devroye, L. and Naderisamani, A. (1980b). A binomial random variate generator, manuscript, McGill University.

Devroye, L. (1981). The computer generation of Poisson random variables. *Computing* **26**, 197–207.

Gnedenko, B. V. (1954). A local limit theorem for probability densities. *Dokl. Akad. Nauk. SSSR* **95**, 5–7.

Kemperman, J. H. B. (1969). On the optimum rate of transmitting information. *Probability and Information Theory*. Springer Lecture Notes in Mathematics **89**, 126–169.

Kullback, S. (1967). A lower bound for discrimination information in terms of variation. *IEEE Transaction on Information Theory* **IT-13**, 126–127.

Lecam, L. (1960). An approximation theorem for the Poisson binomial distribution. *Pacific Journal of Mathematics* **10**, 1181–1197.

Petrov, V. V. (1956). A local theorem for densities of sums of independent random variables. *Theory of Probability and its Applications* **1**, 316–321.

Petrov, V. V. (1975). *Sums of Independent Random Variables*. Springer-Verlag, Berlin.

Prohorov, Yu. V. (1961). Asymptotic behavior of the binomial distribution. *Selected Translations in Mathematical Statistics and Probability* **1**, 87–95.

Romanowska, M. (1979). A note on the upper bound for the distance in total variation between the binomial and the Poisson distribution. *Statistica Neerlandica* **33**, 127–130.

Sahnidarova, N. (1966). Uniform local and global theorems for densities. *Izv. AN-UzSSR Seriya Fiz.-Matem. Nauk.* **5**, 90–91.

Scheffe, H. (1947). A useful convergence theorem for probability distributions. *Annals of Mathematical Statistics* **18**, 434–438.

Schmeiser, B. W. (1980). personal communication.

Serfling, R. J. (1979). A variation on Scheffe's theorem, with application to nonparametric density estimation. Report M502, Department of Statistics, Florida State University.

Sirazdinov, S. H. and Mamatov, M. (1962). On convergence in the mean for densities. *Theory of Probability and its Applications* 1977, **7**, 424–428.

Wheeden, R. L. and Zygmund, A. *Measure and Integral*, Marcel Dekker, New York.