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by

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A METHOD OF SAMPLING CERTAIN PROBABILITY DENSITIES WITHOUT INVERSION OF THEIR DISTRIBUTION FUNCTIONS

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ABSTRACT

A Monte Carlo device is described which bypasses the inversion $x = P^{-1}(r)$ involved in directly sampling the distribution $P(x)$ of a stochastic variable x with given density $p(x)$. The method is practical for all linear and a broad class of quadratic densities.

I. INTRODUCTION

It is a well-known maxim of Monte Carlo practice that one should never compute the square root $x = \sqrt{r}$ of a random number, but rather set x equal to the greater of two such numbers. In general, if $p(x)$ is the density of a stochastic variable x on $[a,b]$, and $P(x) = \int_a^x p(x)dx$ its distribution, the direct way of sampling for x consists in setting a random number $r = P(x)$ and solving for $x = P^{-1}(r)$. This is how the equation $x = \sqrt{r}$ arises from the density $p(x) = 2x$ on $[0,1]$. Since such inversions are usually time consuming if not intractable, it is important to provide simple alternatives when possible. The following is a scheme which generalizes the $\sqrt{r}$ device and applies in particular to the determination $x = \sqrt{1 - (1-\xi^2)r}$ encountered in a previous report[1] on sampling the Klein-Nishina distribution (see Part III below).

II. THE GENERAL METHOD

For a distribution $P(x)$ on $[a,b]$, the function $f(r) = r^{-1}P(x)$, $x = a + (b - a)r$, $0 < r \leq 1$, has the properties

1. $f(0^+) = (b - a)p(a) \geq 0$, $f(1) = 1$
2. $f'(r) = r^{-2}[(x - a)p(x) - P(x)]$
3. $sdr + rds = p(x)dx$, $s = f(r)$, $x = a + (b - a)r$

Hence, if $f(r)$, in particular [by (2)] if $p(x)$, is <u>increasing</u>, then by (1) and (3), the probability $p(x)dx$ of x on $(x, x + dx)$ is the chance of a random point (r', s') of the unit square falling in the lower left region determined by $(r, r + dr)$, $(s, s + ds)$, and the curve $s = f(r)$. But this occurs iff either

(a) r' is on $(r, r + dr)$ and $s' \leq f(r')$, or s' is on $(s, s + ds)$ and $r' \leq f^{-1}(s')$, i.e.,

(b) $f^{-1}(s')$ is on $(r, r + dr)$ and $s' \geq f(r')$.

Thus, x will be obtained with density $p(x)$ if one follows

RULE 1. $\{$Increasing $f(r) = r^{-1}P[a + (b - a)r]\}$

I. Generate random numbers r', s'

II. Define $\rho = \begin{cases} r' \text{ if } s' \leq f(r') \\ f^{-1}(s') \text{ if } s' > f(r') \end{cases}$

III. Set $x = a + (b - a)\rho$.

Analogously, the function $g(r) = r^{-1}Q(x)$, $Q(x) = \int_x^b p(x)dx$, $x = b - (b - a)r$, has properties

(1) $g(0^+) = (b - a)p(b) \geq 0$, $g(1) = 1$

(2) $g'(r) = r^{-2}[(b - x)p(x) - Q(x)]$

(3) $s\,dr + r\,ds = p(x)(-dx) \geq 0, \; s = g(r),$

$x = b - (b - a)r$.

Now, if $g(r)$ is <u>increasing</u>, in particular (by (2)) if $p(x)$ is <u>decreasing</u>, then it is clear that the density $p(x)$ results from

RULE 2. {Increasing $g(r) = r^{-1}Q[b - (b - a)r]$}

I. Generate r', s'

II. Define $\rho = \begin{cases} r' \text{ if } s' \leq g(r') \\ g^{-1}(s') \text{ if } s' > g(r') \end{cases}$

III. Set $x = b - (b - a)\rho$.

III. LINEAR DENSITIES

The method applies to any linear density $p(x) = C^{-1}(c_0 + c_1 x) \geq 0$ on $a \leq x \leq b$, where $c_1 \neq 0$, and $C = (b - a)\left[c_0 + \frac{1}{2}c_1(b + a)\right]$, thus bypassing solution of the quadratic equation $r = P(x) = C^{-1}(x - a)\left[c_0 + \frac{1}{2}c_1(x + a)\right]$ for x.

Case 1. If $c_1 > 0$, then for $x = a + (b - a)r$ one finds

$$f(r) = r^{-1}P(x) = \left[c_0 + c_1 a + \frac{1}{2}c_1(b - a)r\right] \div \left[c_0 + \frac{1}{2}c_1(b + a)\right] ,$$

increasing for $0 \leq r \leq 1$, and RULE 1 defines

$$x = a + \max\left[(b - a)r', \left(b + a + 2c_0c_1^{-1}\right)s' - 2\left(a + c_0c_1^{-1}\right)\right] .$$

In particular, for ξ fixed, $0 \leq \xi < 1$ and $p(x) = 2x/(1 - \xi^2)$ on $[\xi,1]$, this reads

$$x = \xi + \max[(1 - \xi)r', (1 + \xi)s' - 2\xi] .$$

For $\xi > 0$, the latter provides an alternative to the choice $x = \sqrt{\xi^2 + (1 - \xi^2)r}$, while for $\xi = 0$, it becomes $x = \max(r', s')$ in lieu of $x = \sqrt{r}$, the example cited at the outset.

Case 2. If $c_1 < 0$, then for $x = b - (b - a)r$, we have

$$g(r) = r^{-1}Q(x) = \left[c_0 + c_1 b - \frac{1}{2}c_1(b - a)r\right] \div \left[c_0 + \frac{1}{2}c_1(b + a)\right] ,$$

increasing on $[0,1]$, and RULE 2 sets

$$x = b - \max\left[(b - a)r', -\left(b + a + 2c_0c_1^{-1}\right)s' + 2\left(b + c_0c_1^{-1}\right)\right] .$$

IV. QUADRATIC DENSITIES

For a quadratic density $p(x) = C^{-1}\,p_1(x)$, $p_1(x) = c_0 + c_1x + c_2x^2$ on $[a,b]$, with $c_2 \neq 0$,

$$C = (b - a)\left[c_0 + \frac{1}{2}c_1(b + a) + \frac{1}{3}c_2\left(b^2 + ba + a^2\right)\right] ,$$

one obtains

$$f(r) = r^{-1}\,P(x) = (b - a)\left[p(a) + \frac{1}{2}p'(a)\lambda + \frac{1}{6}p''(a)\lambda^2\right], \quad x = a + \lambda, \quad p''(a) = 2C^{-1}c_2,$$

$$\lambda = (b - a)r ,$$

whence

$$f'(r) = (b - a)^2\left[\frac{1}{2}p'(a) + \frac{1}{3}p''(a)\lambda\right],$$

$$f'(0) = \frac{1}{2}(b - a)^2\,p'(a) .$$

Similarly,

$$g(r) = r^{-1}Q(x) = (b - a)\left[p(b) - \frac{1}{2}p'(b)\lambda + \frac{1}{6}p''(b)\lambda^2\right], \; x = b - \lambda, \; p''(b) = 2C^{-1}c_2,$$

$$\lambda = (b - a)r ,$$

with

$$g'(r) = (b - a)^2\left[-\frac{1}{2}p'(b) + \frac{1}{3}p''(b)\lambda\right],$$

$$g'(0) = -\frac{1}{2}(b - a)p'(b) .$$

Now for such a $p(x)$ with $c_2 > 0$, it is evident that, since our method requires either $f'(0) \geq 0$ or

$g'(0) \geq 0$, we must have $p'(a) \geq 0$ or $p'(b) \leq 0$, and therefore $p(x)$ must be monotone on the whole range $[a,b]$. (Graphically, $y = p(x)$ is a parabola opening up.) The method of course applies to such densities, and we omit the obvious details.

More interesting is the fact that quadratic densities with $c_2 < 0$ (parabolas opening down), which are not necessarily monotone, are covered by the rules, provided the interval $[a,b]$ (lying between the zeros of $p(x)$) is sufficiently restricted to render $f(r)$ or $g(r)$ increasing on $[0,1]$. By the above remarks, it is clear that we are limited to the two cases:

Case 1. $f'(0) > 0$, $f'(1) \geq 0$, equivalently, $a < -\frac{1}{2} c_1 c_2^{-1}$ and $b \leq -\frac{1}{2}\left(a + \frac{3}{2} c_1 c_2^{-1}\right)$, with RULE 1 applicable.

Case 2. $g'(0) > 0$, $g'(1) \geq 0$, equivalently, $b > -\frac{1}{2} c_1 c_2^{-1}$ and $a \geq -\frac{1}{2}\left(b + \frac{3}{2} c_1 c_2^{-1}\right)$. Here RULE 2 applies. Obviously no $p(x)$ falls under both cases.

For quadratic $p(x)$, the method, when applicable, avoids solution of the cubic equation

$$r = P(x) = \sum_0^2 \frac{p^{(\nu)}(a)}{(\nu + 1)!} (x - a)^{\nu+1} ,$$

by means of a single square root. Even the latter might be avoided by further application of the rules to a linear density, but this we do not discuss, save to remark that one is led in this way to the well-known alternative $x = \max(r', s', t')$ for $x = r^{1/3}$ in the case of $p(x) = 3x^2$ on $[0,1]$.

The method, for the quadratic densities covered, is summarized below.

$$\text{Define } \alpha = 3\left(a + \frac{c_1}{2c_2}\right),\ \beta = 3\left(b + \frac{c_1}{2c_2}\right)$$

$$\lambda(s) = \frac{1}{2}\left\{-\alpha + \operatorname{sgn} c_2 \sqrt{\alpha^2 + 12c_2^{-1}\left[\frac{C}{b - a} s - p_1(a)\right]}\right\}$$

$$\mu(s) = \frac{1}{2}\left\{\beta + \operatorname{sgn} c_2 \sqrt{\beta^2 + 12c_2^{-1}\left[\frac{C}{b - a} s - p_1(b)\right]}\right\}$$

(a) If $c_2 > 0$, $p_1'(a) \geq 0$, or if $c_2 < 0$, $a < -c_1/2c_2$, $b \leq -\frac{1}{2}\left(a + \frac{3c_1}{2c_2}\right)$

$$\text{set} \qquad x = \begin{cases} a + (b - a)r' \ ; & s' \leq f(r') \\ a + \lambda(s') \ ; & s' > f(r') \end{cases}$$

(b) If $c_2 > 0$, $p_1'(b) \leq 0$, or if $c_2 < 0$, $b > -c_1/2c_2$, $a \geq -\frac{1}{2}\left(a + \frac{3c_1}{2c_2}\right)$

$$\text{set} \qquad x = \begin{cases} b - (b - a)r' \ ; & s' \leq g(r') \\ b - \mu(s') \ ; & s' > g(r') \end{cases}$$

V. NOTE ON STATISTICS

For a general density $p(x)$ on $[a,b]$, the probability of x falling on a particular subinterval $[c,d]$ is $p = \int_c^d p(x)dx$. If, in an experiment of any kind, the event of assigning x to $[c,d]$ has probability p of success, and hence probability $q = 1 - p$ of failure; and if M successes are observed in a large number N of such experiments, then the central limit theorem asserts the approximate relation

$$P\left\{\left|\frac{M}{N} - p\right| < \varepsilon\right\} \cong \frac{2}{\sqrt{2\pi}} \int_0^t e^{-u^2/2} du; \ t = \varepsilon \sqrt{N/pq} ,$$

the difference depending only on N, p, and q.

It follows that the direct method $x = P^{-1}(x)$, and the method of choosing x by the RULES, both involving experiments assigning x to $[c,d]$ with probability p, are of identical statistical reliability. This is reflected in the following part.

VI. TWO EXAMPLES

Example 1. The density

$$p(x) = 2x/(1 - \xi^2) = 8x/3 \text{ on } \xi = \frac{1}{2} \leq x \leq 1$$

was sampled $N = 10{,}000$ times by each of the two methods

$$x = \sqrt{1 - \frac{3}{4} r} \quad , \quad \text{and} \quad x = \frac{1}{2} + \max\left(\frac{1}{2} r', \frac{3}{2} s' - 1\right),$$

the values of x obtained being classified in 10 equal subintervals of $\left[\frac{1}{2}, 1\right]$. The resulting M_i/N with the exact probabilities p_i are tabulated as follows.

i	1	2	3	4	5	6	7	8	9	10
ROOT	0.0695	0.0797	0.0816	0.0884	0.0983	0.0962	0.1088	0.1230	0.1265	0.1280
RULE	0.0688	0.0767	0.0788	0.0898	0.0971	0.1023	0.1152	0.1209	0.1212	0.1292
p_i	0.0700	0.0767	0.0833	0.0900	0.0967	0.1033	0.1100	0.1167	0.1233	0.1300

Example 2. The non-monotone density $p(x) = \frac{3}{164}\left(15 - 2x - x^2\right)$ on $[-2,2]$ was sampled 10,000 times using RULE 2. The value assigned to x by a trial involving r', s' was $x = 2 - 4\rho$, where $\rho = r'$ if $41s' < 21 + r'(36 - 16r')$, and $\rho = \frac{1}{8}\left(9 - \sqrt{165 - 164s'}\right)$ otherwise. The result of classifying the x obtained in 10 equal subintervals of $[-2,2]$ is shown below, with corresponding exact probabilities p_i.

i	1	2	3	4	5	6	7	8	9	10
RULE	0.1139	0.1123	0.1221	0.1156	0.1143	0.1080	0.1002	0.0852	0.0730	0.0554
p_i	0.1123	0.1158	0.1170	0.1158	0.1123	0.1064	0.0982	0.0877	0.0748	0.0596

REFERENCE

1. C. J. Everett, E. D. Cashwell, G. D. Turner, "A New Method of Sampling the Klein-Nishina Probability Distribution for All Incident Photon Energies Above 1 keV," Los Alamos Scientific Laboratory report LA-4663 (May 1971).

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