Cosine with triangulars

MIGUEL A. S. CASQUILHO IST, Universidade Técnica de Lisboa, Ave. Rovisco Pais, IST; 1049-001 Lisboa, Portugal Telephone: (+351)21.8417310; fax: (+351)21.8499242

A simulation by the acceptance-rejection method is presented, applied to a case in which the target density, a cosine, is adopted for its simplicity, and the selected hat function is a truncated symmetrical triangular function, a "roof", to be optimized. Although this simulation would be very easy by the inversion method, the objective is to show that the acceptance-rejection method takes advantage of the preparation of an efficient instrumental density, which is associated with the hat function.

Keywords: acceptance-rejection, cosine, triangular distribution.

1. Fundamental and scope

In Monte Carlo simulation, the two general methods usually mentioned for random number transform are *inversion* and *acceptance-rejection*, while numerous special cases, not addressed here, have been constructed for several known distributions. For a given density to simulate from, the former method is straightforward and simply based on the inversion of the cumulative distribution function of the variable to be simulated (target variable), which may be difficult or computationally unsuitable. The latter method is based on the selection of an instrumental density a multiple of which, the hat function, encloses the target density. With f(x) the *target density*, g(x) the *instrumental density*, c a constant in the context, and h(x) the *hat function*, it is

$$h(x) = c g(x) \qquad h(x) \ge f(x) \qquad \{1\}$$

The instrumental density, g(x), must be chosen such that the inversion method may be easily applied to it, i.e., its cdf may be easily invertible and computationally convenient. Each cdf will be denoted by its corresponding capital, *F*, *G*, and *H*, and the inverse function by superscript "inv", e.g., G^{inv} . The acceptance-rejection algorithm is:

1. Generate a uniform *W* to get $X = G^{inv}(W)$ (inversion transform method).

2. Generate uniform *U*: if $U \cdot h(X) \le f(X)$, then accept *X*; otherwise reject it (go to step 1).

In this study, a simple target density, f(x), a cosine, was adopted,

$$f(x) = \frac{\mathbf{p}}{4a} \cos\left(\frac{\mathbf{p}}{2}z\right) \qquad z = \frac{x - \mathbf{m}}{a}$$
^{2}

i.e., a density centred on its mean, \mathbf{m} with $x \in (\mathbf{m} \pm a)$ and a a positive constant. It was chosen for its simplicity, which permits to compare easily with results from the inversion method. For convenience, the cdf for this variable is presented:

Miguel Casquilho is Assistant Professor in the Departament of Chemical and Biological Engineering, Instituto Superior Técnico, Universidade Técnica de Lisboa (Technical University of Lisbon), Lisbon, Portugal. E-mail address: mcasquilho@ist.utl.pt.

$$F(x) = \int_{-1}^{z} \frac{p}{4a} \cos\left(\frac{p}{2}t\right) (a) dz = \frac{p}{4} \frac{2}{p} \left[\sin\left(\frac{p}{2}t\right)\right]_{-1}^{z} = \frac{1}{2} + \frac{1}{2} \sin\left(\frac{p}{2}z\right)$$
(3)

For the case under study, the instrumental density, g(x), a truncated symmetrical triangular density, or "roof", was selected.

$$g_{1}(x) = y_{M} + saz \qquad z \in (-1, 0)$$

$$g_{2}(x) = y_{M} - saz \qquad z \in (0, +1)$$

$$\{4\}$$

In Eq. {4}, y_M is the mode density (where the two branches meet), *s* is the slope of the left-hand branch and *a* is the half width of the interval of variation of *x*, with *z* already defined (Eq. {2}). The values of y_M and *s* are to be calculated in the application case. The hat function must be as close as possible to the target density, as the smaller the factor (multiplying "constant"), *c* (in Eq. {1}), the smaller the rejection fraction, which is given by r = c - 1. (Ideally, *g* would be identical with *f*, i.e., c = 1, yielding a rejection of 0, but simulating from *f* is precisely what is to be avoided.) Illustrative curves are shown in Fig. 1.



Fig. 1. Target density (cosine), instrumental density (lower "roof") and hat function (upper "roof").

It can be seen from the graph that the slope of the branches of this symmetrical hat function has certainly an effect on c, and thus on the rejection fraction. In the case of a null slope (a horizontal line tangent to the cosine), the instrumental density is a uniform, g(x) = 1/(2a), and the hat function is $h(x) = \max f(x) = \mathbf{p}/(4a)$. The fraction is, of course,

$$r = c - 1 = \frac{\int_{x} h \, \mathrm{d} x}{\int_{x} f \, \mathrm{d} x} - 1 = \frac{(2a)\left(\frac{\mathbf{p}}{4a}\right)}{1} - 1 = \frac{2\mathbf{p}}{4} - 1 \approx 57\%$$
⁽⁵⁾

The rejection fraction, r, given in Eq. {5} for s = 0, say, r(0), may be considered an upper limit, within the reasonable choices (s > 0) for this hat function. The value of s that minimizes r should, therefore, be sought.

The objective of the present study is to show that the acceptance-rejection method takes advantage of the preparation of an "efficient" instrumental density, leading to a rejection fraction as small as possible. In the following sections, the hat function is determined, the rejection fractions are calculated, with their confirmation by simulation, and some conclusions are drawn.

2. Determination of the hat function

A convenient path to find the hat function appears to be:

- **1.** Stipulate a trial value, $z_0 (x_0 = \mathbf{m} + a z_0)$, of the target density, f(z): $(z_0, f(z_0))$
- **2.** Make the hat function, $h(z; z_0)$, tangent to the target density at $z = z_0$ and find its expression.
- **3.** Calculate *c*.
- **4.** Obtain the instrumental density, $g(z; z_0) = h(z; z_0) / c$.

As all the functions are symmetrical about their means, it will be assumed for simplicity that: it is $z_0 \ge 0$; and *s* is the slope of the right-hand branch of *h* (i.e., h_2), at z_0 . Obviously, the slope at $z = -z_0$ is -s (typically positive), and there are two tangency points, although here reference will be to the right-hand side one (so, the slope, *s*, will be typically negative). Thus, the value of z_0 will be sought.

Coordinates of the tangency point (stressing the fact that differentiation is with respect to *x*, so, according to Eq. {2}, $d/dx = dz/dx d/dz = a^{-1} d/dz$):

$$z_{0}; \qquad f_{0} = f(x_{0}) = \frac{\mathbf{p}}{4a} \cos\left(\frac{\mathbf{p}}{2}z_{0}\right) \qquad s = f'(x_{0}) = -\frac{\mathbf{p}^{2}}{8a^{2}} \sin\left(\frac{\mathbf{p}}{2}z_{0}\right) \qquad \{6\}$$

The dimensions of the problem variables, with [x] = [X], are: [a] = [X], $[f, g, h] = [X]^{-1}$, $[s, f^{*}] = [X]^{-2}$. The dimensional coherence of every equation is a way to avoid some mistakes.

Hat function:

$$h_1(x) = f_0 - sa(z + z_0) \qquad z < 0$$

$$h_2(x) = f_0 + sa(z - z_0) \qquad z \ge 0$$
{7}

Integral of the hat function, left-hand branch:

$$H_{1}(x) = \int_{-1}^{z} [f_{0} - sa(t + z_{0})](a) dt = (af_{0} - sa^{2}z_{0})(z + 1) - \frac{1}{2}sa^{2}(z^{2} - 1) =$$

$$= (1 + z) \Big[(af_{0} - sa^{2}z_{0}) + \frac{1}{2}sa^{2}(1 - z) \Big]$$

$$\{8\}$$

or

$$H_{1}(x) = -sa^{2}(1+z)\left[\mathbf{w} - \frac{1}{2}(1-z)\right]$$
^{{9}

with

$$\boldsymbol{w} = \boldsymbol{z}_0 - \frac{f_0}{sa}$$
 {10}

In the extremes:

$$H_{1}(z = -1) = -sa^{2}(1-1)\left[\mathbf{w} - \frac{1}{2}(1+1)\right] = 0$$

$$H_{1}(z = 0) = -sa^{2}(1+0)\left[\mathbf{w} - \frac{1}{2}(1-0)\right] = -sa^{2}\left(\mathbf{w} - \frac{1}{2}\right)$$

$$\{11\}$$

Integral of the hat function, right-hand branch:

$$H_{2}(x) = H_{1}^{T} + \int_{0}^{z} [f_{0} + sa(t - z_{0})](a) dt = H_{1}^{T} + (af_{0} - sa^{2}z_{0})z + \frac{1}{2}sa^{2}z^{2} =$$

$$= -sa^{2} \left(\mathbf{w} - \frac{1}{2}\right) - sa^{2}\mathbf{w}z + \frac{1}{2}sa^{2}z^{2} = -sa^{2} \left(\mathbf{w} - \frac{1}{2} + \mathbf{w}z - \frac{1}{2}z^{2}\right)$$

$$\{12\}$$

with $H_1^{T} = H_1(z = 0)$, given in Eq. {11}, or

$$H_{2}(x) = -sa^{2} \left[w(1+z) - \frac{1}{2}(1+z^{2}) \right]$$
[13]

In the extremes:

$$H_{2}(z=0) = -sa^{2}\left(\mathbf{w} - \frac{1}{2}\right)$$

$$H_{2}(z=1) = -2sa^{2}\left(\mathbf{w} - \frac{1}{2}\right)$$
[14]

Due to symmetry, the total integral, $H_2(z=1)=2H_1(z=0)$, is, of course, as seen above, twice the first one.

The integral of *h*, below designated by $H^{T} = H_{2}(z = 1)$, is, thus,

$$H^{\mathrm{T}} = -2sa^2 \left(\mathbf{w} - \frac{1}{2} \right)$$
 {15}

The previous integral is the factor *c*:

$$c = H^{\mathrm{T}} = -sa^{2}(2\mathbf{w} - 1)$$
 {16}

The instrumental density, g, such that h = c g, is

$$g_{1}(x) = \frac{h_{1}(x)}{c} = \frac{f_{0} - sa(z + z_{0})}{-sa^{2}(2w - 1)} = \frac{1}{a} \frac{w + z}{2w - 1}$$

$$g_{2}(x) = \frac{h_{2}(x)}{c} = \frac{f_{0} + sa(z - z_{0})}{2af_{0} + sa^{2}(1 - 2z_{0})} = \frac{1}{a} \frac{w - z}{2w - 1}$$

$$\{17\}$$

The function G^{inv} , according to the acceptance-rejection algorithm, will be necessary. The cdf G is just

$$G(x) = \frac{H}{c}$$
^{18}

From Eq. $\{9\}$, it is

$$G_{1}(x) = \frac{-sa^{2}(1+z)\left[\mathbf{w} - \frac{1}{2}(1-z)\right]}{-sa^{2}(2\mathbf{w} - 1)} = \frac{1}{2\mathbf{w} - 1}\left(1+z\right)\left(\mathbf{w} - \frac{1}{2} + \frac{1}{2}z\right)$$
^{19}

$$G_{1}(x) = \frac{1}{2\mathbf{w} - 1} \left(\mathbf{w} - \frac{1}{2} + \mathbf{w}z + \frac{1}{2}z^{2} \right)$$

$$\{20\}$$

Inverting, it is

$$\frac{1}{2}z^{2} + wz + w - \frac{1}{2} - (2w - 1)G_{1} = 0$$
^{21}

$$z = -\mathbf{w} \pm \sqrt{\mathbf{w}^2 - 2\left[\mathbf{w} - \frac{1}{2} - (2\mathbf{w} - 1)G_1\right]}$$

$$\{22\}$$

$$z = -\mathbf{w} + \sqrt{\mathbf{w}^2 - 2\mathbf{w} + 1 + 2(2\mathbf{w} - 1)G_1}$$
^{23}

From Eq. $\{13\}$, it is

$$G_{2}(x) = \frac{-sa^{2}\left(\mathbf{w} + \mathbf{w}z - \frac{1}{2} - \frac{1}{2}z^{2}\right)}{-sa^{2}(2\mathbf{w} - 1)} = \frac{1}{2\mathbf{w} - 1}\left(\mathbf{w} + \mathbf{w}z - \frac{1}{2} - \frac{1}{2}z^{2}\right)$$

$$(24)$$

 $G_{2}(x) = \frac{1}{2w-1} \left(w - \frac{1}{2} + wz - \frac{1}{2}z^{2} \right)$

Inverting, it is

$$\frac{1}{2}z^{2} - wz + \frac{1}{2} - w + (2w - 1)G_{2} = 0$$
{25}

$$z = \mathbf{w} - \sqrt{\mathbf{w}^2 - 2\left[\frac{1}{2} - \mathbf{w} + (2\mathbf{w} - 1)G_2\right]}$$

$$\{26\}$$

$$z = \mathbf{w} - \sqrt{\mathbf{w}^2 + 2\mathbf{w} - 1 - 2(2\mathbf{w} - 1)G_2}$$
⁽²⁷⁾

Thus, finally, the inverse, G^{inv} , is

$$G = G_1 \le 1/2 \quad z = -\mathbf{w} + \sqrt{\mathbf{w}^2 - 2\mathbf{w} + 1 + 2(2\mathbf{w} - 1)G_1}$$

$$G = G_2 > 1/2 \quad z = \mathbf{w} - \sqrt{\mathbf{w}^2 + 2\mathbf{w} - 1 - 2(2\mathbf{w} - 1)G_2}$$

$$\{28\}$$

with $w = z_0 - \frac{f_0}{sa}$ (Eq. {10}).

With the availability of h and G^{inv} , the acceptance-rejection algorithm can be applied.

3. Optimization of the hat function

The best hat function is the one "closest" to the target density so as to make the rejection fraction, which is related to the factor c, as small as possible. The hat function in the present case depends on the tangency point, i.e., the value of z_0 . So the minimum value of $c(z_0)$ must be found. From Eq. {16}, with $t = z_0$, and introducing C, it is

$$C(t) = \frac{c}{a^2} = \frac{2}{a} f_0(t) + s(t)(1 - 2t)$$
⁽²⁹⁾

Differentiating, it is

$$\frac{dC}{dt} = \frac{2}{a} \frac{df_0}{dt} + \frac{ds}{dt} (1 - 2t) - 2s = 0$$
(30)

$$\frac{\mathrm{d}f_0}{\mathrm{d}t} = -\frac{\mathbf{p}^2}{8a} \sin\left(\frac{\mathbf{p}}{2}t\right) \qquad \qquad \frac{\mathrm{d}s}{\mathrm{d}t} = -\frac{\mathbf{p}^3}{16a^2} \cos\left(\frac{\mathbf{p}}{2}t\right) \qquad \qquad \{31\}$$

$$\frac{\mathrm{d}C}{\mathrm{d}t} = \frac{2}{a} \frac{-\mathbf{p}^2}{8a} \sin\left(\frac{\mathbf{p}}{2}t\right) + (1-2t)\frac{-\mathbf{p}^3}{16a^2} \cos\left(\frac{\mathbf{p}}{2}t\right) - 2\frac{-\mathbf{p}^2}{8a^2} \sin\left(\frac{\mathbf{p}}{2}t\right) =$$

$$= (1-2t)\frac{-\mathbf{p}^3}{16a^2} \cos\left(\frac{\mathbf{p}}{2}t\right)$$
(32)

$$\frac{\mathrm{d}c}{\mathrm{d}t} = -\frac{\mathbf{p}^3}{16}(1-2t)\cos\left(\frac{\mathbf{p}}{2}t\right) = 0$$
^[33]

Eq. {33} yields $z_0 = t = \frac{1}{2}$ as the useful solution. Some values of c, a function implicitly given in Eq. {29}, are shown in Table 1, with the optimum solution highlighted.

The rejection fraction is c-1, so the smallest fraction, corresponding to $z_0 = 0.5$, is about 11 %.

z_0	$c(z_0)$
0	1.5708
0.1	1.3971
0.2	1.2652
0.3	1.1756
0.4	1.1258
0.5	1.1107
0.6	1.1229
0.7	1.1528

Table 1 – Factor *c* as a function of z_0

The optimum hat function is thus given by Eq. {6} and Eq. {7}, with $z_0 = \frac{1}{2}$ and a minimum rejection rate of about 11 %.

4. Conclusions

In Monte Carlo simulation, the acceptance-rejection transform method depends on a hat function, h. The closer it is to the target function, f, the better, i.e., the smaller is the rejection fraction, r. After its type is chosen, h can itself usually be optimized for minimum r, as in the present case. In this study, r is shown to range, for reasonable choices of h, from 57 % to a much better, optimum value of 11 %.

Acknowledgements

This study was made within the author's teaching and research activities in the "Centro de Processos Químicos" (Centre for Chemical Processes), Department of Chemical and Biological Engineering, Instituto Superior Técnico, Universidade Técnica de Lisboa (Technical University of Lisbon). The computing and Internet publishing was made at the "Centro de Informática do IST" (IST Informatics Centre).

References

- CASQUILHO, Miguel, 2008, Internet webpage: *http://web.ist.utl.pt/mcasquilho/compute/or/Fx-simrejcosine.php*.

*