Generalized Box-Müller Method for Generating $q$-Gaussian Random Deviates

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Abstract

The $q$-Gaussian distribution is known to be an attractor of certain correlated systems, and is the distribution which, under appropriate constraints, maximizes the entropy $S_q$, the basis of nonextensive statistical mechanics. This theory is postulated as a natural extension of the standard (Boltzmann-Gibbs) statistical mechanics, and may explain the ubiquitous appearance of heavy-tailed distributions in both natural and man-made systems. The $q$-Gaussian distribution is also used as a numerical tool, for example as a visiting distribution in Generalized Simulated Annealing. We develop and present a simple, easy to implement numerical method for generating random deviates from a $q$-Gaussian distribution based upon a generalization of the well known Box-Müller method. Our method is suitable for a larger range of $q$ values, $-\infty < q < 3$, than has previously appeared in the literature, and can generate deviates from $q$-Gaussian distributions of arbitrary width and center. MATLAB codes showing a straightforward implementation is also included.

1. Introduction

The Gaussian (normal) distribution is ubiquitous in probability and statistics due to its role as an attractor of independent systems with finite variance. It is also the distribution which maximizes the Boltzmann-Gibbs entropy

$$S_{BG} = E[-\log(f(X))] = -\int_{-\infty}^{\infty} \log[f(x)] f(x) dx$$

under appropriate constraints$^1$. There are many methods available to transform computed pseudorandom uniform deviates into normal deviates, for example the “ziggurat method” of Marsaglia and Tsang$^2$. One of the most popular methods is that of Box and Müller$^3$. Though not optimal in its properties, it is easy to understand and to implement numerically.

The $q$-Gaussian distribution arises as an attractor of certain correlated systems, or when maximizing the entropic form

$$S_q = \frac{1 - \int_{-\infty}^{\infty} p(x)^q \, dx}{q - 1} \quad (q \in \mathbb{R})$$

under appropriate constraints$^4$. Since $q$-Gaussian distributions are ubiquitous within the framework of “non-extensive statistical mechanics”$^5$ there is a need for a $q$-Gaussian generator. One application that has received widespread usage in chemistry, engineering, and computational sciences, is the so called
Generalized Simulated Annealing\textsuperscript{6,7,8}, in which the visiting steps for possible jump acceptance are determined by \( q \)-Gaussians instead of the traditional Gaussians. A recent paper by Deng et. al.\textsuperscript{9} specifies an algorithm to generate \( q \)-Gaussian random deviates as the ratio of a standard normal distribution and square root of an independent \( \chi^2 \) scaled by its degrees of freedom. However, since the resulting Gosset’s Student-\( t \) distribution is a special case of the \( q \)-Gaussian for \( q \) in the range 1 to 3, our method allows the generation of a fuller set of distributions\textsuperscript{10}.

In this paper, we generalize the Box-Müller algorithm to produce \( q \)-Gaussian deviates. Our technique works over the full range of interesting \( q \) values, from \(-\infty \) to 3. In what follows, we show analytically that the algorithm produces random numbers drawn from the correct \( q \)-Gaussian distribution and we demonstrate the algorithm numerically for several interesting values of \( q \). We note here the fact that, while the original Box-Müller algorithm produces pairs of independent Gaussian deviates, our technique produces \( q \)-Gaussian deviate pairs that are uncorrelated but not independent. Indeed, for \( q < 1 \) the joint probability density function of the \( q \)-Gaussian has support on a circle while the marginal distributions have support on intervals. Thus the joint distribution may not be recovered simply as the product of the marginal distributions.

2. Review of the Box-Müller Technique

We first review the well known method of Box-Müller for generating Gaussian deviates from a standard normal distribution. We then present a simple variation of this method useful for generating \( q \)-Gaussian deviates. Our method is easily understood and can be coded very simply using the pseudo-random number generator for uniform deviates available in almost all computational environments.

Box and Müller built their method from the following observations. Given

\[ Z_1, Z_2 \overset{iid}{\sim} N(0,1) \]

uncorrelated (hence in this case independent) standard normal distributions with mean 0 and variance 1, contours of their joint probability density function are circles with \( \Theta \equiv \arctan(Z_1/Z_2) \) uniformly distributed. Also, the square of a standard normal distribution has a \( \chi^2 \) distribution with 1 degree of freedom. Denote a \( \chi^2 \) random variable with \( \nu \) degrees of freedom as \( \chi^2_{\nu} \) and write \( Z^2 \sim \chi^2_1 \). Because the sum of two independent \( \chi^2 \) distributions each with 1 degree of freedom is again \( \chi^2 \) but with 2 degrees of freedom, the random variable defined as \( R^2 = Z_1^2 + Z_2^2 \) has a \( \chi^2_2 \) distribution. Related to this point, if a random variable \( R^2 \) has a \( \chi^2_2 \) distribution then \( U = \exp(-\frac{1}{2}R^2) \) is uniformly distributed. We are led to the Box-Müller transformations

\[
U_1 = \exp\left(-\frac{1}{2}(Z_1^2 + Z_2^2)\right) \\
U_2 = \frac{1}{2\pi} \arctan\left(\frac{Z_2}{Z_1}\right)
\]  

(2a,b)
and inverse transformations

\[ Z_1 = \sqrt{-2 \ln(U_1)} \cos(2\pi U_2), \]  

and

\[ Z_2 = \sqrt{-2 \ln(U_1)} \sin(2\pi U_2). \]  

We now apply these transformations assuming \( U_1 \) and \( U_2 \) are independent, uniformly distributed on the interval \((0,1)\), and show that \( Z_1 \) and \( Z_2 \) are normally distributed. Indeed, given a transformation \((Z_1, Z_2) = T(U_1, U_2)\) between pairs of random variables, we construct the joint density of \((Z_1, Z_2)\), denoted \( f_{Z_1, Z_2}(z_1, z_2) \), as

\[ f_{Z_1, Z_2}(z_1, z_2) = f_{U_1, U_2}(z_1, z_2) |J(z_1, z_2)| \]

where the Jacobian is given by

\[ J(z_1, z_2) = \frac{\partial u_1}{\partial z_1} \frac{\partial u_2}{\partial z_2} - \frac{\partial u_1}{\partial z_2} \frac{\partial u_2}{\partial z_1}. \]  

Since \( U_i \) and \( U_j \) are independent, uniformly distributed random variables on \((0,1)\) we immediately have \( f_{U_1, U_2}(z_1, z_2) = 1 \). Evaluation of the Jacobian yields

\[ f_{Z_1, Z_2}(z_1, z_2) = \frac{1}{2\pi} \exp\left(-\frac{z_1^2 + z_2^2}{2}\right) \]

\[ = \left[ \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z_1^2}{2}\right) \right] \left[ \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z_2^2}{2}\right) \right]. \]  

The Box-Müller method is thus very simple: start with two independent random numbers drawn from the range \((0,1)\), apply the transformations of Eqs. (3)-(4), and one arrives at two random numbers drawn from a standard Gaussian distribution (mean 0 and variance 1). The two random deviates thus generated are independent due to the separation of the terms in Eq. (7).

3. \textbf{The }q\text{-Gaussian Distribution}

Before presenting our generalization of the Box-Müller algorithm, we briefly review the definition and properties of the \(q\)-Gaussian function. First, we introduce the \(q\)-logarithm and its inverse, the \(q\)-exponential\(^{11}\), as

\[ \ln_q(x) \equiv \frac{x^{1-q} - 1}{1 - q} \quad x > 0 \]

and
These functions reduce to the usual logarithm and exponential functions when \(q = 1\). The \(q\)-Gaussian density is defined for \(-\infty < q < 3\) as

\[
p(x; \mu_q, \sigma_q) = A_q \sqrt{B_q} \left[1 + (q-1)B_q (x - \mu_q)^2 \right]^{\frac{1}{2(1-q)}}.
\]

where the parameters \(\mu_q\), \(\sigma_q^2\), \(A_q\), and \(B_q\) are defined as follows. First, the \(q\)-mean \(\mu_q\) is defined analogously to the usual mean, except using the so-called \(q\)-expectation value (based on the escort distribution), as follows

\[
\mu_q = \left\langle x \right\rangle_q = \frac{\int x \left[p(x)\right]^q dx}{\int \left[p(x)\right]^q dx}.
\]

Similarly, the \(q\)-variance, \(\sigma_q^2\) is defined analogously to the usual second order central moment, as

\[
\sigma_q^2 = \left\langle (x - \mu_q)^2 \right\rangle_q = \frac{\int (x - \mu_q)^2 \left[p(x)\right]^q dx}{\int \left[p(x)\right]^q dx}.
\]

When \(q = 1\), these expressions reduce to the usual mean and variance. The normalization factor is given by

\[
A_q = \begin{cases} 
\frac{\Gamma \left[\frac{1}{q-1}\right]}{\sqrt{\pi}} & q = 1 \\
\frac{\Gamma \left[\frac{1}{2(q-1)}\right] \frac{1}{\sqrt{\pi}}} {\Gamma \left[\frac{1}{q-1}\right]} & 1 < q < 3 \\
\frac{\Gamma \left[\frac{1}{q-1}\right]}{\sqrt{\pi}} & q = 0 \\
\frac{\Gamma \left[\frac{1}{2(q-1)}\right]}{\sqrt{\pi}} & q = 1 \\
\end{cases}
\]

Additionally, the \(q\)-Gaussian density is normalized by

\[
\int_{-\infty}^{\infty} p(x; \mu_q, \sigma_q) dx = 1.
\]

Finally, the width of the distribution is characterized by

\[
B_q = \left[(3 - q)\sigma_q^2\right]^{-1}.
\]

Denote a general \(q\)-Gaussian random variable \(X\) with \(q\)-mean \(\mu_q\) and \(q\)-variance \(\sigma_q^2\) as \(X \sim N_q(\mu_q, \sigma_q^2)\), and call the special case of \(\mu_q = 0\) and \(\sigma_q^2 = 1\)
a standard $q$-Gaussian, $Z \sim N_q(0,1)$. The density of the standard $q$-Gaussian distribution may then be written as

$$p(x, \mu_q = 0, \sigma_q = 1) = \frac{A_q}{\sqrt{3-q}} e^{\frac{-x^2}{q(3-q)}} = \frac{1}{\sqrt[3-q]{3-q}} \left[ 1 + \frac{q-1}{q} x^2 \right].$$  \tag{15}$$

We show below (Eq. 23) that the marginal distributions associated with our transformed random variables recover this form with new parameter $q'$. The $q$-Gaussian distribution reproduces the usual Gaussian distribution when $q = 1$, has compact support for $q < 1$, and decays asymptotically as a power law for $1 < q < 3$. For $3 \leq q$, the form given in Eq. (10) is not normalizable. The usual variance (second order moment) is finite for $q < 5/3$, and, for the standard $q$-Gaussian, is given by $\sigma^2 = (3-q)/(5-3q)$. The usual variance of the $q$-Gaussian diverges for $5/3 \leq q < 3$, however the $q$-variance remains finite for the full range $-\infty < q < 3$, equal to unity for the standard $q$-Gaussian.

4. **Generalized Box-Müller for $q$-Gaussian Deviates**

Our generalization of the Box-Müller technique is based on preserving its circular symmetry, while changing the behavior in the radial direction. Our algorithm starts with the same two uniform deviates as the original Box-Müller technique, and applies a similar transformation to yield $q$-Gaussian deviates. Thus it preserves the simplicity of implementation that makes the original Box-Müller technique so useful.

Indeed, given independent uniform distributions $U_1$ and $U_2$ defined on $(0,1)$, we define two new random variables $Z_1$ and $Z_2$ as

$$Z_1 = \sqrt{-2 \ln_q(U_1)} \cos(2\pi U_2) \quad \tag{16}$$

and

$$Z_2 = \sqrt{-2 \ln_q(U_1)} \sin(2\pi U_2). \quad \tag{17}$$

We now show that each of $Z_1$ and $Z_2$ is a standard $q$-Gaussian characterized by a new parameter $q' = \frac{3q-1}{q+1}$. Thus as $q$ (used in the $q$-log of the transformation) ranges over $(-1, \infty)$, the $q$-Gaussian is characterized by $q'$ in the range $(-\infty, 3)$, which is the interesting range for the $q$-Gaussian. For $q' \geq 3$ the distribution can not be normalized.

Proceed as follows. Obtain the inverse transformations as

$$U_1 = \exp_q \left\{ -\frac{1}{2} (Z_1^2 + Z_2^2) \right\} \quad \tag{18}$$

and
so that the Jacobian is

\[ J(z_1, z_2) = -\frac{1}{2\pi} \exp_q \left( -\frac{1}{2} \left( z_1^2 + z_2^2 \right) \right)^{\frac{1}{q}}. \]  

(20)

And, since \( f_{U_1, U_2}(u_1, u_2) = 1 \), we obtain the joint density of \( Z_1 \) and \( Z_2 \) as

\[ f_{Z_1, Z_2}(z_1, z_2) = \frac{1}{2\pi} \left( e^{-\frac{1}{2}(z_1^q + z_2^q)} \right)^{\frac{1}{q}} = \frac{1}{2\pi} e^{\frac{q}{2}(z_1^q + z_2^q)} . \]  

(21)

Note that in the limit as \( q \to 1 \) we recover the product of independent standard normal distributions as required.

The marginal distributions resulting from this joint density are standard \( q \)-Gaussian. As illustrated below for the case \( q > 1 \), one obtains the marginal distributions by integrating the joint density

\[ I = \frac{1}{2\pi} \int_{-\infty}^{\infty} f_{Z_1, Z_2}(z_1, z_2) \, dz_1 \]

\[ = \frac{1}{\sqrt{\pi}} \frac{\Gamma\left(\frac{q+1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)} \sqrt{\frac{1}{q-1}} \left(1-\frac{1}{2}(1-q)z_2^2\right)^{\frac{1}{2}} \left(1-\frac{1}{2}(1-q)z_2^2\right)^{\frac{1}{2}} . \]  

(22)

Note that, by the definition of \( q' \), we have \( \frac{1}{2}(q-1) = \frac{q'-1}{3-q'} \) and

\[ \frac{1}{2} \left( \frac{1+q}{1-q} \right) = \frac{1}{1-q'}, \]  

and so we obtain

\[ I = \frac{1}{\sqrt{\pi}} \frac{\Gamma\left(\frac{1}{q'-1}\right)}{\Gamma\left(\frac{3-q'}{2(q'-1)}\right)} \sqrt{\frac{3-q'}{3-q}} \left(1+\frac{q'-1}{3-q'}x^2\right)^{\frac{1}{2}} = A q' \sqrt{B} e^{-Ax^2}. \]  

(23)

As seen from Eq. 15 this is a standard \( q \)-Gaussian with parameter \( q' \).

An important result is that the standard \( q \)-Gaussian recovers the Student’s-t distribution with \( \eta \) degrees of freedom when \( q \equiv (3+\eta)/(1+\eta) \). Therefore, our method may also be used to generate random deviates from a Student’s-t distribution by taking \( q' = \frac{3+\eta}{1+\eta} \), or \( q = \frac{q'+1}{3-q'} = \frac{2+\eta}{\eta} \). Also, it is interesting to note that, in the limit as \( q' \to -\infty \) the \( q \)-Gaussian recovers a uniform distribution on the interval \((-1, 1)\).
To illustrate our method, we consider the following modified relative frequency histograms (empirical probability density functions) of generated deviates, with $q$-Gaussian density functions superimposed. We present first two typical histograms for $q' < 1$. Figure 1 shows the case $q' = -5.0$ and Figure 2 shows the case $q' = 1/7$. Both the empirical distributions show excellent agreement with the theoretical $q$-Gaussian density, which have compact support since $q' < 1$. For $q' > 1$, the distribution has heavy tails and so a standard modified relative frequency histogram is of little value. We show three different plots of the empirical distribution for the case $q' = 2.75$. In Figure 3 we show a semi-log plot of the empirical density function, which helps to illustrate the behavior in the near tails of the distribution. In Figure 4 we plot the $q$-log of the (appropriately scaled) distribution versus $x^q$, so the resulting distribution function appears as a straight line with slope equal to $-B_q$. Figure 5 provides another validation of the method. We transform as $Y = \log(|X|)$ to produce a random variable without heavy tails, which may be treated with a traditional histogram. This random variable has density

$$f_Y(y) = 2e^{y^q}A_q\sqrt{B_q} \left[ 1 - \frac{1}{2} (1 - q) e^{y^q} \right]^{\frac{1}{2} \left[ \frac{1}{1 - q} \right]}.$$  

(24)

We demonstrate the utility of the $q$-variance $\sigma_q^2$ as a characterization of heavy tail $q$-Gaussian distributions in Figure 6. For standard $q$-Gaussian data generated for various values of parameter $q$, we see that as $q \to 5/3$ the second order central moment (i.e., the usual variance) diverges, whereas the $q$-variance remains steady at unity. For $q \approx 3$ numerical determination of $\sigma_q^2$ is difficult.

The algorithm described in Eqs. 16-17 yields random deviates drawn from a standard $q$-Gaussian distribution. To produce deviates drawn from a general $q$-Gaussian distribution with $q$-mean $\mu_q$ and $q$-variance $\sigma_q^2$, one simply performs the usual transformation $X = \mu_q + \sigma_q Z$. Here $Z \sim N_q(0,1)$ results in $X \sim N_q(\mu_q, \sigma_q^2)$. Figure 7 illustrates this transformation, and also further illustrates the utility of the $q$-variance as a method of characterization. Shown are the variance and $q$-variance of sample data obtained by transforming standard $q$-Gaussian data, $Z \sim N_q(0,1)$ with $q' = 1.4$, via $X = 5 + 3Z \sim N_q(5,9)$. Data were generated for sample sizes $N_3$ ranging from 50 to 2000. As the sample size grows, the $q$-variance converges nicely to the expected value $\sigma^2 = 9$. The sample variances, however, converge relatively slowly to the predicted value $\sigma^2 = \left[ (3 - q')/(5 - 3q') \right] \sigma_q^2 = 18$ (where $(3 - q')/(5 - 3q') = 2$ is the variance of the untransformed data). The utility of the $q$-variance is illustrated even more dramatically in Figure 8 where $q' = 2.75$. Note the variance diverges as $N_3$ grows, whereas the $q$-variance remains at the predicted value of $\sigma_q^2 = 9$. 

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5. Summary and Conclusion

We have presented a method for generating random deviates drawn from a $q$-Gaussian distribution with arbitrary spread and center, and over the full range of meaningful $q$ values $-\infty < q < 3$. The method presented is simple to code and relatively efficient. The relationship between generating $q$ value and target $q'$ value was developed and verified.

It should be noted that the traditional Box-Müller method produces uncorrelated pairs of bivariate normal deviates. For the case of bivariate normality this implies that the deviates so produced are generated in independent pairs. For the $q$-Gaussian, however, even when the second order moment exists (i.e., $q < 5/3$) the deviate pairs are uncorrelated but not independent. It is an interesting question, unresolved at this point, as to whether these pairs are $q$-independent. Random variables which are $q$-independent are actually correlated, but with a special correlation structure. To be $q$-independent, the $q$-Fourier Transform of the sum of the random variables must be the $q$-product of the individual $q$-Fourier Transforms.

Applications of this $q$-Gaussian random number generator include many numerical techniques for which a heavy-tailed distribution is required, most notably for generating the visiting step sizes in generalized simulated annealing.

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![Theoretical density $p(x)$ and histogram of simulated data for a standard $q$-Gaussian distribution with $q' < 0$. The distribution has compact support for this $q'$.](image)
Figure 2: Theoretical density $p(x)$ and histogram of simulated data for a standard $q$-Gaussian distribution with $0 < q' < 1$. The distribution has compact support for this $q'$.

$q = 0.4, q' = 0.14286, N = 5E6$

Figure 3: Theoretical density $p(x)$ and histogram of simulated data for a standard $q$-Gaussian distribution with $1 < q' < 3$, truncated domain.

$q = 15, q' = 2.75, N = 5E6$
q = 15, \( q' = 2.75, N = 5 \times 10^6 

Figure 4: Theoretical density \( \ln \left( \frac{p(x)}{A_q \sqrt{B_q}} \right) \) and histogram of simulated data for a standard \( q \)-Gaussian distribution, as a function of \( x^2 \). Plotted in this form, the \( q \)-Gaussian appears as a straight line. The value of \( q' \) is the same as in Figure 3.

Figure 5: Theoretical density \( f(y) \) of the random variable \( Y = \log(|X|) \), and histogram of simulated data, for a standard \( q \)-Gaussian random variable \( X \). The value of \( q' \) is the same as in Figure 3.
Figure 6: Comparison of computed variance (circles) and $q$-variance (triangles). The usual second order central moment is seen to diverge for generated $q' > 5/3$. For $q \to -\infty$ the $q$-Gaussian approaches a uniform distribution on (-1,1) and so $\sigma^2 \to 1/3$. Very heavy tails for large $q$ renders computation of $q$-variance difficult.

$N_q(5,9), q' = 1.4$

Figure 7: Computed variance and $q$-variance for $q$-Gaussian distributions transformed by $X = 5 + 3Z \sim N_q(5,9)$. The $q$-variance is $\sigma_q^2 = 9$, and since $q' < 5/3$, the variance is finite, $\sigma^2 = 18$ for this value of $q'$. Shown are the results from 30 runs at each sample size, where sample sizes range from 50 to 2000. The $q$-variance shows much faster convergence than the variance.
Figure 8: Computed variance and $q$-variance for $q$-Gaussian distributions transformed by $X = 5 + 3Z \sim N_q(5,9)$. The $q$-variance remains finite, at the predicted value $\tilde{\sigma}_q^2 = 9$. However, since $q' > 5/3$, the variance is infinite. Shown are the results from 30 runs at each sample size, where sample sizes range from 50 to 2000.

6. **Generalized Box-Müller Pseudo Code**

We present, for convenience of implementation, a MATLAB code for the generalized Box-Müller method presented herein. The code shown is intended to demonstrate the algorithm, and is not optimized for speed.

The algorithm is straightforward to implement, and is shown below as two functions. The first function $qGaussianDist$ generates the $q$-Gaussian random deviates, and calls the second function, $log_q$, which calculates the $q$-log. The method relies on a high quality uniform random number generator that produces deviates in the range $(0,1)$. The MATLAB command producing these deviates is called $rand$, and in the default implementation in version 7.1, uses a method due to Marsagalia. The other MATLAB-specific component to the code given below is the built-in value $\texttt{eps}$, whose value is approximately $1E-16$ and which represents the limit of double precision.

```matlab
function qGaussian = qGaussianDist(nSamples,qDist)
    
    % Returns random deviates drawn from a q-gaussian distribution
    % The number of samples returned is nSamples.
    % The q that characterizes the q-Gaussian is given by qDist.
    
    % Check that q < 3
    if qDist < 3
        % Calculate the q to be used on the q-log
        qGen = (1 + qDist)/(3 - qDist);
    end

    % Initialize the output vector
    qGaussian = zeros(1,nSamples);
```

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% Loop through and populate the output vector
for k = 1:nSamples
    % Get two uniform random deviates
    % from built-in rand function
    u1 = rand;
    u2 = rand;

    % Apply the generalized Box-Muller algorithm,
    % taking only one of two possible values
    qGaussian(k) = sqrt(2*log_q(u1,qGen))*sin(2*pi*u2);
end

% Return 0 and give a warning if q >= 3
else
    warning('The input q value must be less than 3')
    qGaussian = 0;
end
end

function a = log_q(x,q)
    
    % Returns the q-log of x, using q
    %
    % Check to see if q = 1 (to double precision)
    if abs(q - 1) < 10*eps
        % If q is 1, use the usual natural logarithm
        a = log(x);
    else
        % If q differs from 1, use the definition of the q-log
        a = (x.^(1-q) - 1)./(1-q);
    end
end

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