Sampling from the Maxwell-Juttner distribution

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ABSTRACT. The Maxwell-Jüttner distribution pertains to the speeds of particles in a hypothetical gas of relativistic particles. We consider the generalized form of this law in $\mathbb{R}^d$, and show how to generate a random variate from this distribution. In particular, one can sample the radius of the d-dimensional random vector in expected time uniformly bounded over all dimensions d and shape parameters (temperatures).

KEYWORDS AND PHRASES. Random variate generation. Simulation. Monte Carlo method. Expected time analysis. Maxwell-Jüttner distribution. Special relativity. Astrophysics. Numerical methods. Probability theory. Energy flux. Plasmas. Maxwell-Boltzmann distribution. Particle distributions.

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1. Introduction

The relativistic Maxwell or Jüttner-Synge distribution, now called the Maxwell-Jüttner distribution (Jüttner, 1911; Synge, 1957; Maxwell, 1860) is a spherically symmetric distribution in $\mathbb{R}^3$ with a density given by

$$\frac{\alpha}{4\pi K_2(\alpha)}\, e^{-\alpha\sqrt{1+(y1^2+y_2^2+y_3^2)}}, y=(y_1,y_2,y_3)\in\mathbb{R}^3,$$

where $\alpha > 0$ is a shape parameter, and K_2 is the modified Bessel function of the second kind, also known as the Macdonald function. In particle simulations, α is inversely proportional to the plasma temperature. The radius $x = \|y\| = \sqrt{y_1^2+y_2^2+y_3^2}$ has density given by

$$f(x) = \frac{\alpha x^2}{4\pi K_2(\alpha)}\, e^{-\alpha\sqrt{1+x^2}}, x \geq 0.$$

Using the the Macdonald function (Abramowitz and Stegun, 1972, p. 376) defined by

$$K_n(z) = \frac{\sqrt{\pi}(z/2)^n}{\Gamma(n+1/2)} \int_1^\infty (t^2-1)^{n-1/2} e^{-zt}\, dt,$$

the d-dimensional generalizations of the densities are

$$\frac{\alpha^{\frac{d-1}{2}}}{2^{\frac{d+1}{2}}\pi^{\frac{d-1}{2}} K_{\frac{d+1}{2}}(\alpha)}\, e^{-\alpha\sqrt{1+\|y\|^2}}, y=(y_1,\ldots,y_d)\in\mathbb{R}^d, \tag{1}$$

and

$$f(x) = \frac{d x^{d-1}\sqrt{\pi}\alpha^{\frac{d-1}{2}}}{2^{\frac{d+1}{2}}\Gamma\left(\frac{d}{2}+1\right) K_{\frac{d+1}{2}}(\alpha)}\, e^{-\alpha\sqrt{1+x^2}}, x \geq 0, \tag{2}$$

respectively. Such d-dimensional generalizations were considered, e.g., by Chacon-Acosta, Dagdug and Morales-Tecotl (2009). In $\mathbb{R}^d$, $1/\alpha$ can be shown to coincide with the thermodynamic definition of temperature.

The objective of this note is to propose two algorithms for generating random variates from the radial density for general $d \geq 3$. The simpler algorithm has expected time proportial to d, uniformly over all values of α. The more advanced algorithm has expected time uniformly bounded over all values of $d \geq 3$ and $\alpha \geq 0$. It should be noted that once the radius R has been generated, a random variate uniformly distributed on (the surface of) the ball in $\mathbb{R}^d$ is easily obtained in time proportional to d. For example, it suffices to generate d i.i.d. standard normal random variables $(X_1,\ldots,X_d)$ and return

$$\frac{R}{||X||}(X_1,\ldots,X_d),$$

where $||X||$ is the L_2 norm of $(X_1,\ldots,X_d)$. Simulations show that for small values of d, the simpler algorithm is faster, but that ranking is flipped for all large values of d.

Simulation from the radial density (2) for $d = 3$ was started by Sobol (1976) and Pozdnyakov, Sobol and Sunyaev (1977, 1983). The first algorithm that was uniformly fast in the parameter α was due to Canfield, Howard and Liang (1987). That algorithm was refined and improved by Zenitani and Nakano (2022). Another uniformly fast algorithm was proposed by Swisdak (2013). That too was refined later by Zenitani (2024).

2. A simple algorithm

We generalize the method first suggested by Canfield, Howard and Liang (1987) for $d = 3$ by applying the transformation

$$z = \alpha\left(\sqrt{1+x^2}-1\right), x = \sqrt{\left(\frac{z+\alpha}{\alpha}\right)^2 - 1}$$

so that density (2) (in x) is transformed into the following density (in z),

$$g(z) = cz^{\frac{d-2}{2}}(z+2\alpha)^{\frac{d-2}{2}}(z+\alpha)e^{-z}, z \geq 0, \tag{3}$$

where c is a constant depending upon α and d. In the remainder of this section, we show how to generate a random variate Z with density (3) in $O(d)$ expected time, uniformly over all values of $\alpha > 0$. A random variate with density (2) can then be obtained by setting

$$X = \sqrt{\left(\frac{Z+\alpha}{\alpha}\right)^2 - 1}.$$

If d is even, then we define $\kappa \stackrel{\text{def}}{=} (d-2)/2$, use the binomial expansion of the factor $(z+2\alpha)^\kappa$, and rewrite g as a mixture of gamma densities. For that purpose, we will use the notation

$$\gamma_a(x) = \frac{x^{a-1}e^{-x}}{\Gamma(a)}, x > 0,$$

for the gamma density with parameter $a > 0$. Then

$$g(z) = \sum_{0 \leq i \leq \kappa, 1 \leq j \leq 2} \frac{q_{i,j}}{q} \gamma_{\kappa+i+j}(z),$$

where

$$q_{i,j} = \binom{\kappa}{i}(2\alpha)^{\kappa-i}\alpha^{2-j}(\kappa+i+j-1)!,$$

and $q = \sum_{0 \leq i \leq \kappa, 1 \leq j \leq 2} q_{i,j}$ is a normalization factor. In other words, one first picks a pair (i, j) with probabilities proportional to $q_{i,j}$ and then returns a gamma random variable with parameter $\kappa + i + j$. The former can be done in time $O(d)$, while for gamma random variables, there is an enormous choice of methods, including the algorithms by Marsaglia and Tsang (1981), Schmeiser and Lal (1980), Cheng and Feast (1979), Cheng (1977), Le Minh (1988), Marsaglia (1977), Ahrens and Dieter (1982), and Devroye (2014). All of the aforementioned methods have expected time uniformly bounded when the gamma parameter is at least one. See the surveys in Devroye (1986) and Luengo (2022) for more references.

When d is odd, we proceed by setting $\kappa = (d-3)/2$, and use the inequality

$$\begin{aligned}
g(z) &= cz^{\kappa+1/2}(z+2\alpha)^{\kappa+1/2}(z+\alpha)e^{-z} \\
&= cz^\kappa(z+2\alpha)^\kappa(z^{3/2}+\alpha\sqrt{z})\sqrt{z+2\alpha}e^{-z} \\
&\leq cz^\kappa(z+2\alpha)^\kappa(z^{3/2}+\alpha\sqrt{z})\left(\sqrt{z}+\sqrt{2\alpha}\right)e^{-z} \\
&= cz^\kappa(z+2\alpha)^\kappa\left(z^2+z^{3/2}\sqrt{2\alpha}+\alpha z+\sqrt{2\alpha^3}\sqrt{z}\right)e^{-z} \\
&\stackrel{\text{def}}{=} h(z).
\end{aligned}$$

If Z is a random variable with density proportional to h, then by von Neumann's rejection method (see, e.g., Devroye, 1986), if we accept Z with probaility

$$\frac{\sqrt{Z+2\alpha}}{\sqrt{Z}+\sqrt{2\alpha}},$$

then, upon acceptance, Z has the desired density g. The expected number of steps in this rejection method does not exceed $\sqrt{2}$.

For h, we can proceed as in the case when d is even, as κ is integer-valued. Using the binomial expansion once again, the density proportional to h can be rewritten as

$$\sum_{0\le i\le\kappa, 3\le j\le 6} \frac{q_{i,j}}{q}\gamma_{\kappa+i+j/2}(z),$$

where

$$q_{i,j} = \binom{\kappa}{i}(2\alpha)^{\kappa-i}\alpha^{\frac{6-j}{2}}(\sqrt{2})^{j \bmod 2}\,\Gamma(\kappa+i+j/2)$$

and $q = \sum_{0\le i\le\kappa,3\le j\le 6} q_{i,j}$ is a normalization factor. So, one first picks a pair (i,j) with probabilities proportional to $q_{i,j}$ and then returns Z, a gamma random variable with parameter $\kappa+i+j/2$.

For $d=3$, and thus $\kappa=0$, we rediscover the method of Canfield, Howard and Liang (1987). For large values of d, the computation of the weights $q_{i,j}$ in the gamma mixture may become cumbersome because of word size limitations. Luckily, one can generate random variates from (2) in constant expected time uniformly over both α and the dimension d, as we will show in the next section.

3. An advanced algorithm

For the advanced algorithm, we once again proceed by first generating a random variate Z with the transformed density g defined in (3). To this end, we note that g is log-concave and thus unimodal. It is convenient to work with $\rho(z) = \log(g(z)/c)$. Observe that, with $\kappa = (d-2)/2$,

$$\rho(z) = \log(z+\alpha) + \kappa\log(z+2\alpha) + \kappa\log(z) - z, \tag{4}$$

$$\rho'(z) = \frac{1}{z+\alpha} + \frac{\kappa}{z+2\alpha} + \frac{\kappa}{z} - 1, \tag{5}$$

and

$$\rho''(z) = -\frac{1}{(z+\alpha)^2} - \frac{\kappa}{(z+2\alpha)^2} - \frac{\kappa}{z^2}. \tag{6}$$

Formally, we have $g(z)=0$ for $z<0$ and thus $\rho(z)=-\infty$ for $z<0$. The mode m occurs as the unique positive real solution of the third order polynomial equation $\rho'(m)=0$, which has three real roots. That equation can be written as

$$m^3 + am^2 + bm + c = 0, a = 3\alpha - 1 - 2\kappa, b = 2\alpha^2 - 2\alpha - 4\alpha\kappa, c = -2\alpha^2\kappa.$$

To this end, we can use Viète's formula (see, e.g., Nickalls, 2006), which describes the three real roots as follows:

$$m = -\frac{a}{3} + 2\sqrt{-\frac{p}{3}}\cos\left(\frac{2}{3}\arctan\sqrt{\frac{\sqrt{-4p^3}-\sqrt{27q^2}}{\sqrt{-4p^3}+\sqrt{27q^2}}} - \frac{2\pi k}{3}\right), k = 0, 1, 2,$$

where

$$p = b - a^2/3, q = \frac{1}{27}(2a^3 - 9ab + 27c).$$

In our case, the unique positive solution occurs for the choice $k = 0$ in Viète's formula.

Since $\rho''' \geq 0$ everywhere, ρ'' is monotonically increasing. Thus, by Taylor's theorem with remainder,

$$\rho(z) \geq \rho(m) - (z-m)^2 \frac{|\rho''(m)|}{2}, z \geq m,$$

and

$$\rho(z) \leq \rho(m) - (z-m)^2 \frac{|\rho''(m)|}{2}, z \leq m.$$

Therefore, for $z \leq m$, there is a simple gaussian bound. This leaves us with the problem of bounding $\rho(z)$ for $z > m$. Taylor's series expansion suggests that around the mode, $\rho(z)$ can be approximated by $\rho(m) + \rho''(m)(z-m)^2/2$. Following the ideas developed in Devroye (2014), we can hope to develop a good upper bound for g by a flat part around the mode and an exponential tail that starts at a point z where $\rho(z) = \rho(m) - 1$. Taylor's approximation suggests the cut-off point $z^+ = m + \Delta$, where

$$\Delta = \sqrt{\frac{2}{|\rho''(m)|}}.$$

The upper bound on g now follows by the concavity of ρ:

$$g(z)/c \leq h(z) \stackrel{\text{def}}{=} \begin{cases} e^{\rho(m) - \frac{(z-m)^2}{\Delta^2}} & \text{if } z < m, \\ e^{\rho(m)} & \text{if } m \leq z \leq z^+ - \delta \ , \\ e^{\rho(m) + \rho'(z^+)(z - z^+ + \delta)} & \text{if } z > z^+ - \delta. \end{cases}$$

Here, $\delta = (\rho(m) - \rho(z^+))/|\rho'(z^+)|$ is picked such that the bounding line is tangential to $\log(h)$ at the point z^+.

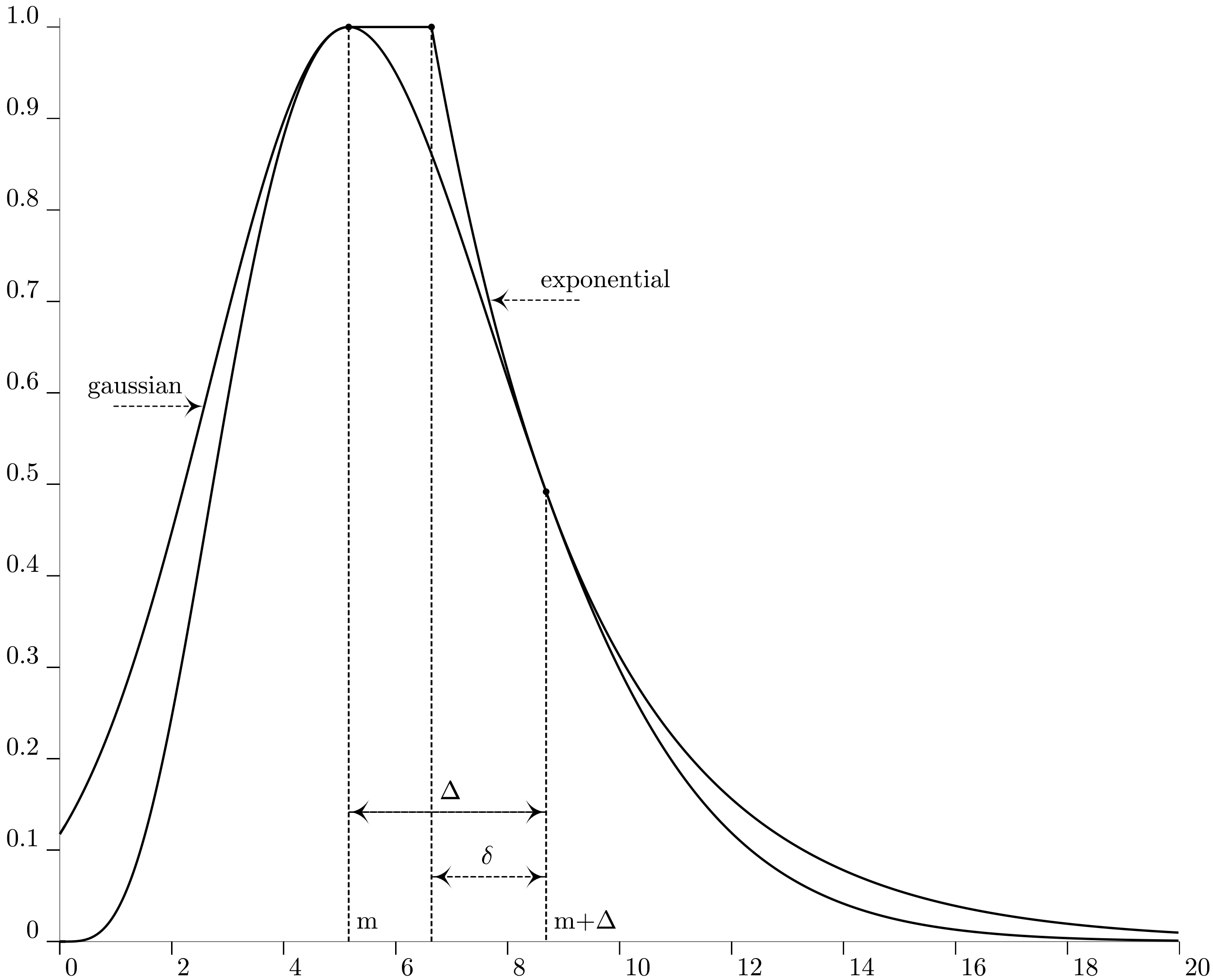

Figure 1. The transformed Maxwell-Jüttner density (3) is shown for $\alpha = 10$ and dimension $d = 10$, after rescaling the value at the mode m to one. The top curve is used for rejection: it consists of a gaussian left tail, an exponential right tail, and a flat mid-section.

When the upper bound h is used in von Neumann's rejection method, one realizes that the cumbersome constant c does not matter. The areas under the left and right tail bound and the flat middle section of h are, respectively,

$$p_\ell = \frac{e^{\rho(m)}\sqrt{\pi}\Delta}{2}, p_r = \frac{e^{\rho(m)}}{|\rho'(z^+)|}, \text{and } p_m = e^{\rho(m)}\,(\Delta - \delta).$$

We summarize the proposed algorithm in which we use the fact that an exponential random variable E is distributed as $\log(1/U)$, where U is uniformly distributed on $[0,1]$. Also, we note that if N is standard normal, then $N^2/2$ can be obtained by the Box-Müller method (see, e.g., Devroye, 1986), as $E\cos^2(\pi U)$ or as $E(1+\cos(\pi U))/2$.

the algorithm for density (2)

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input:  parameter α > 0, dimension d ≥ 3
set κ = (d − 2)/2
define the functions ρ, ρ' and ρ'' as in (4-6)
let m be the location of a mode of g by solving a cubic equation
define Δ = √(2/|ρ''(m)|), z⁺ = m + Δ, δ = (ρ(m) − ρ(z⁺))/|ρ'(z⁺)|
set p_ℓ = e^{ρ(m)} Δ √π / 2, p_r = e^{ρ(m)} / |ρ'(z⁺)|, p_m = (Δ − δ) e^{ρ(m)}, p = p_ℓ + p_m + p_r
repeat let V be uniform on [0,1]
        if V < p_ℓ/p then
                    set Z ← m − Δ|N|/√2
                    where N is a standard normal random variate
                    Accept ← [Z ≥ 0] ∩ [ρ(m) − N²/2 − E' ≤ ρ(Z)]
                    where E' is standard exponential
        if V > 1 − p_r/p then
                    set Z ← m + Δ − δ + E/|ρ'(z⁺)|
                    where E is standard exponential
                    Accept ← [ρ(m) − E − E' ≤ ρ(Z)]
                    where E' is standard exponential
        if p_ℓ/p ≤ V ≤ 1 − p_r/p then
                    set Z ← m + U(Δ − δ)
                    where U is uniform on [0,1]
                    Accept ← [ρ(m) − E' ≤ ρ(Z)]
                    where E' is standard exponential
until Accept
        (Z now has density (3))
return X ← √(((Z + α)/α)² − 1)
        (X has density (2))
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The design was based on a heuristic. We are now left with the task of showing that the expected number of iterations in the rejection algorithm is bounded by a constant, uniformly over all $\alpha > 0$ and $d \geq 3$.

THEOREM 1. *The algorithm given above halts after an expected number of iterations not exceeding*

$$e\left(3+\sqrt{\frac{\pi}{4}}+\sqrt{\frac{8}{\kappa}}\right),$$

where $\kappa = (d-2)/2$.

Proof. As pointed out above, $\rho(z^+) \geq \rho(m) - 1$. As the expected number of steps is

$$\frac{\int_0^\infty h(z)\,dz}{\int_0^\infty (g(z)/c)\,dz},$$

we first lower bound $\int_0^\infty g/c = \int_0^\infty e^{\rho(z)}\,dz$ by $\Delta e^{\rho(z^+)} \geq (\Delta/e)e^{\rho(m)}$, ignoring the contributions from all other parts of the halfline but $[m, z^+]$. Since $p_r = e^{\rho(m)}/|\rho'(z^+)|$, we upper bound $\int h$ by $p = p_\ell + p_r + p_m \leq (1/|\rho'(z^+)| + (\Delta - \delta)(1 + \sqrt{\pi/4}))e^{\rho(m)}$. The ratio of upper over lower bound is not more than

$$e(1 + \sqrt{\pi/4}) + \frac{e}{\Delta|\rho'(z^+)|}.$$

Now,

$$|\rho'(m + \Delta)| = |\rho'(m + \Delta) - \rho'(m)| \geq \frac{\kappa}{m} - \frac{\kappa}{m + \Delta} = \frac{\kappa\Delta}{m(m + \Delta)}.$$

Thus,

$$\Delta|\rho'(z^+)| \geq \frac{\kappa\Delta^2}{m(m + \Delta)} = \frac{2\kappa}{m(m + \Delta)|\rho''(m)|}.$$

Since $\kappa \geq 1/2$ and $\rho''(m) \leq (2\kappa + 1)/m^2$, we have

$$\Delta|\rho'(z^+)| \geq \frac{2\kappa}{(2\kappa + 1)(1 + \Delta/m)} \geq \frac{1}{2(1 + \Delta/m)} \geq \frac{1}{2(1 + \sqrt{2/\kappa})},$$

where in the last inequality, we used the fact that $\Delta \leq \sqrt{2m^2/\kappa}$. Therefore, the expected number of iterations in the algorithm is not more than

$$e(1 + \sqrt{\pi/4}) + 2e(1 + \sqrt{2/\kappa}).$$

□

We observe that the proof above uses various loose bounds and can be tightened. We also note that as the dimension tends to ∞, the bound in Theorem 1 tends to $e(3 + \sqrt{\pi/4})$. In addition, the algorithm can be tightened a bit by optimizing the position of the tangent point z^+ for the bounding function. Finally, the design principle for log-concave densities based on the manner of obtaining Δ can be used in many other examples as well.

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