On transforming random variables

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2024-04-08

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Consider a random vector $\mathbf{X}$ in the d-dimensional space, whose components $\{X_i, i = 1, \cdots, d\}$ are independent normal random variables. To start with, the components are assumed to follow standard normal distributions, namely their common variance is one. The probability density function (PDF) of $\mathbf{X}$ is

$$p_{\mathbf{X}}(x_1, \cdots, x_d) = \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2}\sum_{i=1}^{d} x_i^2\right)$$

What is the PDF of the modulus squared of $\mathbf{X}$? We are searching for the CDF of the random variable Q:

$$Q = \sum_{i=1}^{d} X_i^2$$

We indicate with $F_Q(q)$ the cumulative distribution function (CDF):

$$F_Q(q) = \Pr(Q \leq q) = \Pr\left(\sum_{i=1}^{d} X_i^2 \leq q\right) \tag{1}$$

The probability in Equation 1 can be computed as follows:

$$F_Q(q) = \int_{\sum_i x_i^2 \leq q} \cdots \int p_{\mathbf{R}}(x_1, x_2, \cdots, x_d)\, dx_1\, dx_2 \cdots dx_d$$

We can pass to spherical coordinates by setting:

$$\sum_{i=1}^{d} x_i^2 = r$$

Because of the spherical symmetry of both the multivariate Gaussian PDF and the domain of integration (a hypersphere), the integrand is angle-independent and we need to integrate just over the radius of the hypersphere. It is known from differential geometry that an element of volume dV integrated over the angles in the d-dimensional space is equal to:

$$dV = Dr^{d-1}dr \tag{2}$$

where D is a constant. Therefore:

$$F_Q(q) = F_0 \int_0^{\sqrt{q}} \exp(-r^2/2)\, r^{d-1} dr$$

If we change variable in the integral:

$$r = \sqrt{q'}, \quad dr = \frac{1}{2\sqrt{q'}} dq'$$

and collect all the constants into F_0', we obtain:

$$F_Q(q) = F_0' \int_0^{q} \exp(-q'/2)\, (q')^{\,d/2-1} dq'$$

The PDF of Q is then

$$p_Q(q) = F_0' \exp(-q/2)\, q^{\,d/2-1}$$

The constant F_0' can be derived from the condition of normalization:

$$F_0' \int_0^{\infty} \exp(-q/2)\, q^{\,d/2-1} dq = 1$$

Recall the definition of the **gamma function**:

$$\Gamma(p) = \int_0^{\infty} \exp(-x) x^{p-1} dx$$

Gamma function and normalization factor

Some useful properties of the gamma function to remember are the following:

$$\begin{aligned}
\Gamma(1) &= 1 \\
\Gamma(1/2) &= \sqrt{\pi} \\
\Gamma(p+1) &= p\,\Gamma(p) \\
\Gamma(p+1) &= p! \quad p \in \mathbb{N} \\
\Gamma(p+1) &= p(p-1)(p-2)\cdots\frac{3}{2}\cdot\frac{1}{2}\sqrt{\pi} \quad p \text{ half-integer}
\end{aligned}$$

For the calculations to follow, related to the cases when $d = 1, 2, 3$, the normalization factor $1/(2^{d/2}\Gamma(d/2))$ in Equation 3 is equal to

$$\begin{aligned}
d = 1 \rightarrow F_0' &= \frac{1}{\sqrt{2\pi}} \\
d = 2 \rightarrow F_0' &= \frac{1}{2} \\
d = 3 \rightarrow F_0' &= \frac{1}{\sqrt{2\pi}}
\end{aligned}$$

In conclusion:

$$\boxed{p_Q(q) = \frac{1}{2^{d/2}\Gamma(d/2)}\exp(-q/2)\,q^{d/2-1}, \quad q \geq 0} \tag{3}$$

This is the PDF of the χ-squared random variable with d degrees of freedom. The mean value and the variance of Q are:

$$\begin{cases} E[Q] = d \\ \mathrm{Var}(Q) = 2d \end{cases} \tag{4}$$

Functions of a random variable

Let X be a continuous random variable with PDF $p_X(x)$ and let Z be the random variable depending on X through the functional relation:

$$Y = f(X)$$

For each $z \in \mathbb{R}$, find the values of x that solve the equation $x = f^{-1}(z)$ (we assume that

$f^{-1}(\cdot)$ exists and that it is differentiable):

$$x_i = f^{-1}(z), i = 1, \cdots, n$$

It can be proven that:

$$\boxed{p_Z(z) = \sum_{i=1}^{n} \frac{p_X(x_i)}{|f'(x_i)|}} \tag{5}$$

The analogous rule in the multivariate case $\mathbf{Z} = \mathbf{f}(\mathbf{X})$ ($\mathbf{Z} \in \mathbb{R}^m, \mathbf{X} \in \mathbb{R}^m$) is written:

$$\boxed{p_{\mathbf{Z}}(\mathbf{z}) = \sum_{i=1}^{n} p_{\mathbf{X}}(\mathbf{x}_i) \big| \det \mathbf{J}(\mathbf{x}_i) \big|} \tag{6}$$

where $\mathbf{x}_i = \mathbf{f}^{-1}(\mathbf{z}), i = 1, \cdots n$. If all functions $f_i(\cdot)$ are assumed to be differentiable, the ij-element of the $m \times m$ Jacobian matrix $\mathbf{J}$ is given by:

$$J_{ij} = \frac{\partial f_i^{-1}}{\partial z_j} \tag{7}$$

The Jacobian matrix is calculated for each $\mathbf{x}_i = \mathbf{f}^{-1}(\mathbf{z})$.
It is worth noting that the calculation of the integrals over the angular coordinates in Equation 2 can be managed by passing from Cartesian coordinates to polar coordinates ($d = 2$) or spherical coordinates ($d = 3$), which requires to consider, in place of the differential element $dx\,dy$ in $\mathbb{R}^2$, the differential element $|\det \mathbf{J}(r, \theta)| dr\, d\theta$ and, in place of the differential element $dx\, dy\, dz$ in $\mathbb{R}^3$, the differential element $|\det \mathbf{J}(r, \phi, \theta)| dr\, d\phi\, d\theta$ (see below for details about the calculations).

Now, we want to consider specifically the following three cases.

Unidimensional case ($d = 1$)

Apparently, we do not have any angle over which to integrate. However, we have:

$$dV = 2r\, dr$$

Namely in Equation 2, we have $D = 2$:

$$q = r^2 \rightarrow dq = 2r\, dr$$

The reason for the factor $D = 2$ is that, in geometrical terms, for any vector aligned in one direction, we always have another vector, with the same modulus, oriented in the opposite direction.

We can take another route for the calculation. For $d = 1$, the density of the modulus squared Q can be obtained from the density of the standard normal variable by using Equation 5 for the case when $Q = X^2$. Inverting $f(\cdot)$ gives rise to two values for x, namely $x_1 = \sqrt{q}$ and $x_2 = -\sqrt{q}$:

$$p_Q(q) = \frac{p_X(\sqrt{q})}{|f'(\sqrt{q})|} + \frac{p_X(-\sqrt{q})}{|f'(-\sqrt{q})|}$$

In conclusion:

$$\boxed{p_Q(q) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{q}}\exp(-q/2), \quad q \geq 0}$$

This is the same as Equation 3, with $d = 1$ ($F_0' = 1/\sqrt{2\pi}$). The mean value and the variance of the random variable Q are, see Equation 4:

$$\begin{cases} E[Q] = 1 \\ \mathrm{Var}(Q) = 2 \end{cases}$$

Bidimensional case ($d = 2$)

When $d = 2$, the Cartesian coordinates $x = x_1, y = x_2$ can be expressed in terms of the polar coordinates (r, θ) using the algorithm, see Figure 1:

$$\begin{cases} x = r\cos\theta \\ y = r\sin\theta \end{cases} \tag{8}$$

The Jacobian associated to the transformation is written:

$$J(r,\theta) = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{bmatrix} \to |\det J(r,\theta)| = r$$

The integral Equation 2 is then:

$$dV = \int_0^{2\pi} r\, d\theta\, dr = 2\pi r\, dr \to D = 2\pi$$

The χ squared density with two degrees of freedom is:

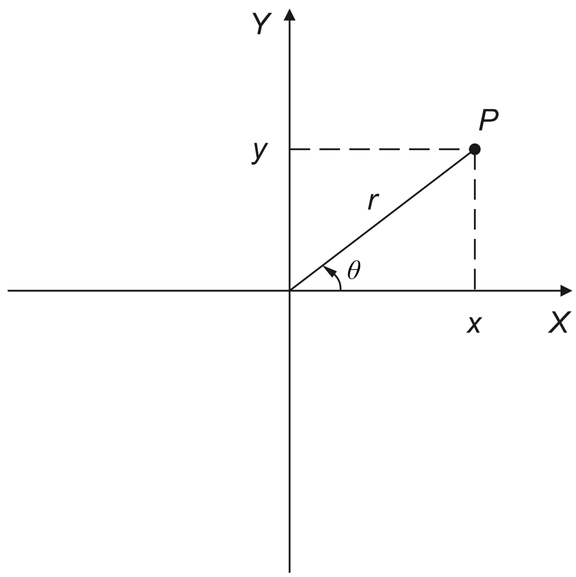

Figure 1: The generic point P is identified by the two coordinates r, θ.

$$\boxed{p_Q(q) = \frac{1}{2}\exp(-q/2), \quad q \geq 0}$$

The mean value and the variance of the random variable Q are, see Equation 4:

$$\begin{cases} E[Q] = 2 \\ \mathrm{Var}(Q) = 4 \end{cases}$$

Tridimensional case ($d = 3$)

When $d = 3$, the Cartesian coordinates $x = x_1, y = x_2, z = x_3$ can be expressed in terms of the spherical coordinates (r, ϕ, θ) ($r \geq 0, \phi \in [0, 2\pi], \theta \in [0, \pi]$) using the algorithm, see Figure 2.

$$\begin{cases} x = r \sin\theta \cos\phi \\ y = r \sin\theta \sin\phi \\ z = r \cos\theta \end{cases} \tag{9}$$

The Jacobian associated to the transformation is written:

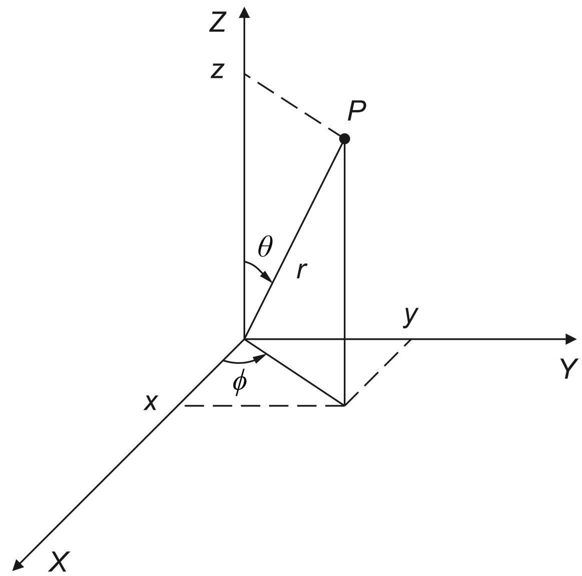

Figure 2: The generic point P is identified by the three coordinates r, ϕ, θ.

$$J(r,\theta) = \begin{bmatrix} \dfrac{\partial x}{\partial r} & \dfrac{\partial x}{\partial \phi} & \dfrac{\partial x}{\partial \theta} \\ \dfrac{\partial y}{\partial r} & \dfrac{\partial y}{\partial \phi} & \dfrac{\partial y}{\partial \theta} \\ \dfrac{\partial z}{\partial r} & \dfrac{\partial z}{\partial \phi} & \dfrac{\partial z}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \sin\theta\cos\phi & -r\sin\theta\sin\phi & r\cos\theta\cos\phi \\ \sin\theta\sin\phi & r\sin\theta\cos\phi & r\cos\theta\sin\phi \\ \cos\theta & 0 & -r\sin\theta \end{bmatrix} \to |\det J(r,\theta)| = r^2\sin\theta$$

The integral Equation 2 is then:

$$dV = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \, r^2 \, dr = 4\pi r^2 \, dr \to D = 4\pi$$

The χ squared density with three degrees of freedom is:

$$\boxed{p_Q(q) = \sqrt{\frac{q}{2\pi}} \exp(-q/2), \quad q \geq 0}$$

The mean value and the variance of the random variable Q are, see Equation 4:

$$\begin{cases} E[Q] = 3 \\ \mathrm{Var}(Q) = 6 \end{cases}$$

Rather than the modulus squared Q of $\mathbf{R}$, we can be interested in determining the PDF of the modulus R. We consider the transformation $R = \sqrt{Q}$ and the rule exposed in Equation 5

$$\boxed{p_R(r) = \frac{p_Q(r^2)}{1/2r} = \frac{2}{2^{d/2}\Gamma(d/2)} \exp(-r^2/2)\, r^{d-1}, \quad r \geq 0}$$

In Table 1 we report the expression of the PDF of R in the three spaces $\mathbb{R}, \mathbb{R}^2, \mathbb{R}^3$ examined so far. For the sake of broader generality, the PDFs are written for the case when the components of $\mathbf{R}$ are non-standard, namely their common variance is not one, but σ^2: in the calculation, we need to change r' in $r' = r/\sigma$, with a factor $1/\sigma$ appearing in the expression of the PDF (this is due to $dr' = dr/\sigma$).

Table 1: PDF of the modulus of random vectors whose components are independent, normally distributed with common variance σ^2.

dimension	name	PDF
$d = 1$	1D-Maxwell	$p_R(r) = \frac{2}{\sqrt{2\pi}\sigma} \exp(-r^2/2\sigma^2)$
$d = 2$	Rayleigh	$p_R(r) = \frac{r}{\sigma^2} \exp(-r^2/2\sigma^2)$
$d = 3$	3D-Maxwell	$p_R(r) = \frac{2}{\sqrt{2\pi}} \frac{r^2}{\sigma^3} \exp(-r^2/2\sigma^2)$

Exercise 0.1. Find the energy density of the molecules of an ideal gas at the absolute temperature T.

In an ideal gas the velocity components V_x, V_y, V_z of the molecules are random variables that satisfy the condition of the central limit theorem. Hence, thee components are independent normal. Their common variance σ^2 is:

$$\sigma^2 = \frac{k_B T}{m}$$

where m is the mass of the molecules. This relationship comes from the thermodynamics equation that links the variance and temperature.

We can further consider the relationship existing between kinetic energy and velocity (**equipartition law**):

$$E = \frac{1}{2}mv^2, \quad v = \sqrt{\frac{2E}{m}}, \quad mv\,dv = dE$$

The energy density is then:

$$p_E(E) = \frac{p_V(\sqrt{2E/m})}{m\sqrt{2E/m}}$$

We also know that the modulus of the velocity follows the Maxwellian distribution. Therefore:

$$\boxed{p_E(E) = \frac{2}{\sqrt{\pi}}\frac{1}{k_BT}\sqrt{\frac{E}{k_BT}}\exp(-E/k_BT)}$$

This is the density of the **Boltzmann distribution**.

Exercise 0.2. Randomly generate points uniformly distributed in a circle of radius R, with constant density ρ. The circle is assumed to be centered in the origin of the Cartesian coordinate system.

To define the position of a generic point P within a circle, we use the polar coordinates (r, θ):

$$\begin{cases} 0 \leq r \leq R \\ 0 \leq \theta \leq 2\pi \end{cases}$$

To determine the PDFs $p(r)$ and $p(\theta)$, we first observe that $p(\theta)\,d\theta$ is given by the ratio between the number of points contained in the circular sector with central angle $d\theta$ and the total number of points within the circle. On the other hand, $p(r)\,dr$ is given by the ratio between the number of points within the annulus of width dr and radius r and the total number of points within the circle, see Figure 3:

$$\begin{cases} p(\theta)d\theta = \dfrac{\rho(d\theta/2)R^2}{\rho\pi R^2} = \dfrac{d\theta}{2\pi} \\ p(r)dr = \dfrac{\rho(2\pi r dr)}{\rho\pi R^2} = \dfrac{2r}{R^2}dr \end{cases}$$

The corresponding CDFs are:

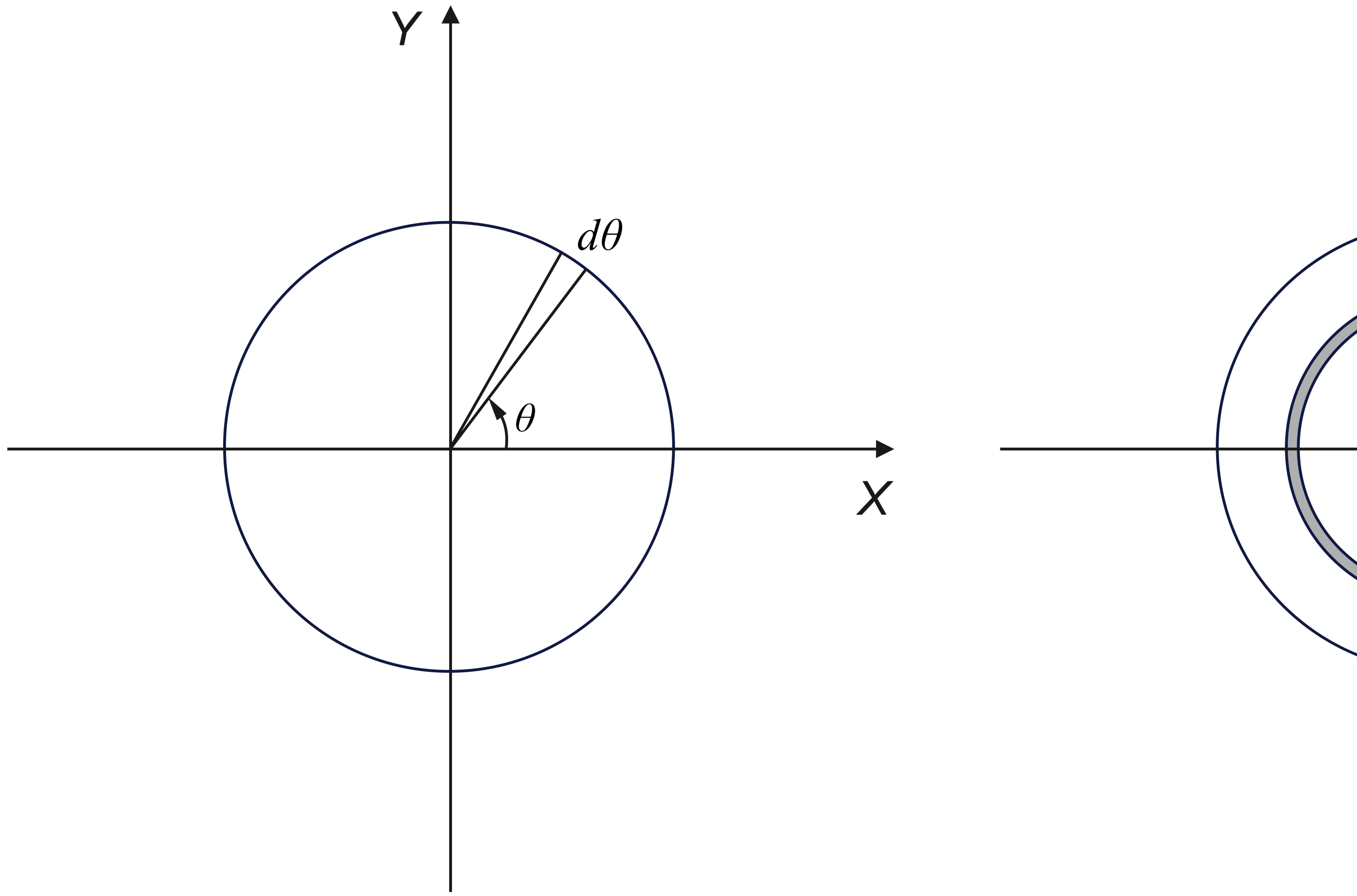

Figure 3: When points are uniformly distributed in the circle, $p(\theta)\,d\theta$ and $p(r)\,dr$ can be easily derived by geometrical arguments.

$$\begin{cases} F(\theta) = \int_0^\theta p(\theta)\, d\theta = \dfrac{\theta}{2\pi} & 0 \le \theta \le 2\pi \\ F(r) = \int_0^r p(r)\, dr = \dfrac{r^2}{R^2} & 0 \le r \le R \end{cases}$$

If ξ_1 and ξ_2 are independent draws from a standard uniform pseudo-number generators:

$$\begin{cases} \theta = 2\pi\xi_1 \\ r = R\sqrt{\xi_2} \end{cases}$$

The points in Cartesian coordinates are calculated using Equation 8. Figure 4 shows the cloud of points generated from 5000 draws.

It is worth noting that an isotropic point distribution in the circle implies uniformity in θ but not in r. Uniformity in r would imply to have the same number of points for two circular sectors with different radii and then a higher density for the one closer to the center of the sphere.

Exercise 0.3. Randomly generate isotropically distributed on a spherical surface of radius R and uniformly within the spherical volume. The sphere is assumed to be centered in the origin of the Cartesian coordinate system.

To define the position of a generic point P located on a spherical surface, we use the spherical coordinates (r, ϕ, θ):

$$\begin{cases} 0 \le r \le R \\ 0 \le \phi \le 2\pi \\ 0 \le \theta \le \pi \end{cases}$$

If we denote by n_t and dn the total number of points on the sphere and in the elemental volume $dV = r^2 \sin\theta\, dr\, d\phi\, d\theta$, respectively, we have:

$$p(r, \phi, \theta) = \frac{3r^2 \sin\theta}{4\pi R^3}$$

The marginal densities are given by:

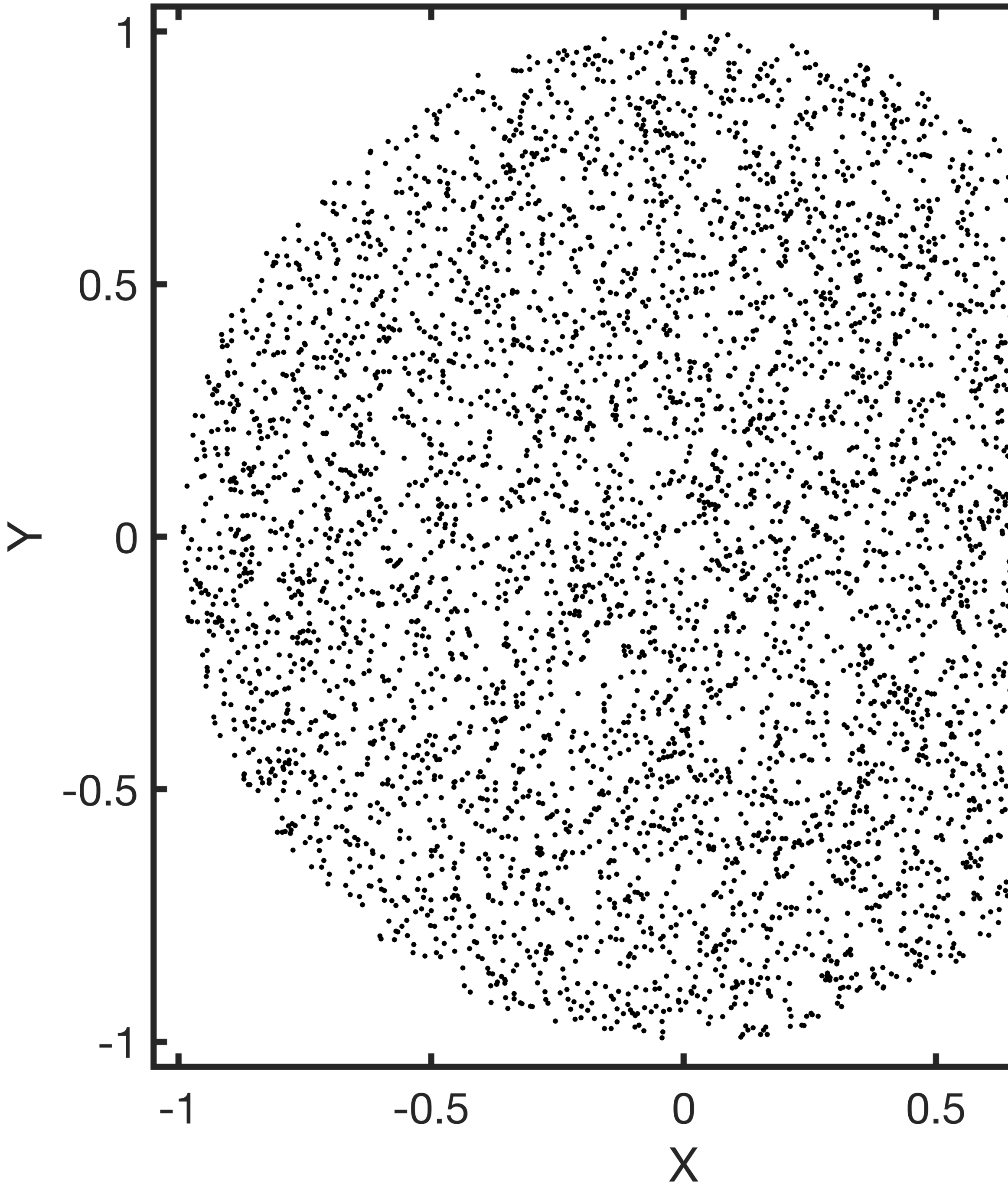

Figure 4: Cloud of points distributed uniformly in a circle of radius \$R\$ (\$R=1\$).

$$
\begin{cases}
p_R(r) = \dfrac{3r^2}{4\pi R^3}\displaystyle\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta = \dfrac{3r^2}{R^3}, & 0 \le r \le R \\
p_\Phi(\phi) = \dfrac{3}{4\pi R^3}\displaystyle\int_0^{\pi} \sin\theta\, d\theta \int_0^{R} r^2 dr = \dfrac{1}{2\pi}, & 0 \le \phi \le 2\pi \\
p_\Theta(\theta) = \dfrac{3\sin\theta}{4\pi R^3}\displaystyle\int_0^{2\pi} d\phi \int_0^{R} r^2 dr = \dfrac{\sin\theta}{2}, & 0 \le \theta \le \pi
\end{cases}
$$

The corresponding CDFs are:

$$
\begin{cases}
F_R(r) = \dfrac{r^3}{R^3}, & 0 \le r \le R \\
F_\Phi(\phi) = \dfrac{\phi}{2\pi}, & 0 \le \phi \le 2\pi \\
F_\Theta(\theta) = \dfrac{1-\cos\theta}{2}, & 0 \le \theta \le \pi
\end{cases}
$$

The formulae for the random generation of (r, ϕ, θ) follow from three independent standard uniform draws ξ_1, ξ_2 and ξ_3:

$$
\begin{cases}
r = R^3 \xi_1^{1/3} \\
\phi = 2\pi\, \xi_2 \\
\theta = \arccos(1 - 2\xi_3)
\end{cases}
$$

The points in Cartesian coordinates are calculated using Equation 9. Figure 5 shows the cloud of points generated from 5000 draws.

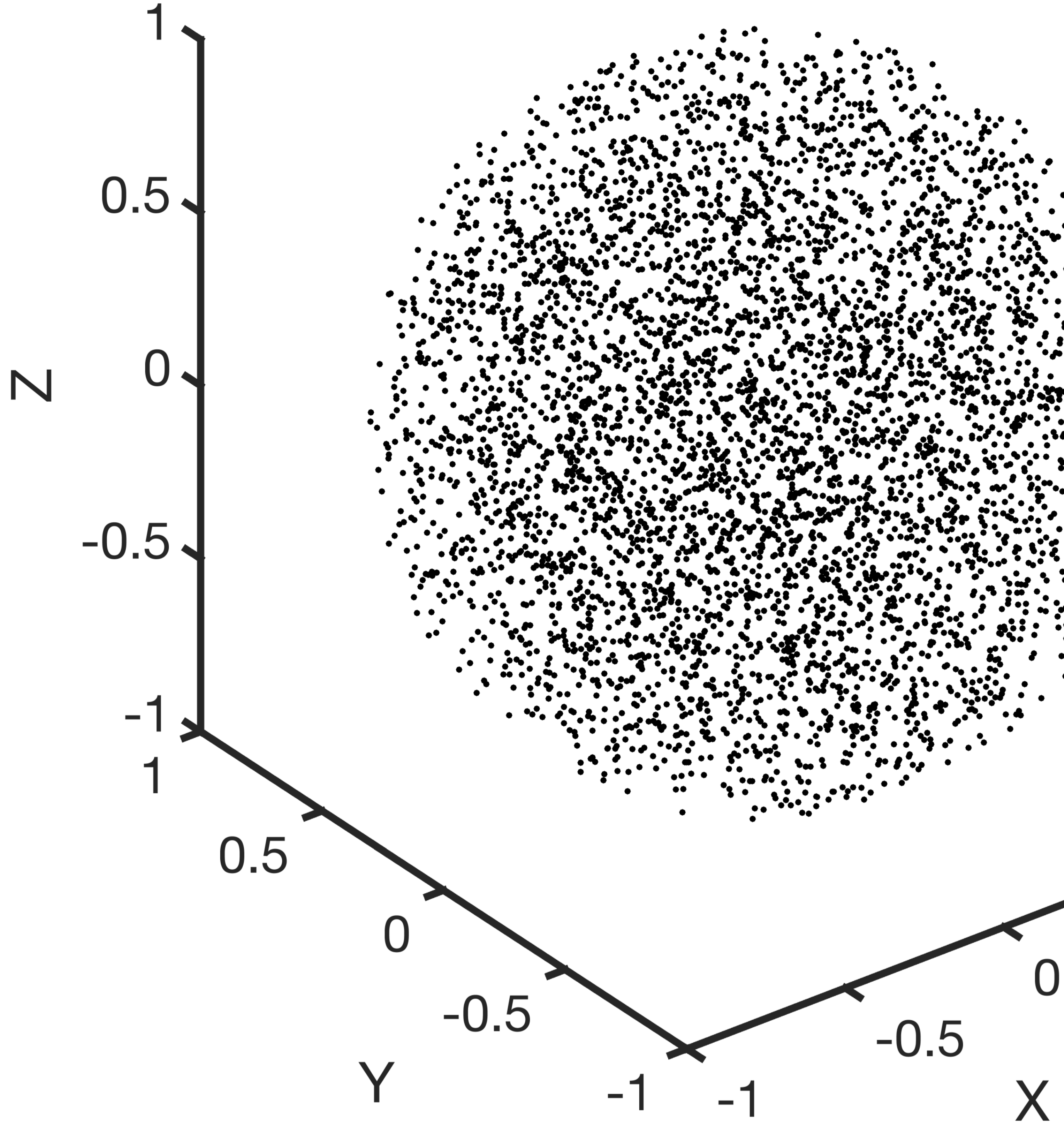

Figure 5: Cloud of points distributed uniformly on the spherical surface and uniformly within the spherical volume of radius R ($R = 1$).