Objectives

1. Evaluate normalization constant of a 3D normal distribution.
2. Evaluate different moments.

Consider the following function:

$$e^{-bx^2}$$

where b is a constant. We would like to know the following integral:

$$\int_{-\infty}^{\infty} e^{-bx^2} dx$$

It can rewritten in polar coordinate, with the knowledge that $x = r\cos\theta$, $y = r\sin\theta$. The corresponding Jacobian matrix has the following form:

$$\begin{bmatrix} \cos\theta & -r\sin\theta \\ \sin\theta & r\cos\theta \end{bmatrix}$$

Determinant of the Jacobian matrix is therefore r.

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-b(x^2+y^2)}dxdy = \int_0^{2\pi}\int_0^{\infty} e^{-br^2} r dr d\theta$$
$$= 2\pi \cdot \Big[-\frac{e^{-br^2}}{2b} \Big]_0^{\infty} = \frac{\pi}{b}$$

This shows that:

$$\boxed{\int_{-\infty}^{\infty} e^{-bx^2}dx = \sqrt{\frac{\pi}{b}}} \tag{1}$$

Then, we know for three dimensional case that:

$$\boxed{\int_{-\infty}^{\infty} e^{-bx^2}dx \int_{-\infty}^{\infty} e^{-by^2}dy \int_{-\infty}^{\infty} e^{-bz^2}dz = \left(\frac{\pi}{b}\right)^{1.5}} \tag{2}$$

Therefore, a 3D normal distribution must be normalized as follows:

$$\left(\frac{b}{\pi}\right)^{1.5} e^{-b(x^2+y^2+z^2)}dxdydz$$

We know that in spherical coordinate:

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} r\sin\theta\cos\psi \\ r\sin\theta\sin\psi \\ r\cos\theta \end{bmatrix} \tag{3}$$

With this Jacobian matrix, this can be transformed to spherical coordinate:

$$\mathbf{J} = \begin{bmatrix} \sin\theta\cos\psi & r\cos\psi\cos\theta & -r\sin\theta\sin\psi \\ \sin\theta\sin\psi & r\cos\theta\sin\psi & r\sin\theta\cos\psi \\ \cos\theta & -r\sin\theta & 0 \end{bmatrix} \tag{4}$$

The determinant of $\mathbf{J}$ is $r^2\sin\theta$. Then, we have:

$$\boxed{\left(\frac{b}{\pi}\right)^{1.5} e^{-br^2} r^2 \sin\theta dr d\theta d\psi}$$

We are interested in the mean value $\langle r \rangle$:

$$\langle r \rangle = 4\pi \left(\frac{b}{\pi}\right)^{1.5} \int_0^\infty e^{-br^2} r^3 dr$$

Pay attention to the integral:

$$\int_0^\infty e^{-br^2} r^3 dr$$

That it can be solved by integration by part. In integration by part, we have:

$$\int_a^b u dv = uv\Big|_a^b - \int_a^b v du \tag{5}$$

By setting:

$$\boxed{dv = e^{-br^2} r dr}, \ \boxed{v = -\frac{e^{-br^2}}{2b}}$$

$$\boxed{u = r^2}, \ \boxed{du = 2rdr}$$

We then have:

$$\int_0^\infty e^{-br^2} r^3 dr = -\frac{r^2 e^{-br2}}{2b}\Big|_0^\infty + \int_0^\infty \frac{e^{-br^2} 2r}{2b} dr$$
$$= \int_0^\infty \frac{e^{-br^2}}{2b} dr^2$$

This gives us:

$$\int_0^\infty e^{-br^2} r^3 dr = \Big[-\frac{e^{-br^2}}{2b^2} \Big]_0^\infty = \frac{1}{2b^2}$$

Finally,

$$\boxed{\langle r \rangle = 4 \cdot \pi^{1-1.5} \cdot b^{1.5-2} \cdot 0.5 = \sqrt{\frac{4}{\pi b}}}$$

Now, we are interested in the mean square value $\langle r^2 \rangle$:

$$\langle r^2 \rangle = 4\pi \left(\frac{b}{\pi}\right)^{1.5} \int_0^\infty r^4 e^{-br^2} dr$$

Integration by part:

$$\boxed{dv = e^{-br^2} r dr}, \quad \boxed{v = \frac{-e^{-br^2}}{2b}}$$

$$\boxed{u = r^3}, \quad \boxed{du = 3r^2 dr}$$

We get:

$$\int_0^\infty r^4 e^{-br^2} dr = \frac{-r^3 e^{-br^2}}{2b}\Big|_0^\infty + \int_0^\infty \frac{3r^2 e^{-br^2}}{2b} dr = \frac{3}{2b} \int_0^\infty r^2 e^{-br^2} dr$$

Integration by part for the second time:

$$\boxed{dv = e^{-br^2} r dr}, \quad \boxed{v = \frac{-e^{-br^2}}{2b}}$$

$$\boxed{u = r}, \quad \boxed{du = dr}$$

We have:

$$\begin{aligned}\frac{3}{2b}\int_0^\infty r^2 e^{-br^2} dr &= \frac{3}{2b}\Big(\frac{-r^2 e^{-br^2}}{2b}\Big|_0^\infty + \int_0^\infty \frac{e^{-br^2}}{2b} dr\Big) \\ &= \frac{3}{2b}\frac{1}{4b}\sqrt{\frac{\pi}{b}}\end{aligned}$$

This is because $\int_{-\infty}^{\infty} e^{-br^2} dr = \sqrt{\frac{\pi}{b}}$, therefore $\int_0^\infty e^{-br^2} dr = \frac{1}{2}\sqrt{\frac{\pi}{b}}$.

Finally, this gives us:

$$\boxed{\langle r^2\rangle = 4\pi\left(\frac{b}{\pi}\right)^{1.5}\frac{3}{8b^2}\sqrt{\frac{\pi}{b}} = \frac{3}{2}\cdot b^{1.5-2-0.5}\cdot \pi^{1-1.5+0.5} = \frac{3}{2b}}$$

One interesting question to ask: what are $\langle xy\rangle$, $\langle xz\rangle$ and $\langle yz\rangle$? Let us start with $\langle xy\rangle$.

$$\begin{aligned}\langle xy\rangle &= \left(\frac{b}{\pi}\right)^{1.5}\int_0^{2\pi}\sin\psi\cos\psi d\psi\int_0^{\pi}\cos\theta\sin^3\theta d\theta\int_0^{\infty}r^4 e^{-br^2}dr\\ &= \frac{3}{8b^2}\sqrt{\frac{\pi}{b}}\left(\frac{b}{\pi}\right)^{1.5}\int_0^{2\pi}\sin\phi\cos\phi d\phi\int_0^{\pi}\cos\theta\sin^3\theta d\theta\end{aligned}$$

Solve the integral for θ:

$$\int_0^{\pi}\cos\theta\sin^3\theta d\theta = \int_0^{\pi}\sin^3\theta d\sin\theta = \frac{\sin^4\theta}{4}\Big|_0^{\pi} = 0$$

Therefore, $\langle xy\rangle = 0$

$$\langle xz \rangle = \left(\frac{b}{\pi}\right)^{1.5} \int_0^{2\pi} \cos\psi d\psi \int_0^{\pi} \sin\theta\cos\theta d\theta \int_0^{\infty} r^4 e^{-br^2} dr$$

It can be found that:

$$\int_0^{\pi} \sin\theta\cos\theta d\theta = \int_0^{\pi} \cos\theta d\cos\theta = -\frac{\cos^2\theta}{2}\Big|_0^{\pi} = 0$$

Again we obtain $\langle xz \rangle = 0$.

$$\langle yz \rangle = \left(\frac{b}{\pi}\right)^{1.5} \int_0^{2\pi} \sin\psi d\psi \int_0^{\pi} \sin\theta\cos\theta d\theta \int_0^{\infty} r^4 e^{-br^2} dr$$

Again, $\int_0^{\pi} \sin\theta\cos\theta d\theta = 0$, $\langle yz \rangle = 0$. Maybe a good question to ask is 'What are the values of $\langle x^2 \rangle$, $\langle y^2 \rangle$, $\langle z^2 \rangle$?'

$$\langle xx \rangle = \left(\frac{b}{\pi}\right)^{1.5} \int_0^{2\pi} \cos^2\psi d\psi \int_0^{\pi} \sin^3\theta d\theta \int_0^{\infty} r^4 e^{-br^2} dr$$

$$\begin{aligned}
\int_0^{2\pi} \cos^2\psi d\psi &= \int_0^{2\pi} \frac{(e^{i\psi} + e^{-i\psi})^2}{4} \\
&= \int_0^{2\pi} \frac{e^{2i\psi} + e^{-2i\psi} + 2}{4} d\psi \\
&= \frac{e^{2i\psi}}{8i}\bigg|_0^{2\pi} - \frac{e^{-2i\psi}}{8i}\bigg|_0^{2\pi} + \int_0^{2\pi} \frac{d\psi}{2} = \pi
\end{aligned}$$

$$\int_0^{\pi} \sin^3\theta d\theta = -\int_0^{\pi} (1 - \cos^2\theta) d\cos\theta = \frac{4}{3}$$

Then, these give us:

$$\boxed{\langle xx \rangle = \frac{4\pi}{3}\left(\frac{b}{\pi}\right)^{1.5} \int_0^{\infty} r^4 e^{-br^2} dr = \frac{1}{2b}}$$

It is also interesting to evaluate $\langle xyxy \rangle$, as later this is useful in evaluating the viscosity of ideal gas.

$$\langle xyxy \rangle = \Big(\frac{b}{\pi}\Big)^{1.5} \int_0^{2\pi} \cos^2\psi \sin^2\psi d\psi \int_0^{\pi} \sin^5\theta d\theta \int_0^{\infty} r^6 e^{-br^2} dr$$

$$\begin{aligned}
\cos^2\psi \sin^2\psi &= \Big(\frac{e^{i\psi} + e^{-i\psi}}{2}\Big)^2 \Big(\frac{e^{i\psi} - e^{-i\psi}}{2i}\Big)^2 \\
\int_0^{2\pi} \cos^2\psi \sin^2\psi d\psi &= -\frac{1}{16} \int_0^{2\pi} \big[(e^{4i\psi} + e^{-4i\psi}) - 2\big] d\psi \\
&= -\frac{1}{16} \Big[\frac{e^{4i\psi}}{4i} - \frac{e^{-4i\psi}}{4i} - 2\theta\Big]_0^{2\pi} \\
&= -\frac{1}{16} \Big(\frac{2i\sin 4\psi}{2}\Big)_0^{2\pi} = \frac{\pi}{4}
\end{aligned}$$

Next integral to solve:

$$
\begin{aligned}
\int_0^\pi \sin^5\theta d\theta &= -\int_0^\pi (1-\cos^2\theta)^2 d\cos\theta \\
&= -\int_0^\pi (1-2\cos^2\theta+\cos^4\theta) d\cos\theta \\
&= -\Big(\cos\theta\Big)_0^\pi + \frac{2}{3}\Big(\cos^3\theta\Big)_0^\pi - \frac{1}{5}\Big(\cos^5\theta\Big)_0^\pi \\
&= -(-1-1) + \frac{2}{3}(-1-1) - \frac{1}{5}(-1-1) = 2 - \frac{4}{3} + \frac{2}{5} \\
&= \frac{16}{15}
\end{aligned}
$$

Therefore:

$$\langle xyxy \rangle = \frac{4\pi}{15}\Big(\frac{b}{\pi}\Big)^{1.5} \int_0^\infty r^6 e^{-br^2} dr$$

$$
\begin{aligned}
\int_0^\infty r^6 e^{-br^2} dr &= \int_0^\infty \frac{e^{-br^2}}{2b} 5r^4 dr \\
&= \frac{5}{2b} \int_0^\infty \frac{e^{-br^2}}{2b} 3r^2 dr \\
&= \frac{15}{4b^2} \int_0^\infty e^{-br^2} r^2 dr \\
&= \frac{15}{4b^2} \int_0^\infty \frac{e^{-br^2}}{2b} dr \\
&= \frac{15}{8b^3} \cdot \frac{1}{2} \sqrt{\frac{\pi}{b}} = \frac{15}{16b^3} \sqrt{\frac{\pi}{b}}
\end{aligned}
$$

Then, we have:

$$
\langle xyxy \rangle = \frac{4\pi}{15} \left(\frac{b}{\pi} \right)^{1.5} \frac{15}{16b^3} \sqrt{\frac{\pi}{b}} = \frac{1}{4b^2}
$$

In summary, we have the following values:

Average	Value
$\langle r \rangle$	$\sqrt{\frac{4}{\pi b}}$
$\langle r^2 \rangle$	$\frac{3}{2b}$
$\langle xy \rangle = \langle xz \rangle = \langle yz \rangle$	0
$\langle xx \rangle = \langle yy \rangle = \langle zz \rangle$	$\frac{1}{2b}$
$\langle xyxy \rangle$	$\frac{1}{4b^2}$