On The Gaussian Distribution from Diffusion Equation

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Note on Divergence Theorem

$$\iint_S \vec{F} \cdot \hat{n} \, dS = \iiint_V \nabla \cdot \vec{F} \, dV \tag{1}$$

$\vec{F}$ is a mass flux vector (flow of mass through the unit surface per unit time), $\nabla \cdot \vec{F}$ is a divergence of $\vec{F}$ (an outflow of mass from a volume element dV per the volume element dV per unit time), S is the complete boundary of the volume V, $\hat{n}$ is a unit vector normal to the surface S pointing outside the volume V.

Note on Mass Conservation Equation

The total mass in the volume V is

$$\iiint_V C(\vec{r}, t) \, dV \tag{2}$$

where $C(\vec{r}, t)$ is the mass concentration in point $\vec{r}$ at time t. The total increase of the mass in the volume V per unit time is

$$\frac{\partial}{\partial t} \iiint_V C(\vec{r}, t) \, dV \tag{3}$$

The total decrease of mass in the volume V per unit time is

$$-\frac{\partial}{\partial t} \iiint_V C(\vec{r}, t) \, dV \tag{4}$$

The total outflow of mass from the volume V is

$$\iint_S \vec{F} \cdot \hat{n} \, dS = \iiint_V \nabla \cdot \vec{F} \, dV \tag{5}$$

If the total decrease of mass in the volume V is solely due to the total outflow of mass from the volume V then by comparing the two appropriate expressions we have

$$-\frac{\partial}{\partial t}\iiint_V C(\vec{r},t)\,dV = \iiint_V \nabla\cdot\vec{F}\,dV \tag{6}$$

what leads to

$$\iiint_V (\frac{\partial C}{\partial t} + \nabla\cdot\vec{F})\,dV = 0 \tag{7}$$

Since the volume V is arbitrary

$$\frac{\partial C}{\partial t} + \nabla\cdot\vec{F} = 0 \tag{8}$$

what is the mass conservation equation.

Note on Fick's Law

$$\vec{F} = -D\,\nabla C \tag{9}$$

The flux $\vec{F}$ is proportional to the negative gradient of the mass concentration where D is a constant coefficient.

Note on Diffusion Equation

Applying the mass conservation equation and the Fick's Law we get

$$\frac{\partial C}{\partial t} + \nabla\cdot(-D\,\nabla C) = 0 \tag{10}$$

what leads to the *diffusion equation*

$$\frac{\partial C}{\partial t} = D\,\nabla^2 C \tag{11}$$

In one dimension we have

$$\frac{\partial C}{\partial t} = D\,\frac{\partial^2 C}{\partial x^2} \tag{12}$$

Solving The Diffusion Equation in One Dimension and Obtaining The Gaussian Distribution of Mass Concentration

We solve the diffusion equation as suggested in [1]

$$\frac{\partial C}{\partial t} = D\,\frac{\partial^2 C}{\partial x^2} \qquad -\infty < x < \infty \tag{13}$$

with the initial condition

$$C(x,0) = C_0\,\delta(x) \tag{14}$$

where $\delta(x)$ is the Dirac's delta function. We will use the pair of Fourier transforms

$$\hat{C}(k,t) = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} C(x,t) e^{-ikx}\,dx \tag{15}$$

$$C(x,t) = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} \hat{C}(k,t) e^{ikx}\,dk \tag{16}$$

Using the properties of Fourier transform operator $\mathcal{F}$

$$\mathcal{F}(f(x)) = \hat{f}(k) \tag{17}$$

$$\mathcal{F}(f'(x)) = ik\hat{f}(k) \tag{18}$$

$$\mathcal{F}(f''(x)) = -k^2\hat{f}(k) \tag{19}$$

and applying the Fourier transform to the diffusion equation we receive

$$\frac{\partial \mathcal{F}(C(x,t))}{\partial t} = -Dk^2\mathcal{F}(C(x,t)) \tag{20}$$

what is

$$\frac{\partial \hat{C}(k,t)}{\partial t} = -Dk^2\hat{C}(k,t) \tag{21}$$

We solve the above equation obtaining

$$\hat{C}(k,t) = \hat{C}(k,0)\,e^{-Dk^2 t} \tag{22}$$

where

$$\hat{C}(k,0) = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} C(x,0) e^{-ikx}\, dx = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} C_0\, \delta(x) e^{-ikx}\, dx = \frac{C_0}{\sqrt{2\,\pi}} \tag{23}$$

and

$$\hat{C}(k,t) = \frac{C_0}{\sqrt{2\,\pi}}\, e^{-Dk^2 t} \tag{24}$$

We now invert the transform

$$C(x,t) = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} \hat{C}(k,t) e^{ikx}\, dk = \frac{1}{\sqrt{2\,\pi}} \int_{-\infty}^{\infty} \frac{C_0}{\sqrt{2\,\pi}}\, e^{-Dk^2 t} e^{ikx}\, dk \tag{25}$$

$$C(x,t) = \frac{C_0}{2\,\pi} \int_{-\infty}^{\infty} e^{-Dk^2 t} e^{ikx}\, dk = \frac{C_0}{2\,\pi} \int_{-\infty}^{\infty} e^{-Dk^2 t} (\cos(kx) + i \sin(kx))\, dk \tag{26}$$

We arrive at the equation

$$C(x,t) = \frac{C_0}{2\,\pi} \int_{-\infty}^{\infty} e^{-Dtk^2} \cos(xk)\, dk \tag{27}$$

We use the formula

$$\int_{-\infty}^{\infty} e^{-az^2} cos(\mu z)\, dz = \sqrt{\frac{\pi}{a}}\, e^{-(\mu^2/4a)} \tag{28}$$

and we write the solution

$$C(x,t) = \frac{C_0}{2\,\pi} \sqrt{\frac{\pi}{Dt}} e^{-x^2/4Dt} \tag{29}$$

$$C(x,t) = \frac{C_0}{2\sqrt{\pi Dt}} \exp(-x^2/4Dt) \tag{30}$$

$$C(x,t) = \frac{C_0}{\sqrt{2\pi}\sqrt{2Dt}} \exp(-x^2/4Dt) \tag{31}$$

$$C(x,t) = \frac{C_0}{\sigma\sqrt{2\pi}} \exp(-x^2/2\sigma^2) \tag{32}$$

where

$$\sigma = \sqrt{2Dt} \tag{33}$$

is the standard deviation of the Gaussian distribution of the concentration $C(x,t)$.

Solving The Integral $\int_{-\infty}^{\infty} \mathbf{e^{-az^2} cos(\mu z)\, dz}$

The integral $\int_{-\infty}^{\infty} e^{-az^2} cos(\mu z)\, dz$ has been solved in [2] on page 309

$$I(\mu) = \int_0^{\infty} e^{-z^2} cos(\mu z)\, dz \tag{34}$$

Differentiation with respect to μ behind the integral sign gives:

$$I'(\mu) = -\int_0^{\infty} z e^{-z^2} sin(\mu z)\, dz \tag{35}$$

The differentiation is legitimate because the resulting integral is uniformly convergent in μ.

Now we integrate by parts applying the formula:

$$\int u' v dz = uv - \int u v' dz \tag{36}$$

$$\begin{gathered} I'(\mu) = -\int_0^{\infty} z e^{-z^2} sin(\mu z)\, dz = \\ \left| \begin{array}{rcl} -ze^{-z^2} = (\frac{1}{2} e^{-z^2})' & = & u' \\ sin(\mu z) & = & v \end{array} \right| \left| \begin{array}{rcl} u & = & (\frac{1}{2} e^{-z^2}) \\ v' & = & \mu cos(\mu z) \end{array} \right| = \\ \frac{1}{2} [e^{-z^2} sin(\mu z)]_{z=0}^{z=\infty} - \frac{\mu}{2} \int_0^{\infty} e^{-z^2} cos(\mu z)\, dz \end{gathered} \tag{37}$$

and we get

$$I'(\mu) = -\frac{\mu}{2}\, I(\mu) \tag{38}$$

$$\frac{dI}{I} = -\frac{\mu}{2}\, d\mu \tag{39}$$

After integration we obtain

$$I(\mu) = C\, e^{-(\mu^2/4)} \tag{40}$$

To find a constant C we set $\mu = 0$. This gives

$$C = I(0) = \int_0^{\infty} e^{-z^2}\, dz = \frac{1}{2}\sqrt{\pi} \tag{41}$$

and

$$I(\mu) = \int_0^{\infty} e^{-z^2} cos(\mu z)\, dz = \frac{1}{2}\sqrt{\pi}\, e^{-(\mu^2/4)} \tag{42}$$

$$\int_0^\infty e^{-az^2} cos(\mu z)\, dz = \int_0^\infty e^{-(\sqrt{a}z)^2} cos(\mu z)\, dz = \left| \begin{array}{ccc} \sqrt{a}\, z & = & w \\ \sqrt{a}\, dz & = & dw \end{array} \right| = \quad (43)$$

$$\frac{1}{\sqrt{a}} \int_0^\infty e^{-w^2} cos(\frac{\mu}{\sqrt{a}} w)\, dw = \frac{1}{2}\sqrt{\frac{\pi}{a}}\, e^{-(\mu^2/4a)}$$

and we have the integral

$$\int_{-\infty}^\infty e^{-az^2} cos(\mu z)\, dz = \sqrt{\frac{\pi}{a}}\, e^{-(\mu^2/4a)} \quad (44)$$

References

[1] McQuarrie, D.A. (1976) *Statistical Mechanics* Harper & Row, New York, NY

[2] Tolstov, G.P. (1976) *Fourier Series* Translation by Silverman, R.A., Dover Publications, Inc., New York, NY

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