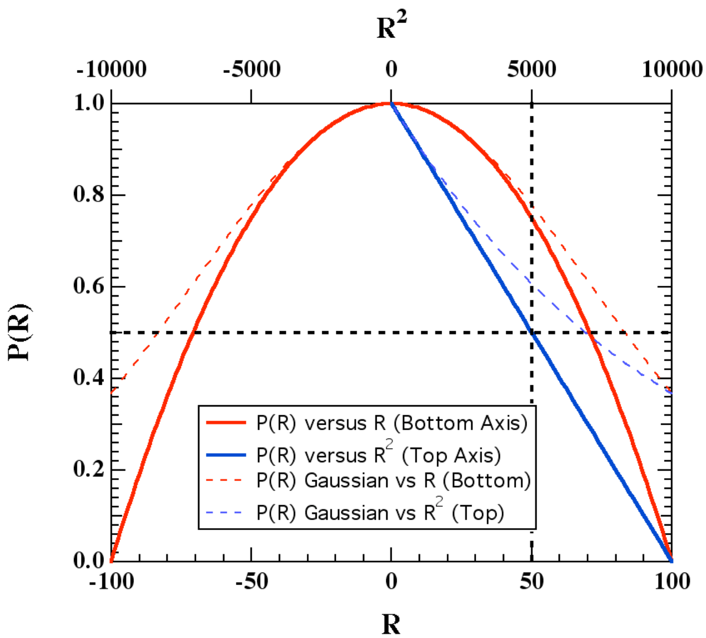
Gaussian Probability Function for End-to-End Distance of a Random Walk.

Consider a collection of 1-d random walks that go along the x-axis. We would like to determine the probability of a walk of length R. The walk is composed of n steps of length ℓ. The maximum distance that can be traveled is n ℓ.

1) A random walk has a maximum probability of having traversed a distance of R = 0 since it is equally probable that the walk goes forward as backward. We can arbitrarily set the probability of a walk of distance R = 0 at P(R) = 1.
2) P(R) must decay from the value of 1 at R=0 in both positive and negative x and the decay must be monotonic (no peaks or valleys) and symmetric about 0 (there is no preference to positive or negative walks). P(R) can only be a function of even orders (powers) of R due to symmetry.
3) We can propose the lowest order approximation from a power-series expansion of P(R),

$$P(R) = 1 - \frac{R^2}{k^2} + \ldots \qquad (1)$$

This function follows rule "1" since P(R = 0) = 1 and follows the symmetry rule "2" since positive and negative R have the same probability. Equation (1) suggests a plot of P(R) versus R^2, top axis and blue curve in plot below for k = 100. This curve intercepts the x-axis at R = 100 = k.



4) A random distribution of end to end distances, R, will follow the Gaussian distribution which is approximately equal to equation (1) at low values of R/k,

$$P_G(R) = \exp\left(-\frac{R^2}{k^2}\right) = 1 - \frac{R^2}{k^2} + \frac{R^4}{2!k^4} - \frac{R^6}{3!k^6} \ldots \qquad (2)$$

5) Using $P_G(R)$ we can calculate $\langle R^2 \rangle$.

$$\langle R^2\rangle = \frac{\int_{-\infty}^{\infty} R^2 P_G(R)dR}{\int_{-\infty}^{\infty} P_G(R)dR} = \frac{\int_{-\infty}^{\infty} R^2 \exp\left(\frac{R^2}{k^2}\right)dR}{\int_{-\infty}^{\infty} \exp\left(\frac{R^2}{k^2}\right)dR} \tag{3}$$

These integrals require a trick to solve. First the integral is squared in x and y:

$$G(\alpha) = \int_{-\infty}^{\infty} \exp\left(-\alpha x^2\right)dx$$

$$\left(G(\alpha)\right)^2 = \int_{-\infty}^{\infty} \exp\left(-\alpha x^2\right)dx \int_{-\infty}^{\infty} \exp\left(-\alpha y^2\right)dy = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \exp\left(-\alpha\left(y^2 + x^2\right)\right)dy$$

Then Cartesian coordinates are replaced with circular coordinates, r and θ,

$$\left(G(\alpha)\right)^2 = \int_0^{\infty} rdr \int_0^{2\pi} d\theta \exp\left(-\alpha r^2\right) = 2\pi \int_0^{\infty} rdr \exp\left(-\alpha r^2\right)$$

$$= \frac{-2\pi}{2\alpha}\int_0^{\infty} -2\alpha r dr \exp\left(-\alpha r^2\right) = \frac{-\pi}{\alpha}\left[\exp\left(-\alpha r^2\right)\right]_0^{\infty} = \frac{\pi}{\alpha}$$

The integral in the numerator can be solved by another trick,

$$H(\alpha) = \int_{-\infty}^{\infty} x^2 \exp\left(-\alpha x^2\right)dx = -\frac{dG(\alpha)}{d\alpha}$$

and since $G(\alpha) = (\pi/\alpha)^{1/2}$, then $H(\alpha) = \frac{\pi^{1/2}}{2\alpha^{3/2}}$ so, with $\alpha = 1/k^2$ and $x = R$,

$$\langle R^2\rangle = \frac{\int_{-\infty}^{\infty} R^2 \exp\left(\frac{R^2}{k^2}\right)dR}{\int_{-\infty}^{\infty} \exp\left(\frac{R^2}{k^2}\right)dR} = \frac{H(\alpha)}{G(\alpha)} = \frac{k^3\pi^{1/2}/2}{k\pi^{1/2}} = \frac{k^2}{2} \tag{4}$$

6) So,

$$P_G(R) = \exp\left(-\frac{R^2}{2\langle R^2\rangle}\right) \approx 1 - \frac{R^2}{2\langle R^2\rangle} + \ldots \tag{5}$$

7) We can calculate $\langle R^2\rangle$ from a consideration of the random walk in 1d which is composed of n steps,

$$\langle R^2\rangle = \sum_{i=1}^{n}\sum_{j=1}^{n} l_i \bullet l_j = \sum_{i=1}^{n} l_i \bullet l_i + \left(\sum_{i=1}^{n}\sum_{j=1}^{n} l_i \bullet l_j\right)_{for j \neq i} = nl^2 + 0$$

so,

$$P_G(R) = \exp\left(-\frac{R^2}{2nl^2}\right) \tag{6}$$

8) Equation (6) is not normalized meaning that the integral does not equal 1. To normalize this function we consider a prefactor such that the integral is equal to 1 and solve for this prefactor,

$$1 = \int_{-\infty}^{\infty} K \exp\left(-\frac{R^2}{2nl^2}\right) = K\left(2\pi nl^2\right)^{1/2}$$

so the normalized 1d Gaussian probability function is

$$P_G(R) = \left(2\pi nl^2\right)^{-1/2} \exp\left(-\frac{R^2}{2nl^2}\right) \quad (7)$$

9) A real Gaussian chain is in 3d space rather than in 2d space. But each of the 3 dimensions is independent of the others so the three probabilities just multiply as independent 1d probabilities. This cubes the exponential and adds a factor of 3 to the prefactor as well as changing the power to -3/2,

$$P_G(R) = \left(2\pi nl^2/3\right)^{-3/2} \exp\left(-\frac{3R^2}{2nl^2}\right) \quad (8)$$

10) Using equation (8) we can calculate any moment of the distribution such as the second moment, $\langle R^2 \rangle$,

$$\langle R^2 \rangle = 4\pi \int_0^\infty R^4 P_G(R) dR = nl^2$$

Where the integral can be solved in a similar way,

$$U(\alpha) = \int_{-\infty}^{\infty} x^4 \exp\left(-\alpha x^2\right) dx = -\frac{dH(\alpha)}{d\alpha} = \frac{3}{4}\pi^{1/2}\alpha^{-5/2}$$

All even order moments of the Gaussian can be solved using this approach.