Exercise | We derive the 1D nearest neighbor distribution. (Source: Undergrad Stat mech)

Suppose we have $N \gg 1$ points uniformly distributed over an interval of length L. We want to find the probability that the closest particle is a distance x away from an arbitrarily chosen point (not close to the boundary).

To compute the probability that the closest particle is a distance x away, we need

- the probability that $N-1$ particles are not within x
- the probability that one particle is between x and $x+dx$

The first term is given by $(1-2x/L)^{N-1}$, and the second is given by $2dx/L$. Combining them, we get the probability

$$dP = 2dx/L\,(1-2x/L)^{N-1}.$$

(Both factors of 2 come from the fact that we don't care if the closest particle is to the right or left.)

The probability density is given by

$$\rho(x) = \frac{dP}{dx} = \frac{2}{L}(1-2x/L)^{N-1} \approx \frac{2}{L}e^{-2Nx/L},$$

where we have used the approximation $(1-x)^n \approx e^{-nx}$ for small x and large n. Thus, the nearest neighbor distribution is given by

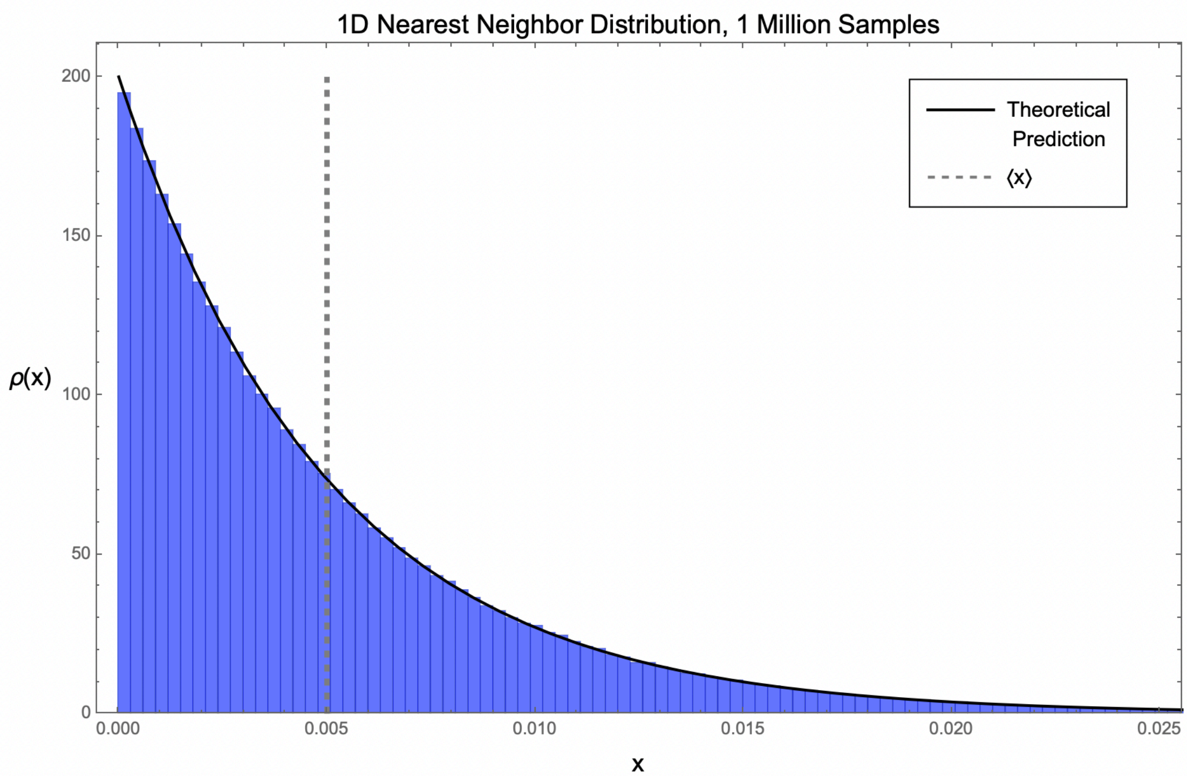
$$\boxed{\rho(x) = \frac{2N}{L} e^{-2Nx/L}}$$

The additional factor of N is simply a normalization constant. We can see it only depends on the density, which makes sense!

The mean nearest neighbor distance is given by

$$\langle x \rangle = \int_0^\infty \frac{2N}{L} \cdot x\, e^{-2Nx/L}\, d\left(\frac{2Nx}{L}\right) \cdot \frac{L}{2N} = \boxed{\frac{L}{2N}}$$

We compare our theoretical prediction with a Monte Carlo simulation at density $N/L = 1000$.



<u>Exercise</u> We derive the nearest neighbor distribution in n dimensions.

We follow the same procedure as before. The probability that $N-1$ particles are not within a distance r is given by

$$\left(1 - V_n(r)/L^n\right)^{N-1},$$

and the probability that one particle is between r and $r+dr$ is $S_n(r)\,dr/L^n$, where $V_n(r)$, $S_n(r)$ are the volume and surface areas of spheres in n dimensions.

It follows that the probability is given by

$$dP_n = \left(1 - V_n(r)/L^n\right)^{N-1} S_n(r)\,dr/L^n,$$

and that the PDF is given by

$$\tilde{\rho}_n(r) = \frac{dP_n}{dr} = \left(1 - V_n(r)/L^n\right)^{N-1} S_n(r)/L^n \approx$$

$$\frac{S_n(r)}{L^n} e^{-N V_n(r)/L^n}, \quad \text{up to normalization.}$$

The formulas for n-sphere surface area and volume are given by

$$S_n(r) = \frac{2\pi^{n/2} r^{n-1}}{\Gamma(n/2)}, \quad V_n(r) = \frac{\pi^{n/2}}{\Gamma(n/2+1)} r^n$$

So, our nearest neighbor distribution is given by

$$\tilde{\rho}_n(r) = \mathcal{N} \frac{2\pi^{n/2} r^{n-1}}{\Gamma(n/2) L^n} \exp\left(-\frac{N\pi^{n/2} r^n}{\Gamma(n/2+1) L^n}\right)$$

where $\mathcal{N}$ is the normalization constant, which can simply be found by integrating over r. (No Jacobian is required for this integration, since the angular information is already captured in $S_n(r)$.) We find that

$$\boxed{\rho_n(r) = \frac{N}{L^n} \frac{2\pi^{n/2} r^{n-1}}{\Gamma(n/2)} \exp\left(-\frac{N}{L^n}\frac{\pi^{n/2} r^n}{\Gamma(n/2+1)}\right)}$$

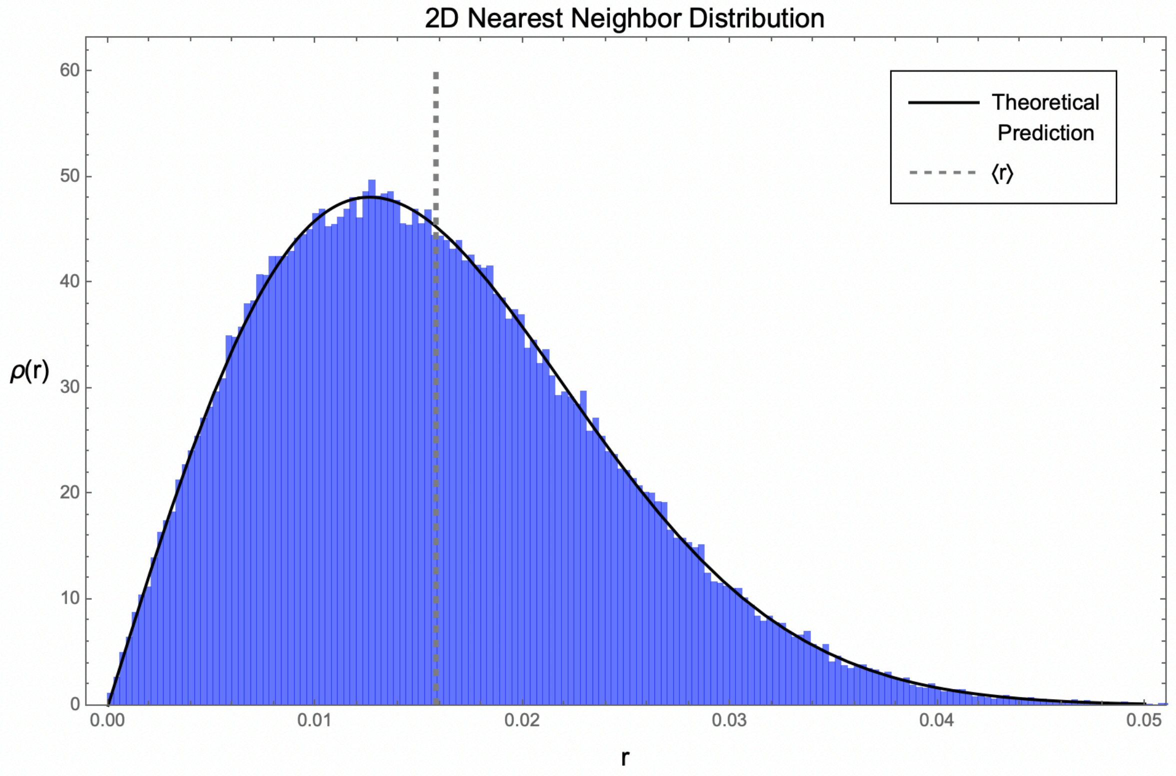
We now see that our result only depends on the density and the spatial dimension. The mean distance of the nearest neighbor in n-dimensions is given by

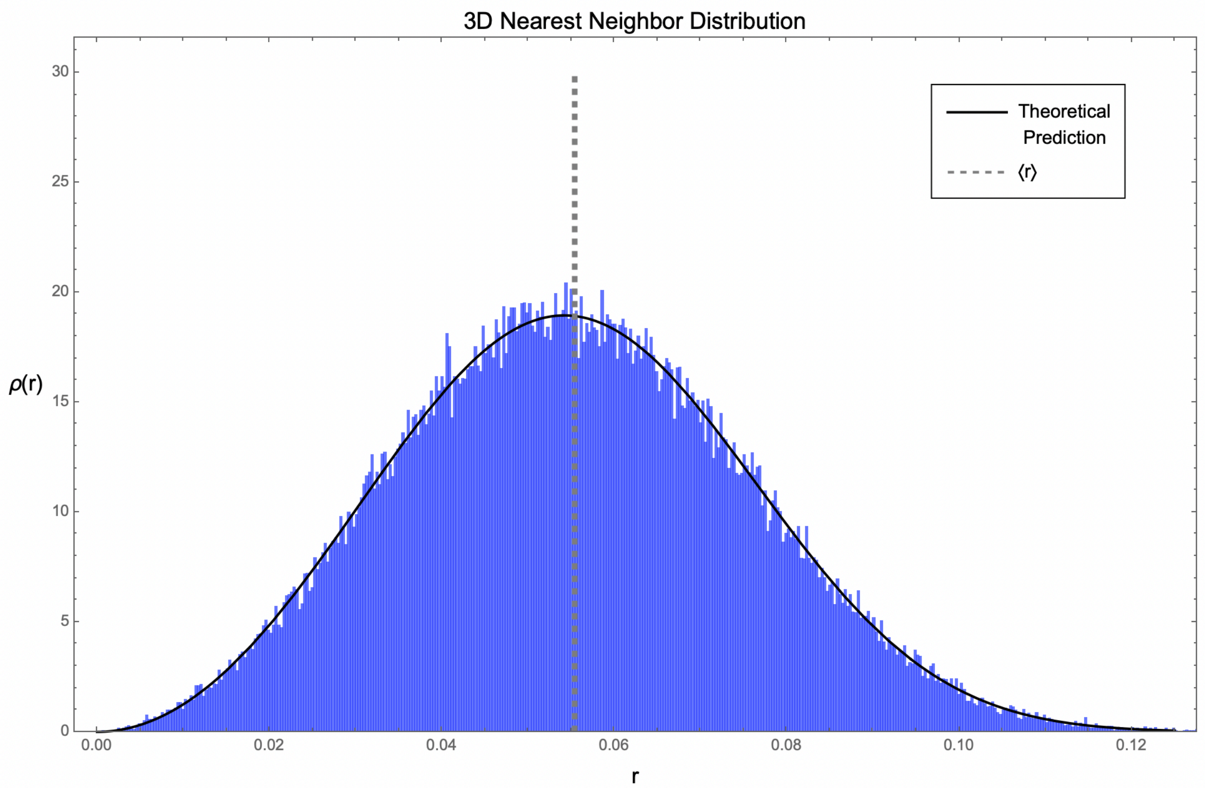
$$\langle r_n \rangle = \int_0^\infty r\rho_n(r)\,dr = \int_0^\infty \frac{N}{L^n} \cdot \frac{2\pi^{n/2} r^n}{\Gamma(n/2)} \exp\left(-\frac{N}{L^n}\frac{\pi^{n/2} r^n}{\Gamma(n/2+1)}\right) dr .$$

$$u = \frac{N}{L^n}\frac{\pi^{n/2} r^n}{\Gamma(n/2+1)} \Rightarrow du = \frac{N}{L^n}\frac{2\pi^{n/2} r^{n-1}}{\Gamma(n/2)} \Rightarrow$$

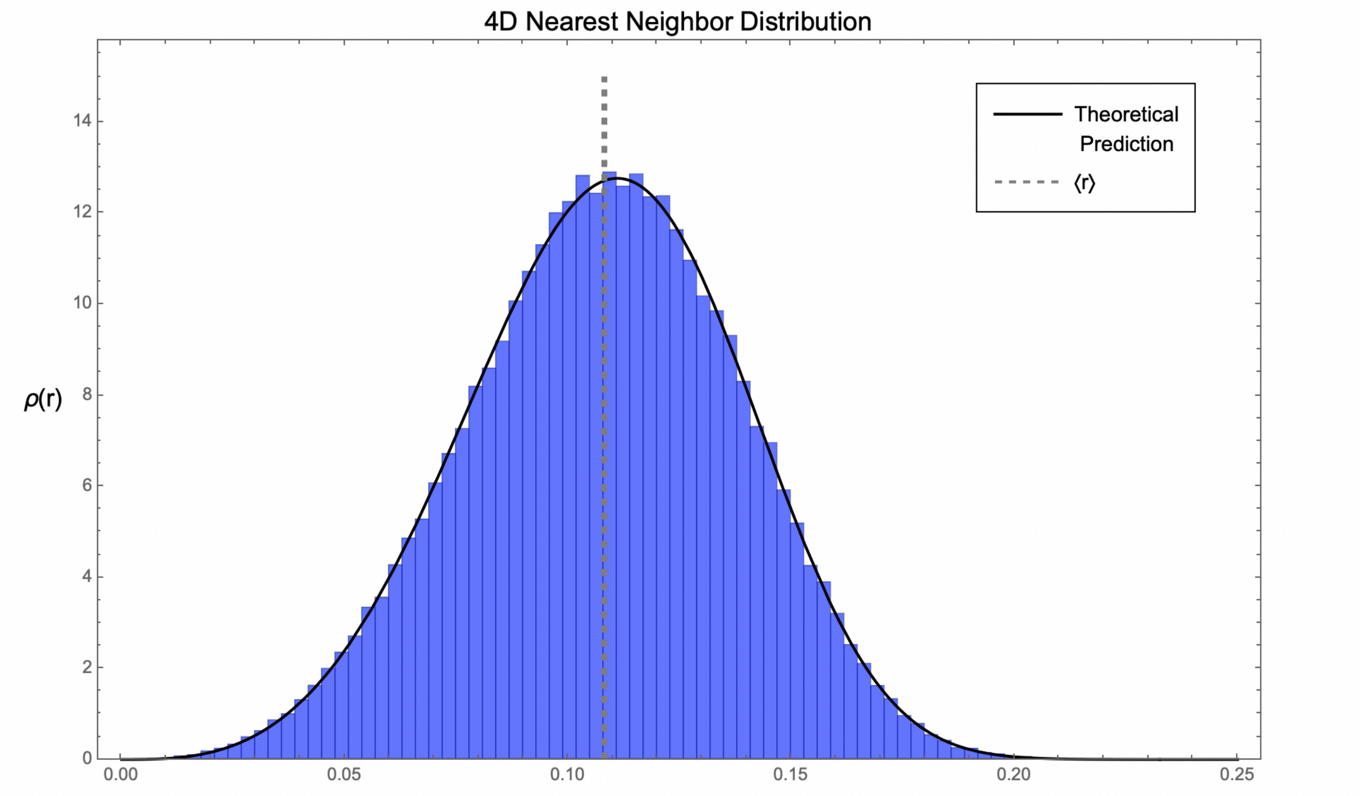
$$\langle r_n \rangle = \int_0^\infty u^{1/n} e^{-u}\,du \cdot \frac{L}{N^{1/n}} \frac{\Gamma(n/2+1)^{1/n}}{\sqrt{\pi}} = \boxed{\Gamma(1+1/n)\left(\frac{L^n}{N}\cdot\frac{\Gamma(n/2+1)}{\pi^{n/2}}\right)^{1/n}}$$

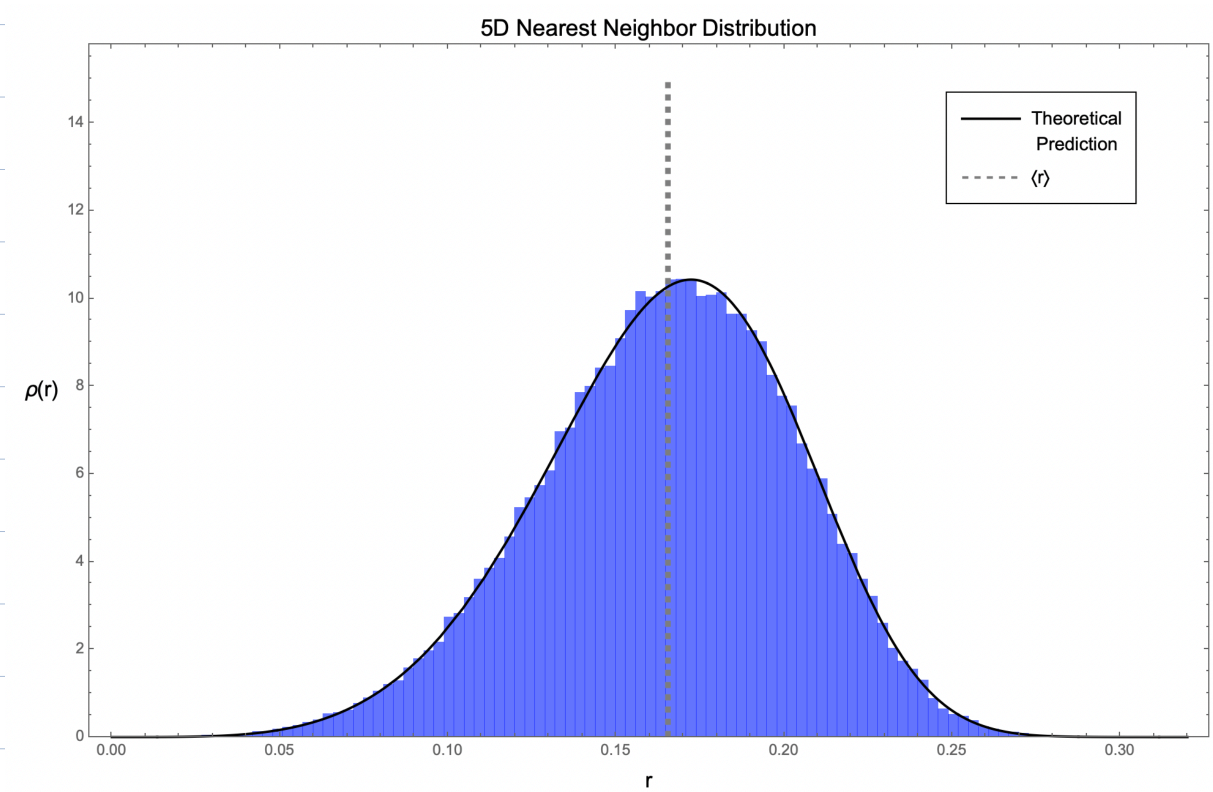
We now perform several Monte Carlo simulations to test these results.

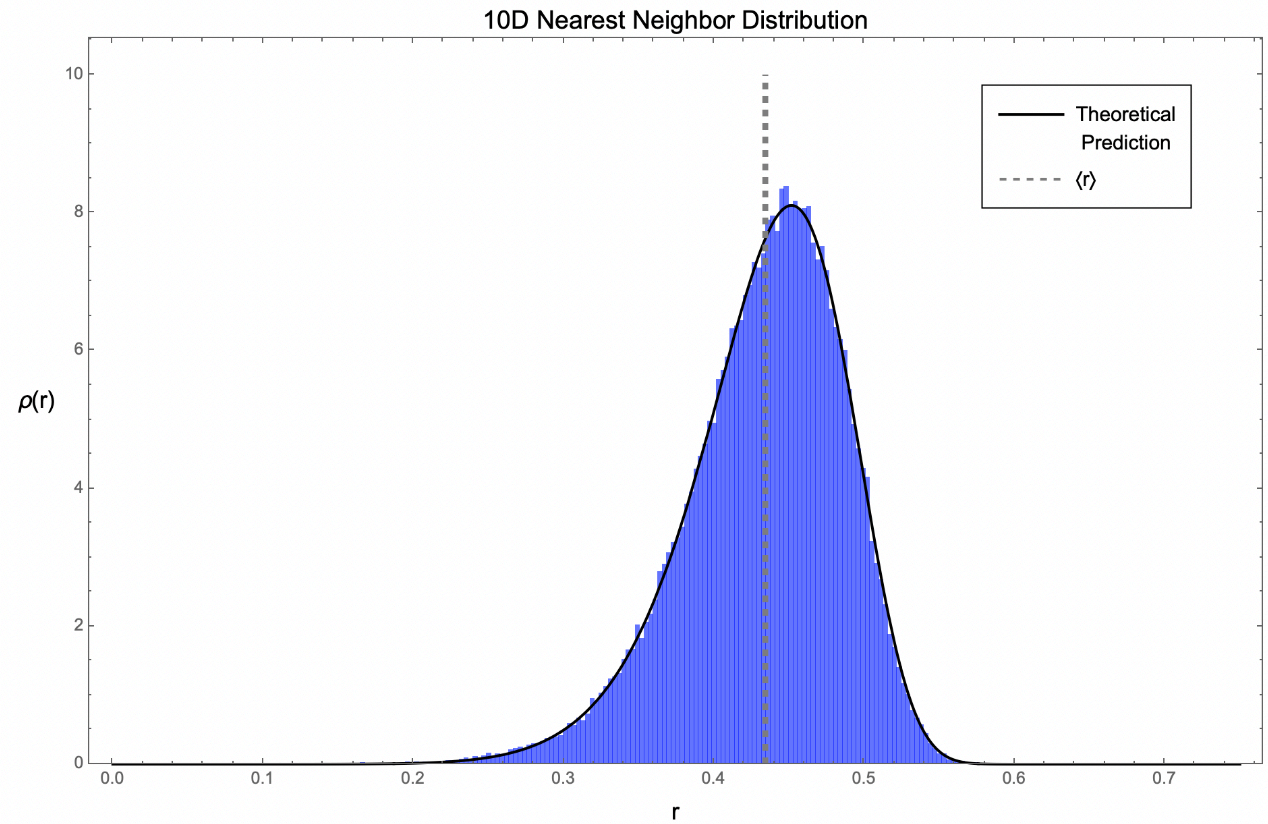




It is less likely that higher dimensions will be relevant, but we include a few cases out of general interest.







It is perhaps not surprising that the mean increases with spatial dimension (N fixed, $L=1$), but I have no idea why the distributions would become left-skewed in higher dimensions!