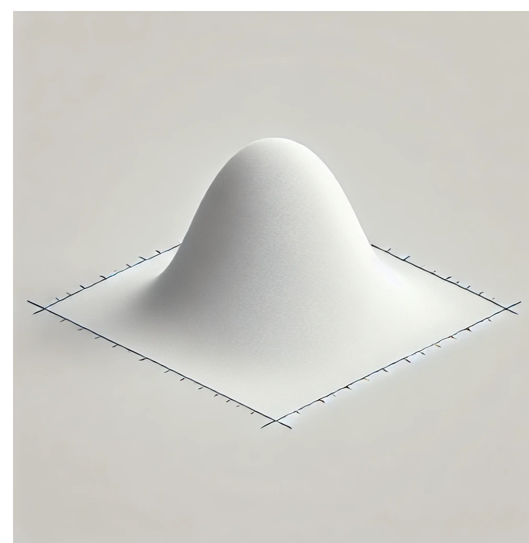
Presse Lab

Pressé Lab
@LabPresse

CBP Summer School
Aug 5-16
Lecture 5

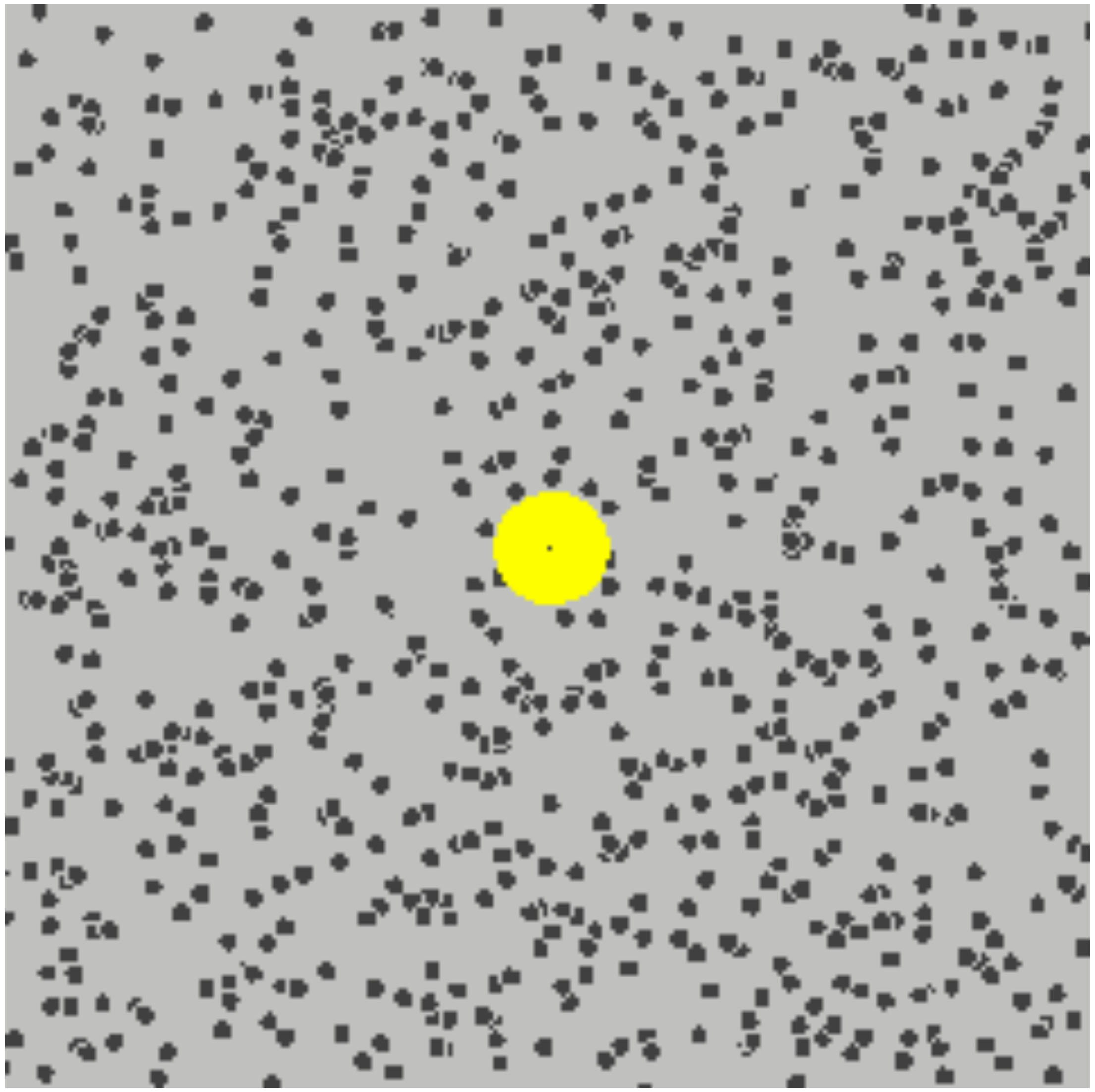


S. Pressé

Physics Dept., ASU
School of Mol. Sciences, ASU
Center for Biological Physics, ASU

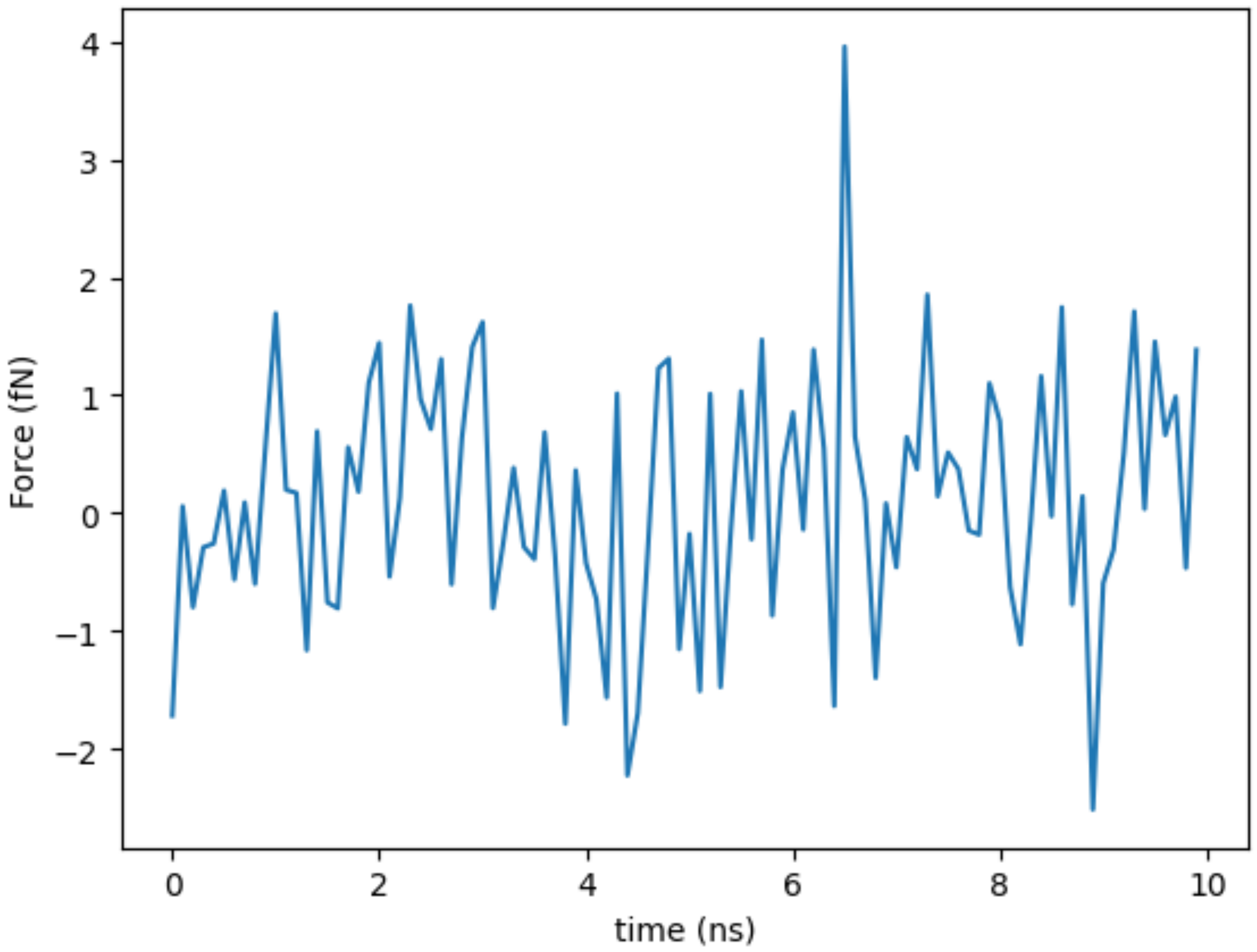
Recall from Lecture 2….

Here's a "Brownian particle".



https://upload.wikimedia.org/wikipedia/commons/c/c2/Brownian_motion_large.gif

If I were to plot the force on the particle induced by the fluid



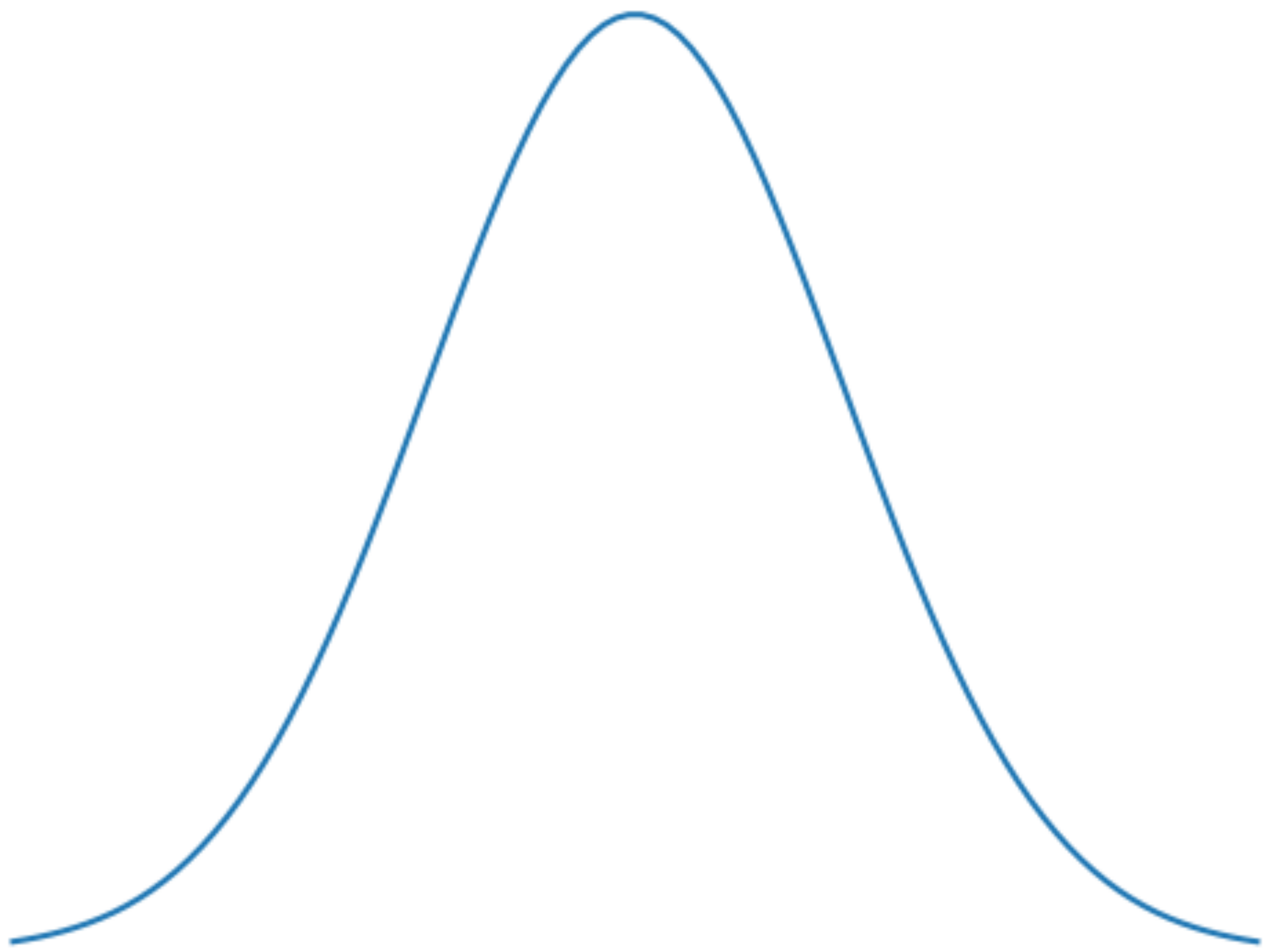
If I were to plot force

```
import numpy as np
import matplotlib.pyplot as plt

# Generate time series data
time = np.arange(0, 10, 0.1)
data = np.random.normal(0, 1, len(time))

# Plot the time series
plt.plot(time, data)
plt.xlabel('time (ns)')
plt.ylabel('Force (fN)')
plt.title('')
plt.show()
```

These forces are typically drawn from a “Gaussian” probability distribution



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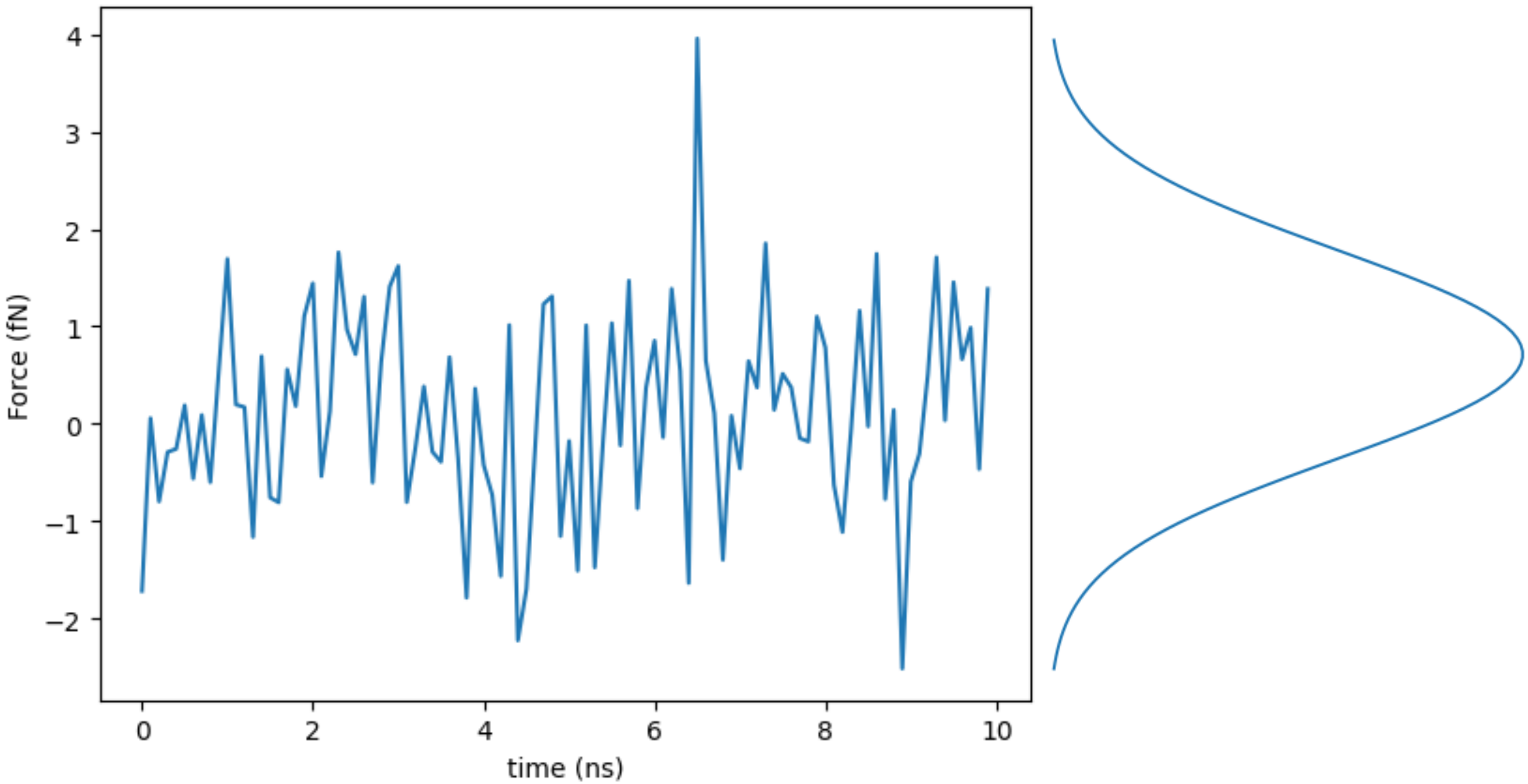

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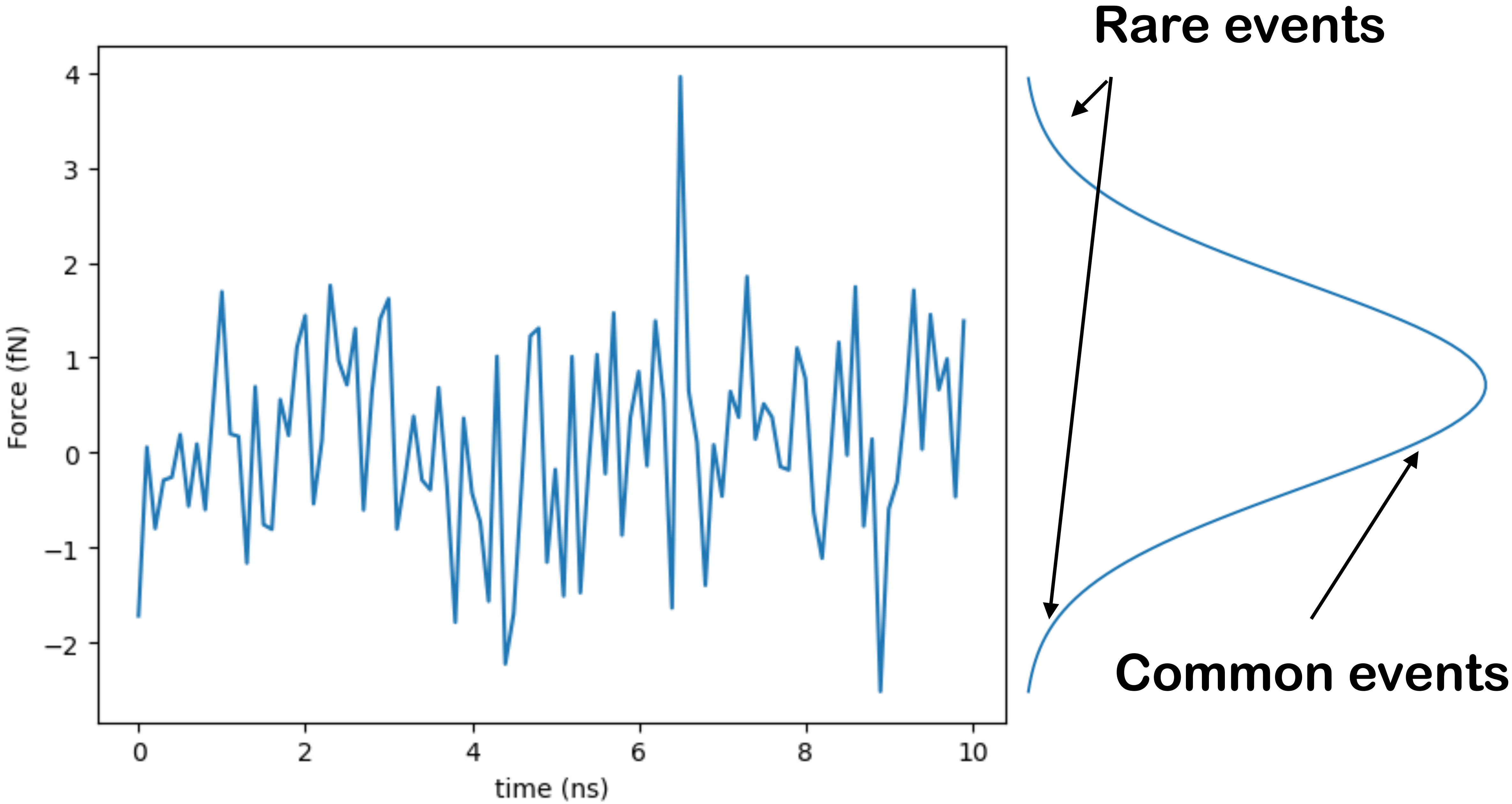

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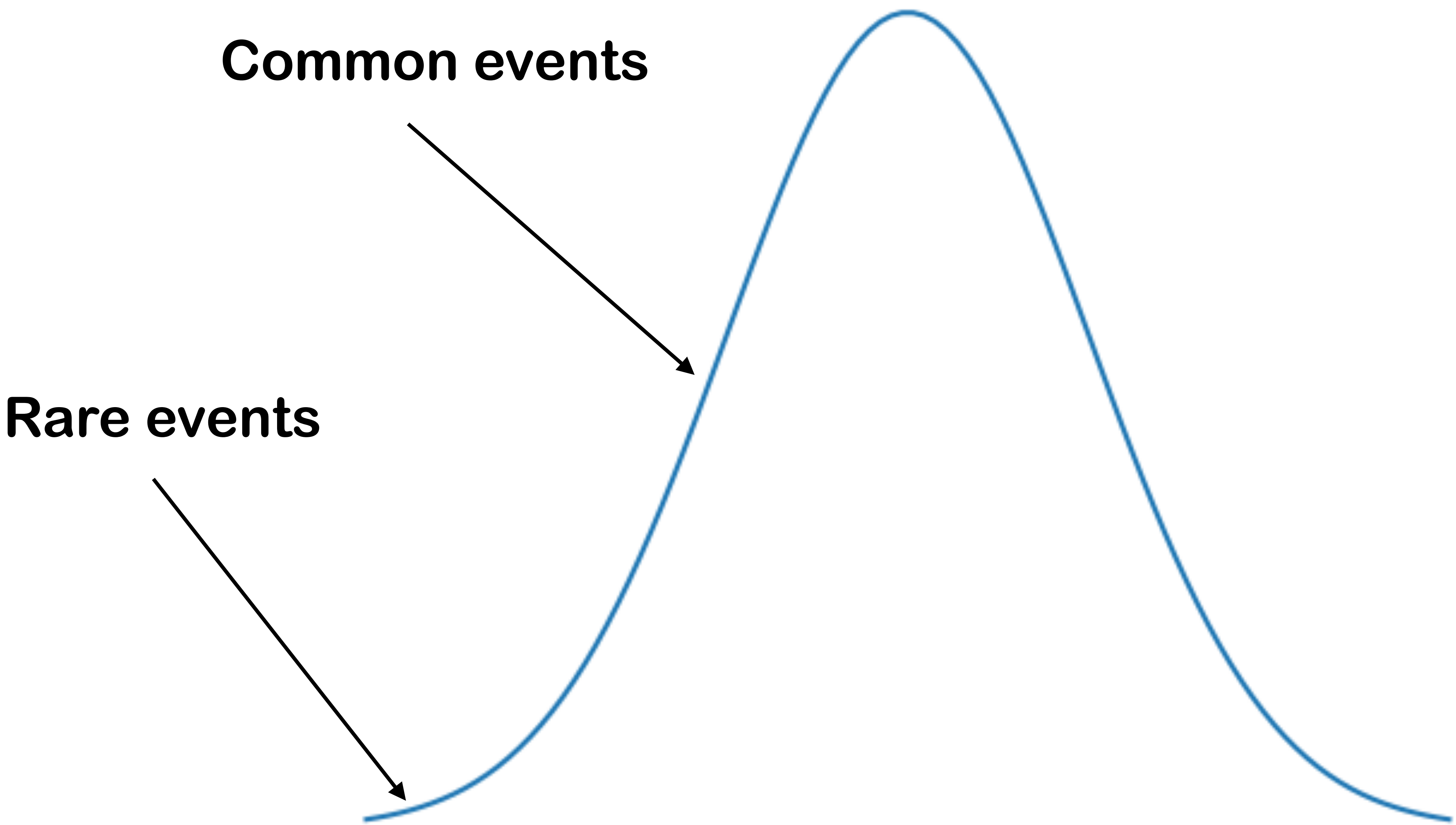

What does a Gaussian look like?

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

variance

mean

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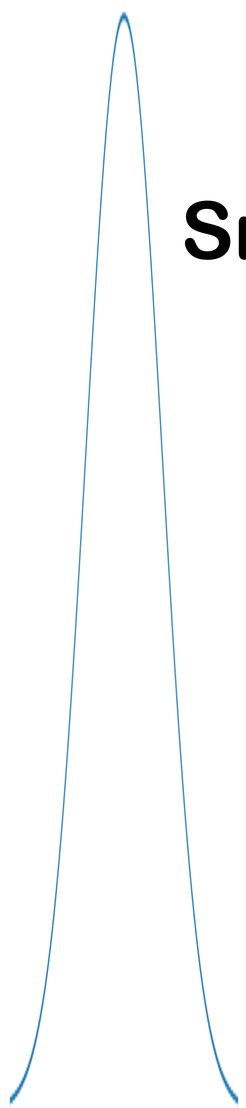
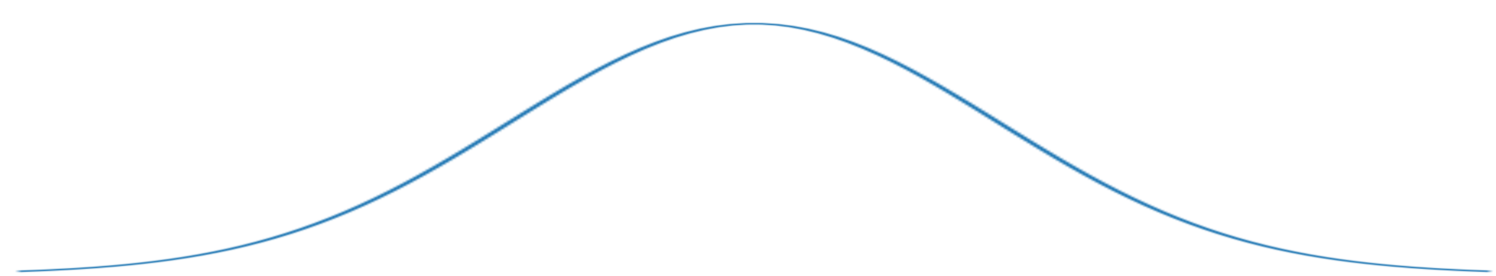


Small variance

Big variance



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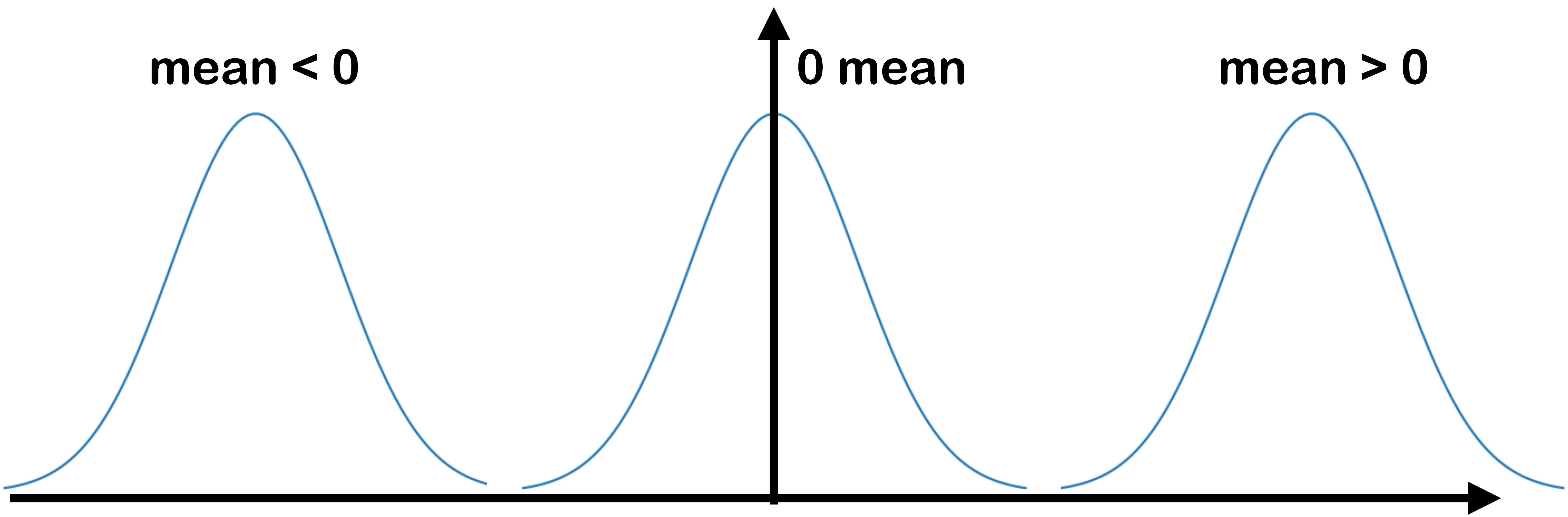
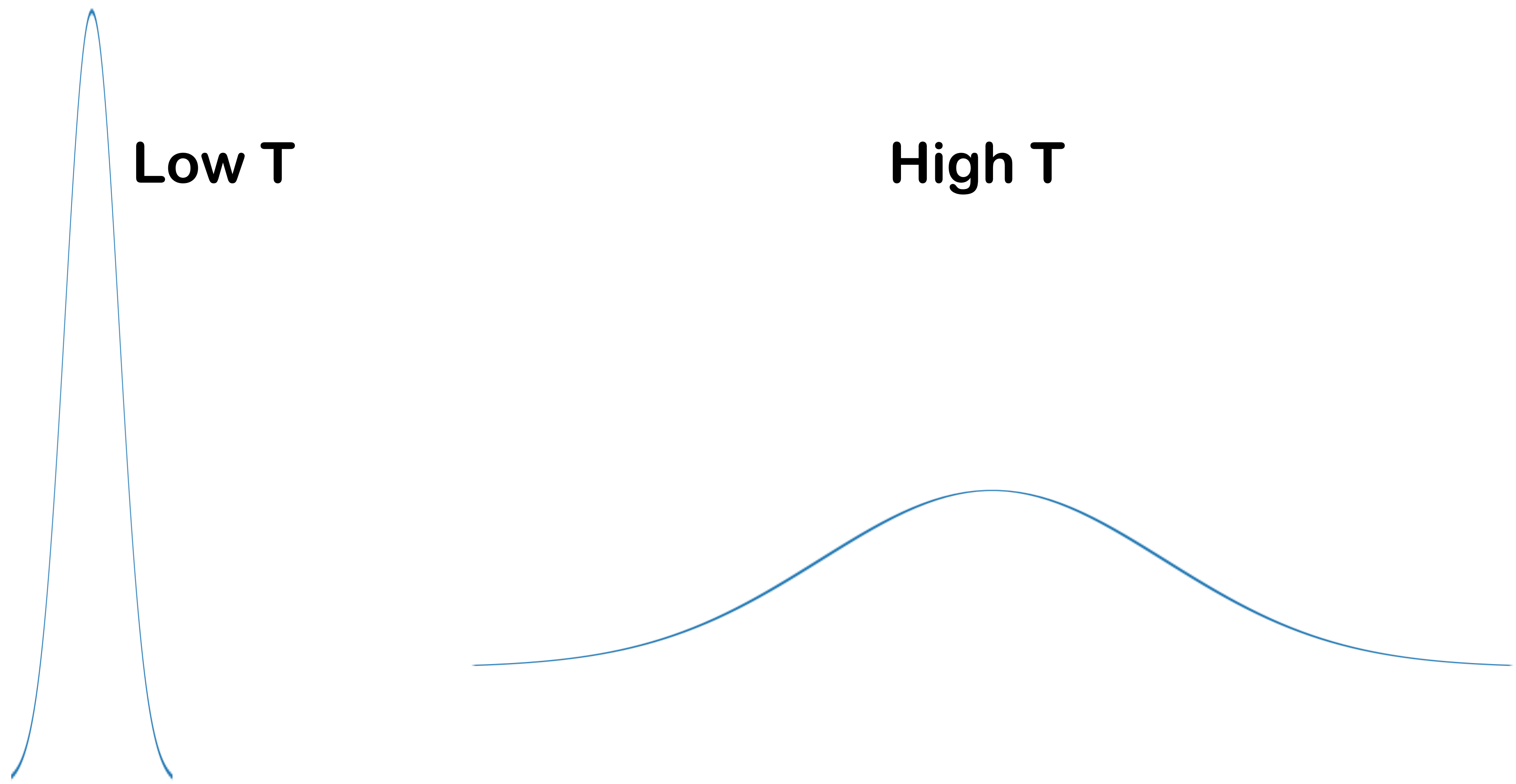


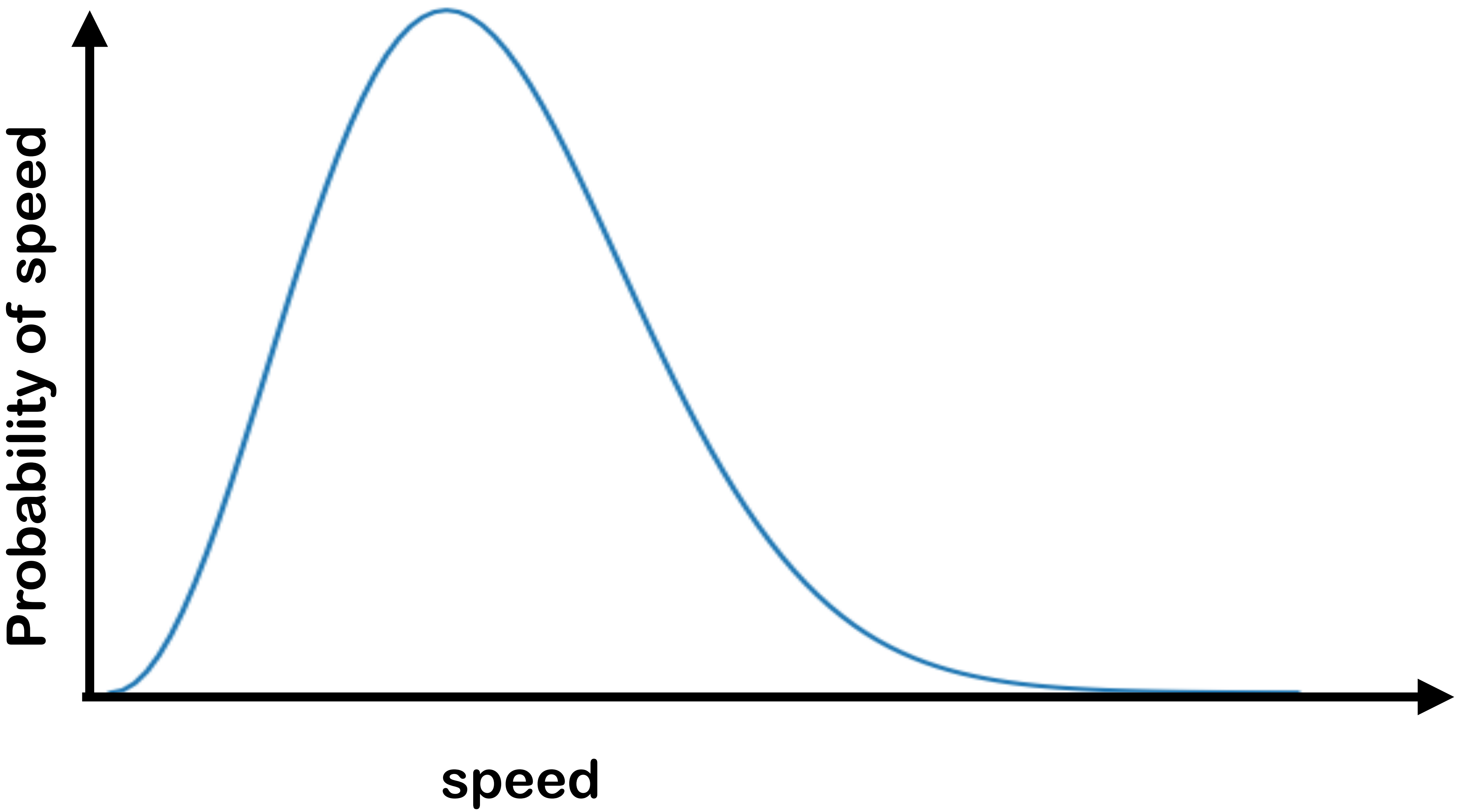
How is the variance related to temperature?

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$



Because of the “kicks” provided by the environment, the speeds of molecules are usually quickly randomized.

So if the force kicks follow a Gaussian, the speed is distributed according to a Maxwell Boltzmann



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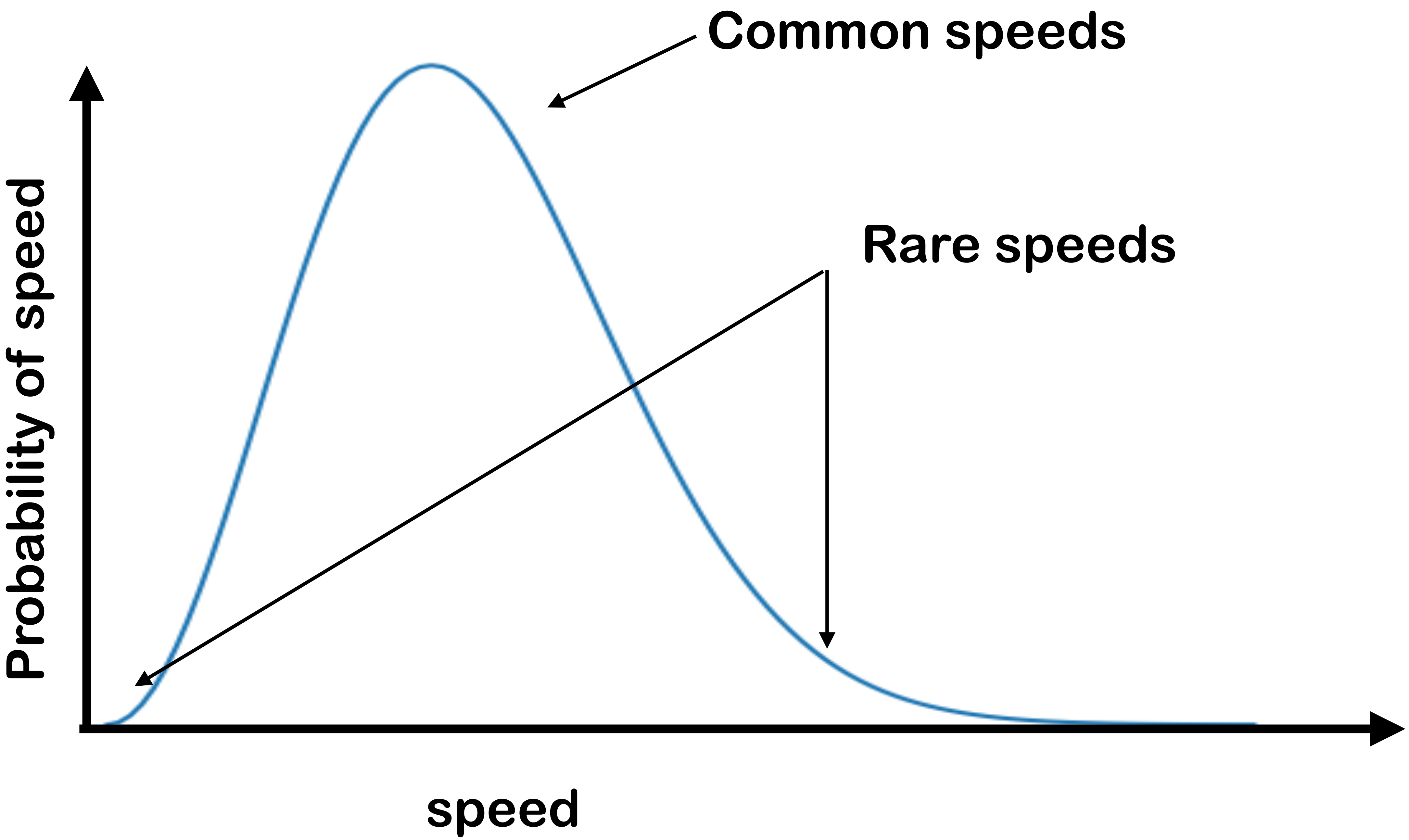

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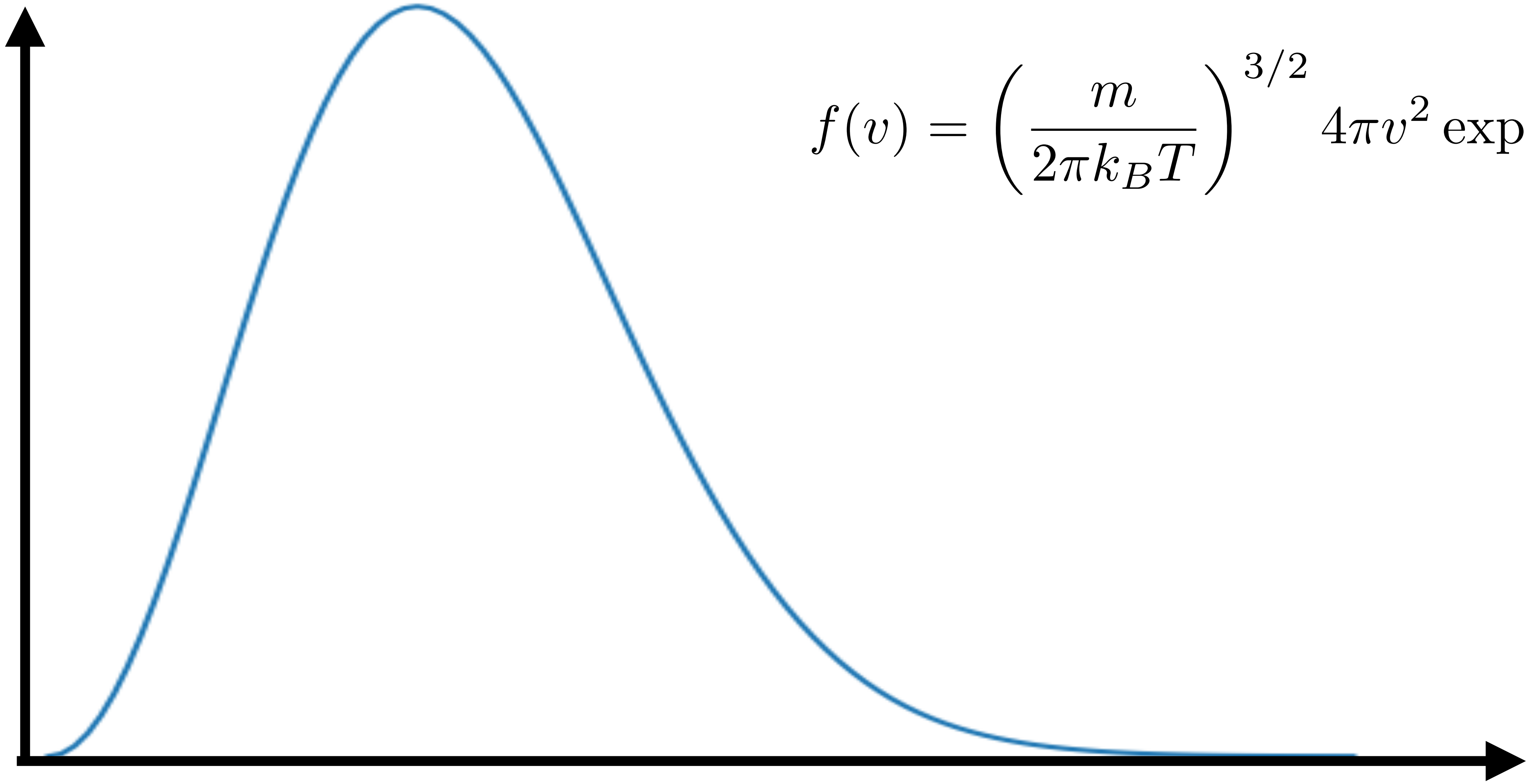
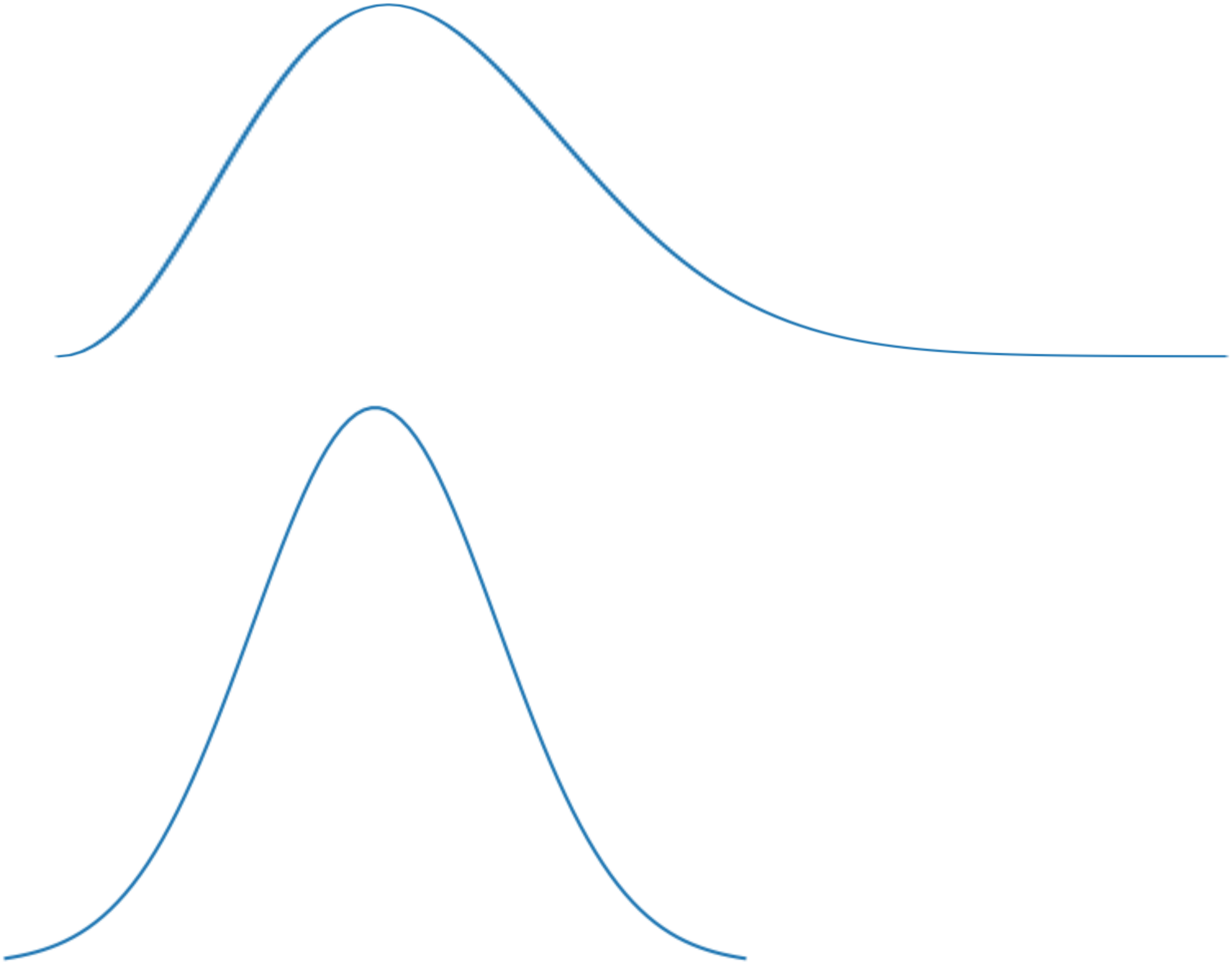


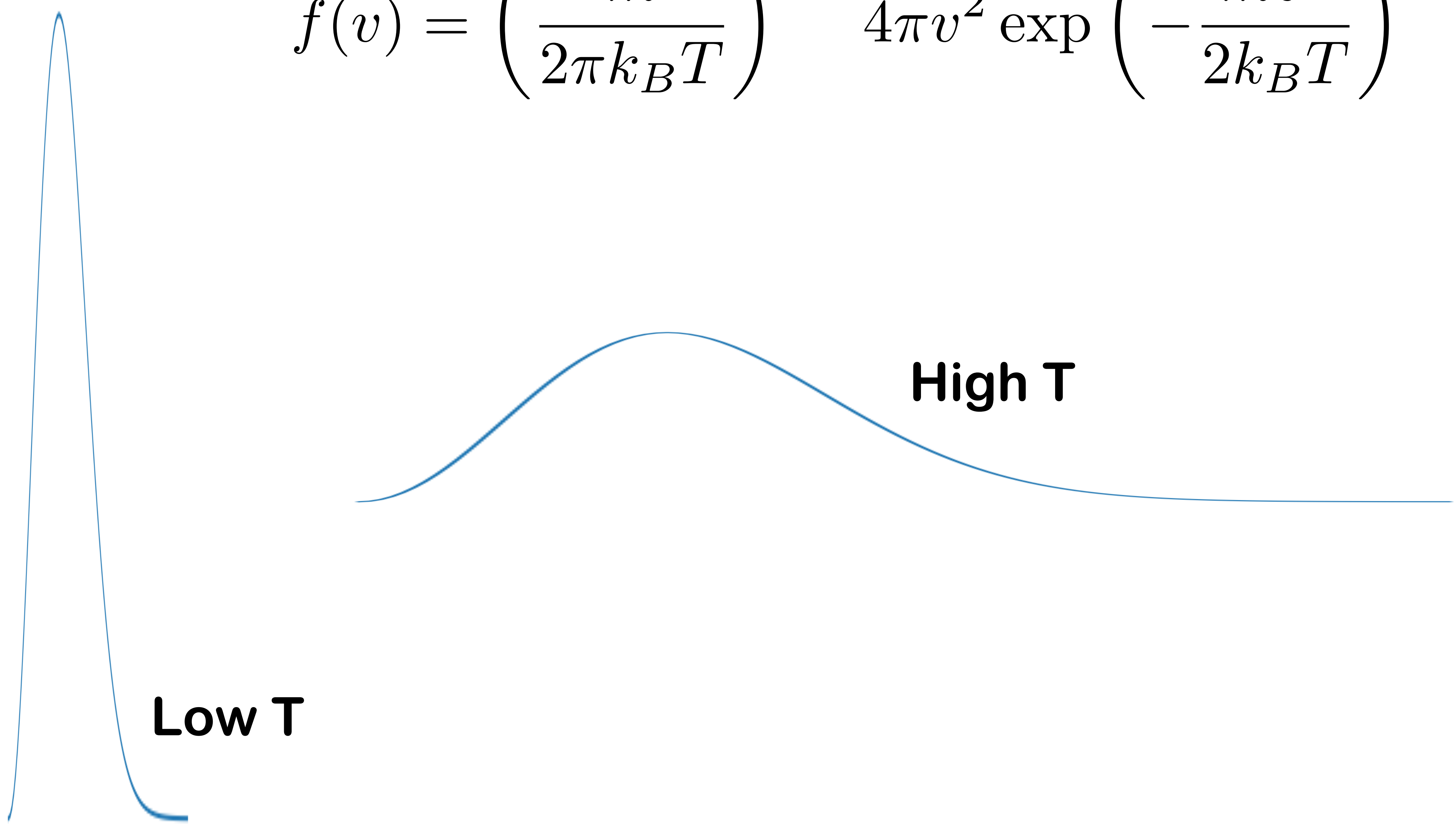
$$f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$

What do you notice is the difference between Maxwell Boltzmann and Gaussian distribution?

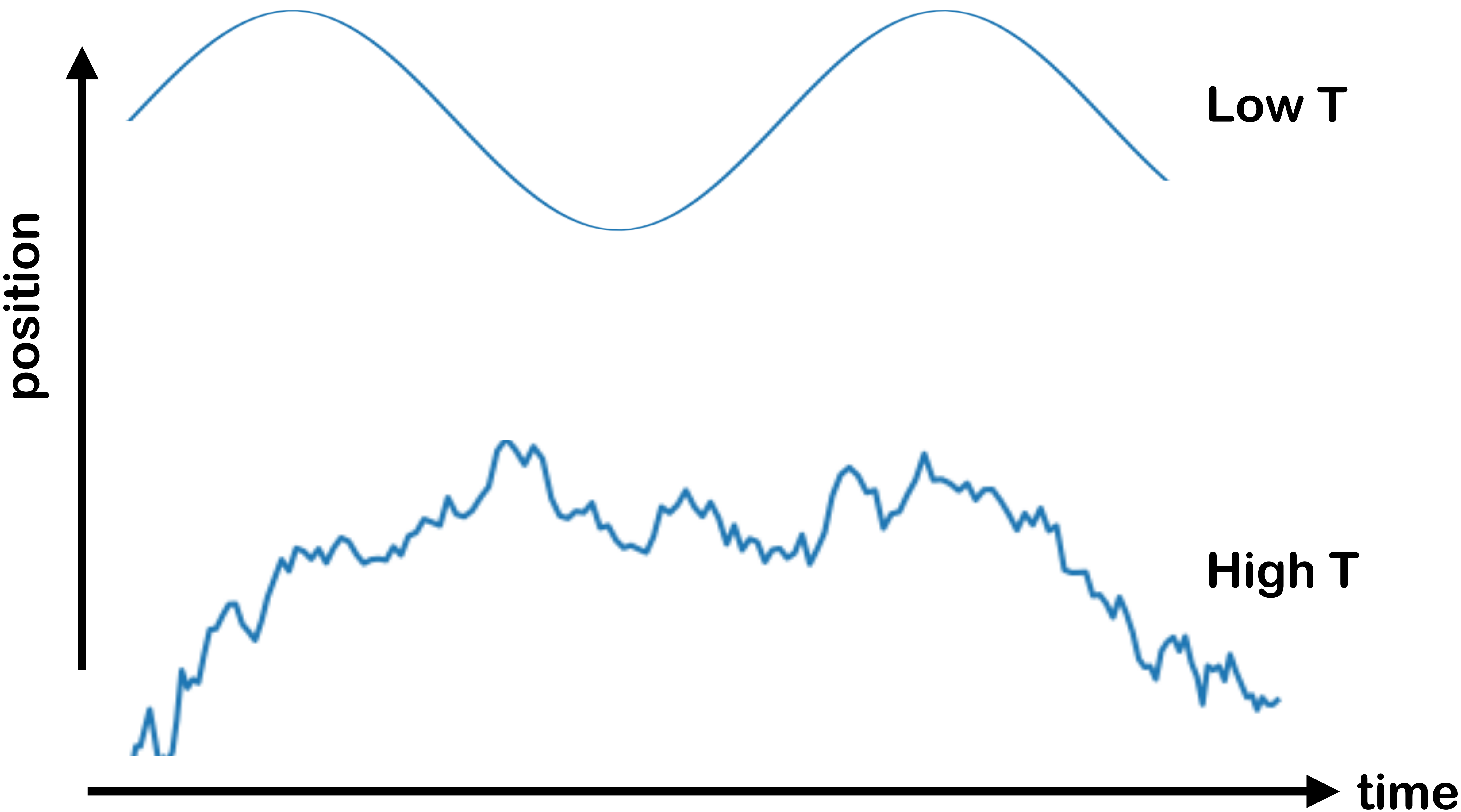


High versus low temperature Maxwell Boltzmann

$$f(v) = \left(\frac{m}{2\pi k_B T}\right)^{3/2} 4\pi v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$



Here is the motion of a particle in a harmonic potential



When we simulate a protein, how do we simulate the effect of temperature and bombardment due to water molecules (i.e., the environment)?

Draw the velocity in each direction (x,y,z) from a Maxwell-Boltzmann. Then simulate the position of every atom (from the fluid and protein) according to

$$v_{\text{old}} \sim \text{Maxwell-Boltzmann}$$

Iterate
$$\left[\begin{array}{l} v_{\text{new}} \approx v_{\text{old}} + \dfrac{F(x_{\text{old}})}{m}\Delta t \\ x_{\text{new}} \approx x_{\text{old}} + v_{\text{new}}\Delta t \end{array}\right.$$

$$v_{\text{old}} \sim \text{Maxwell-Boltzmann}$$

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What do we do exactly?

How do we initiate positions of atoms? How many velocities do we need to initialize?

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Positions for all atoms (from protein and fluid) can be initialized from "crystal structures".

# of velocities initialized: 3 velocities for each of the three directions of each (!) atom. So for N atoms, we need to initialize 3N velocities.

How do we draw samples from a random variable?

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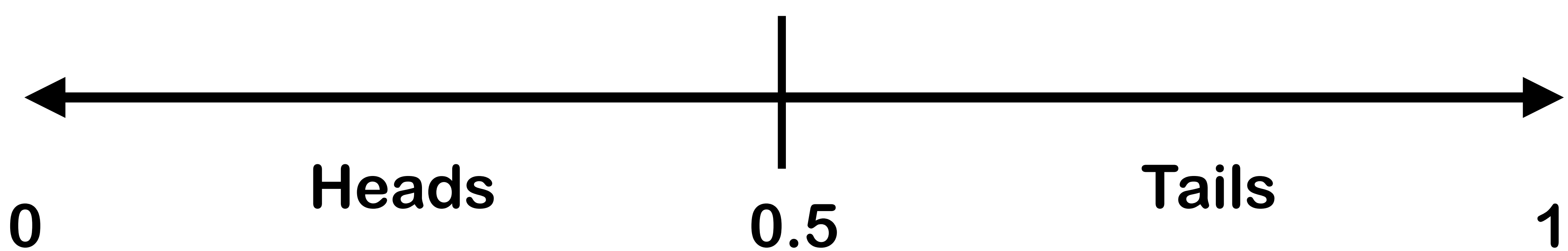
Draw a random number from 0 to 1. If it falls below the line, picks heads. Otherwise pick tails.



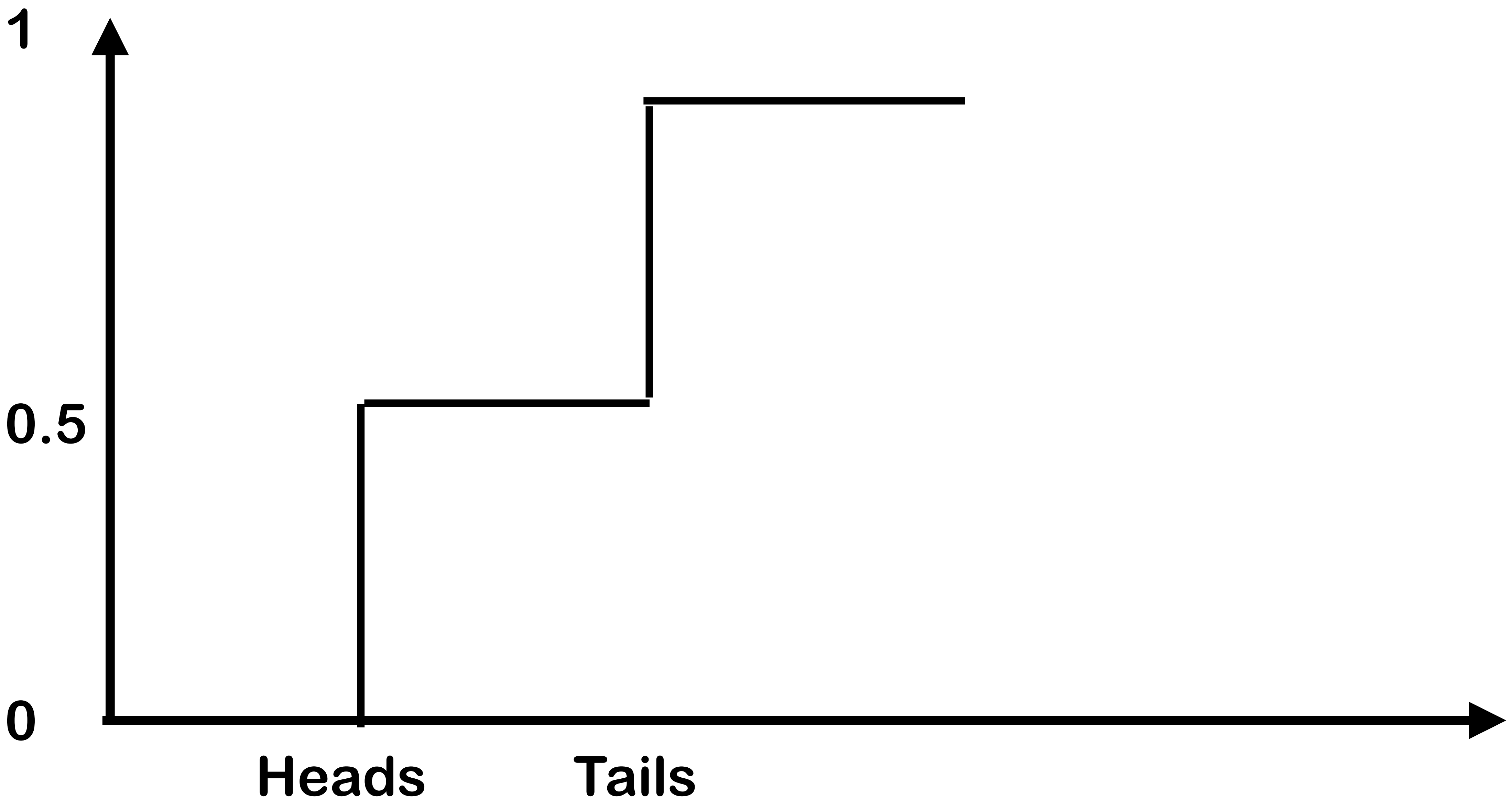
How do we draw samples from a random variable?

$$u \sim \mathrm{Uniform}_{[0,1]}$$

If u> 0.5, pick Heads.

Otherwise, pick Tails.

Let's get some intuition for how this works



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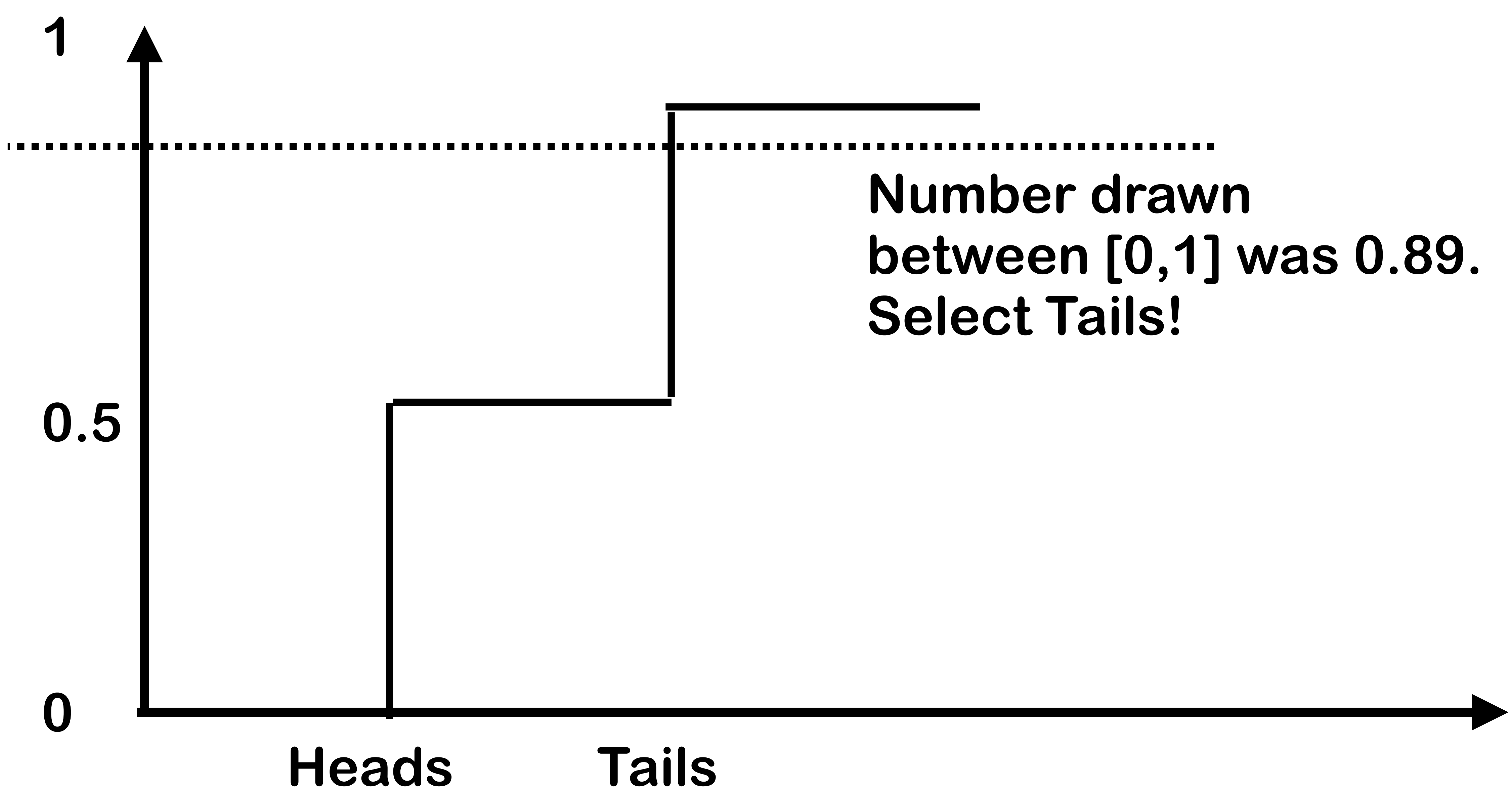

Now imagine a roll of a dice.

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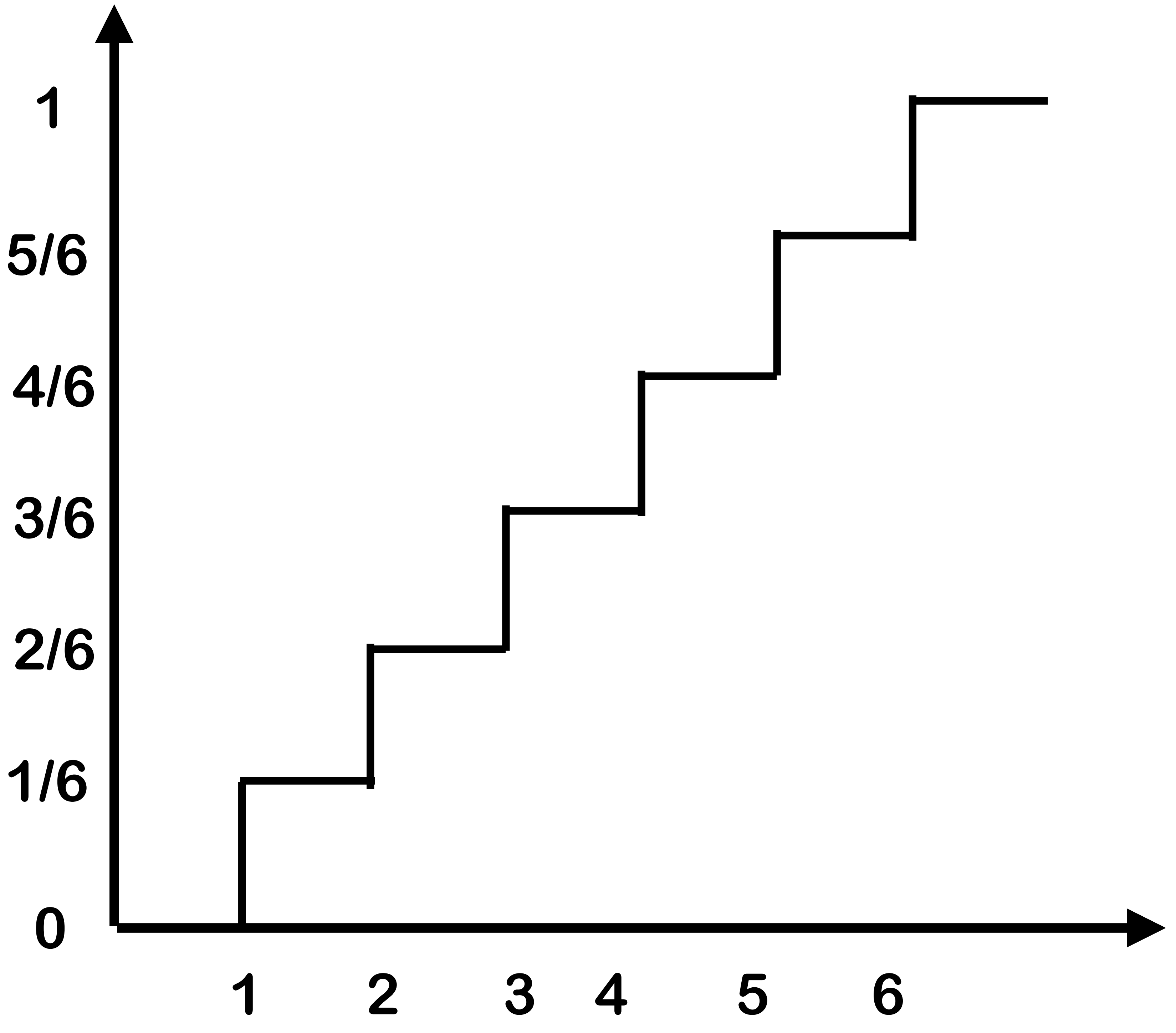

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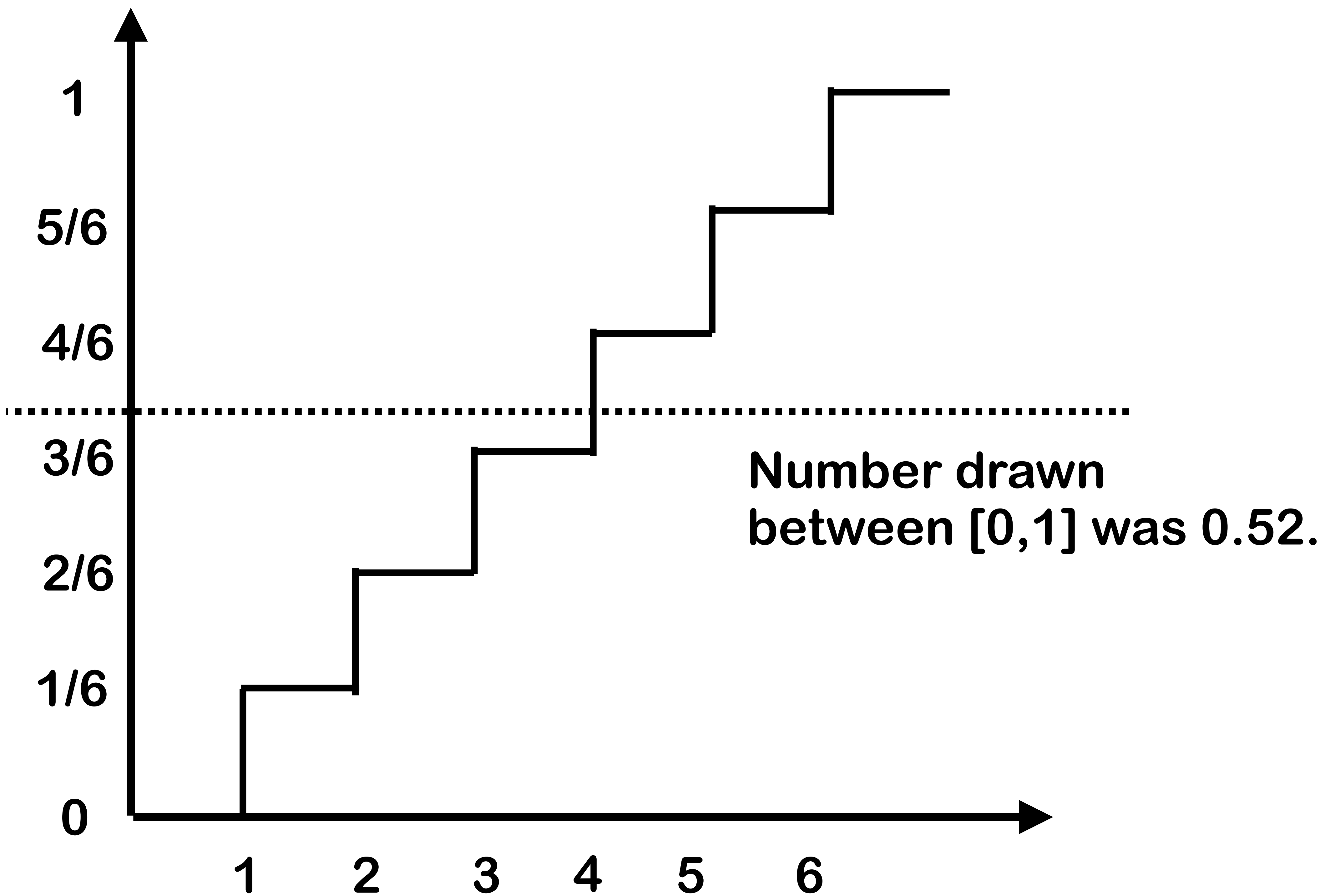

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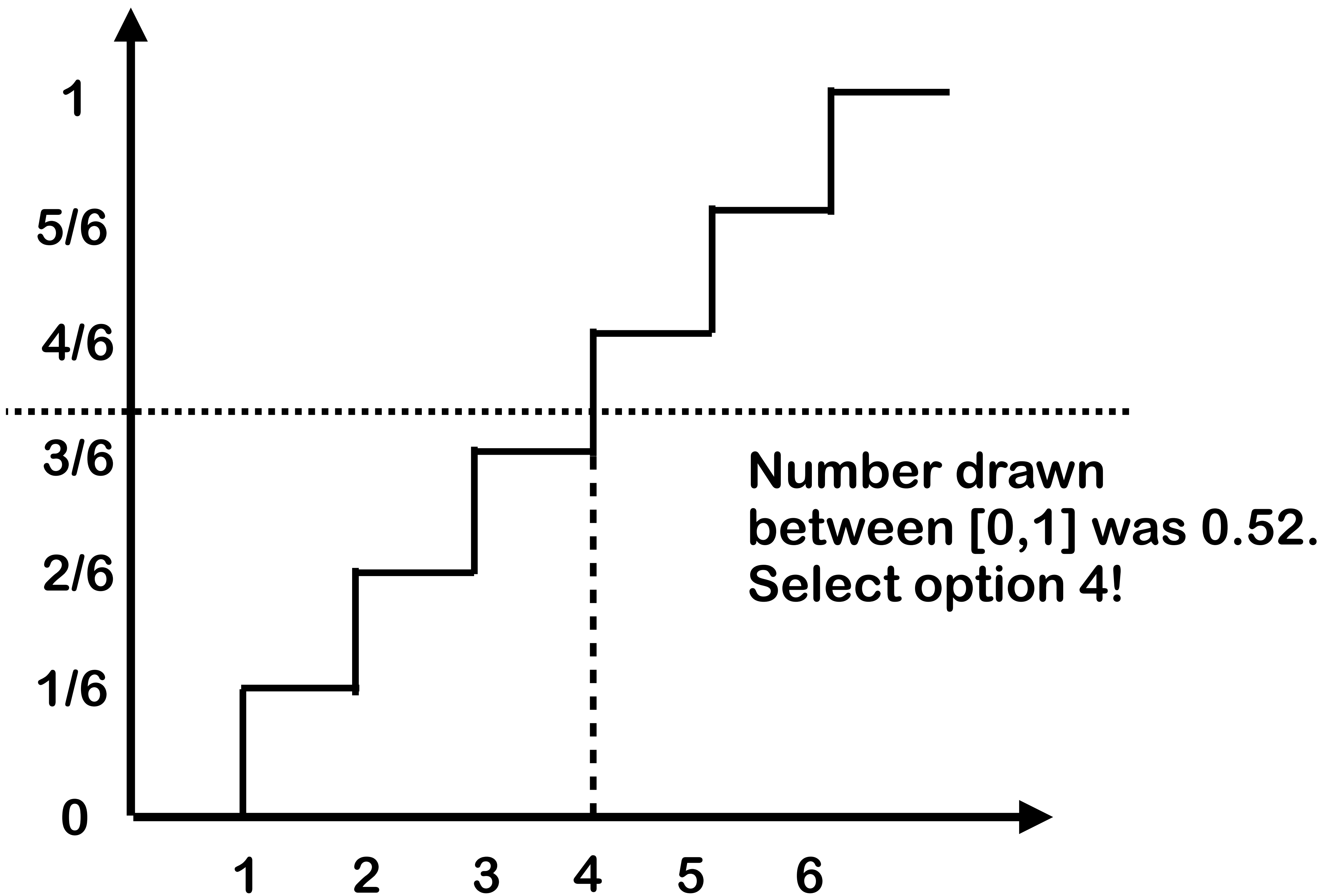
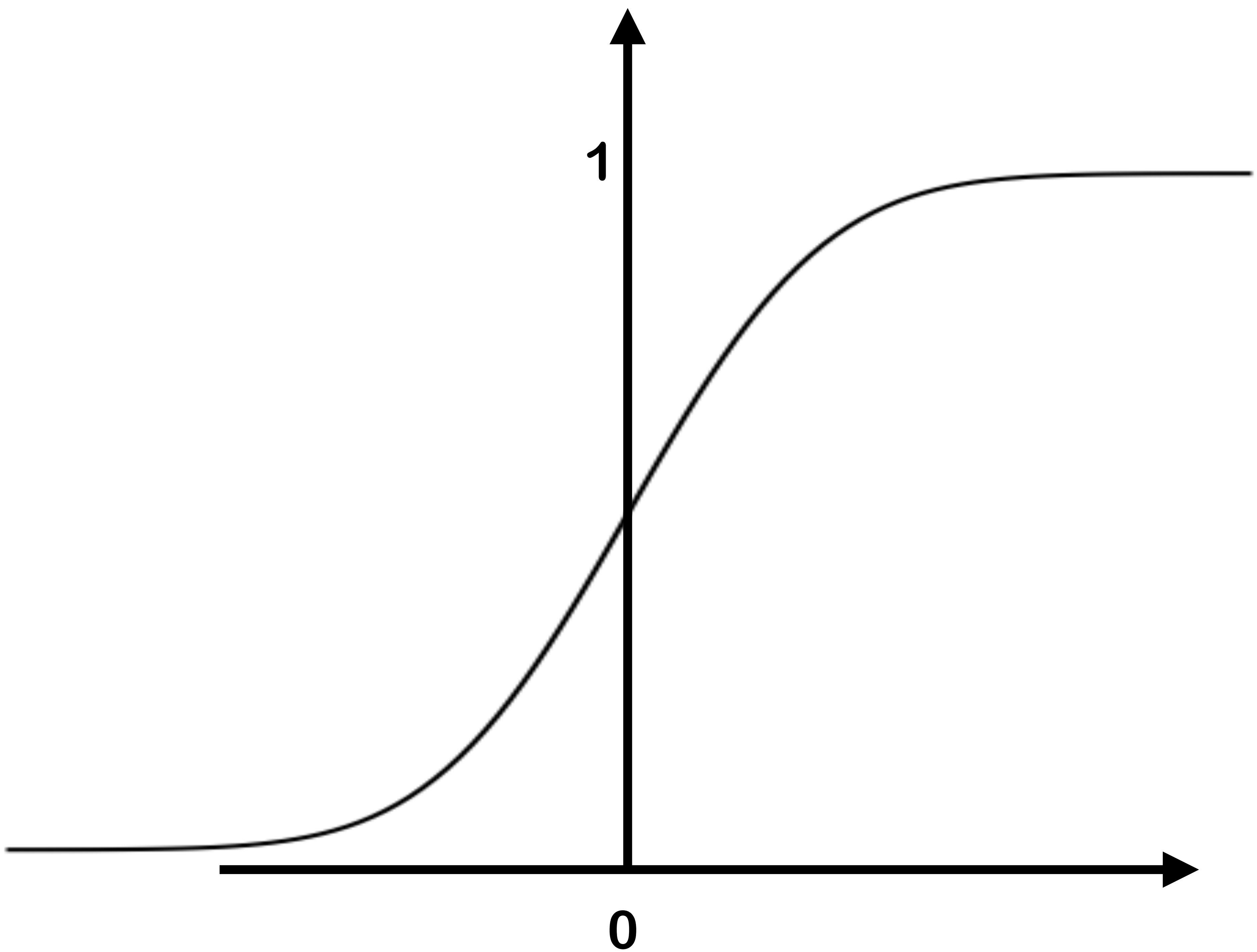


How many “options” does a Gaussian have? Infinity!



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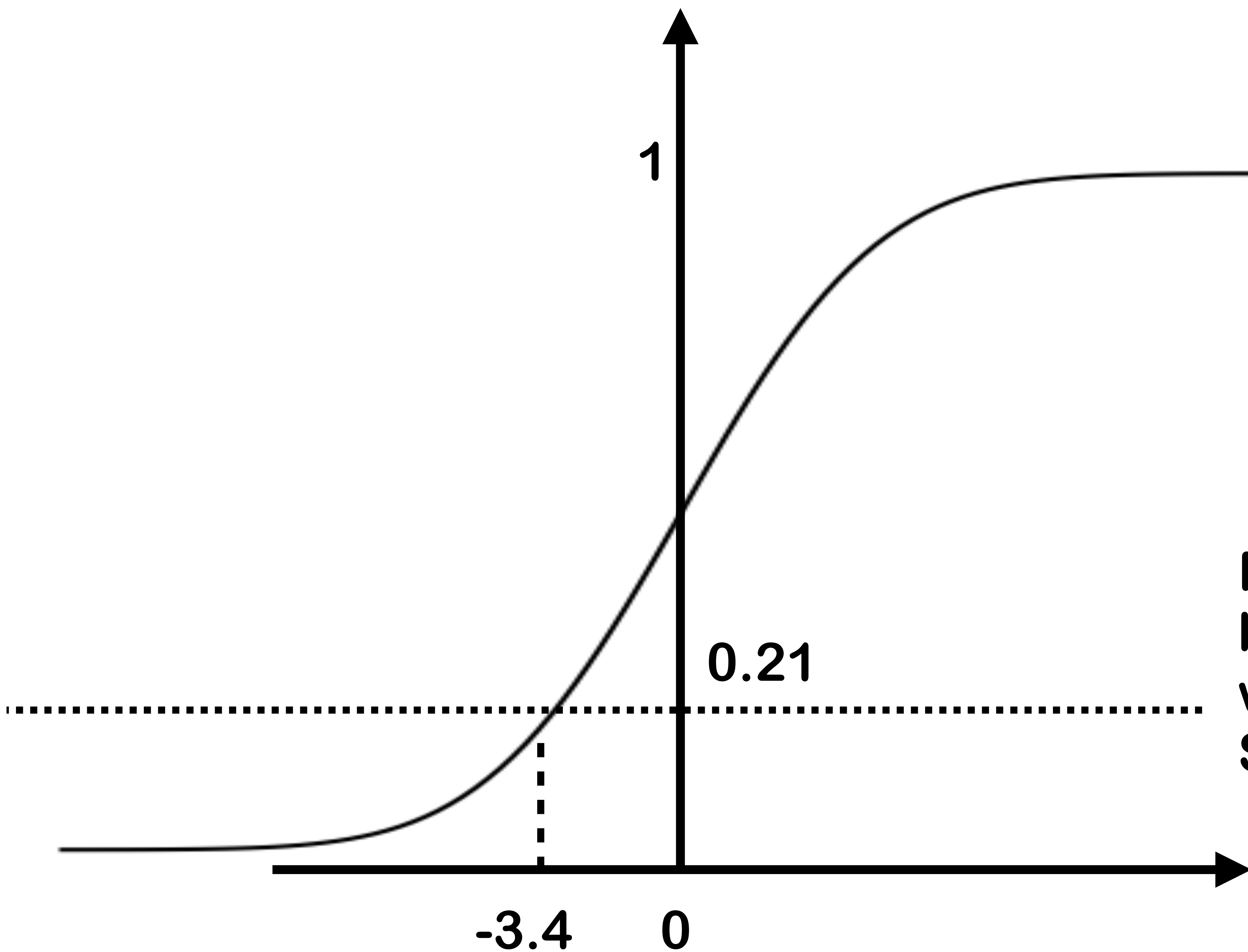
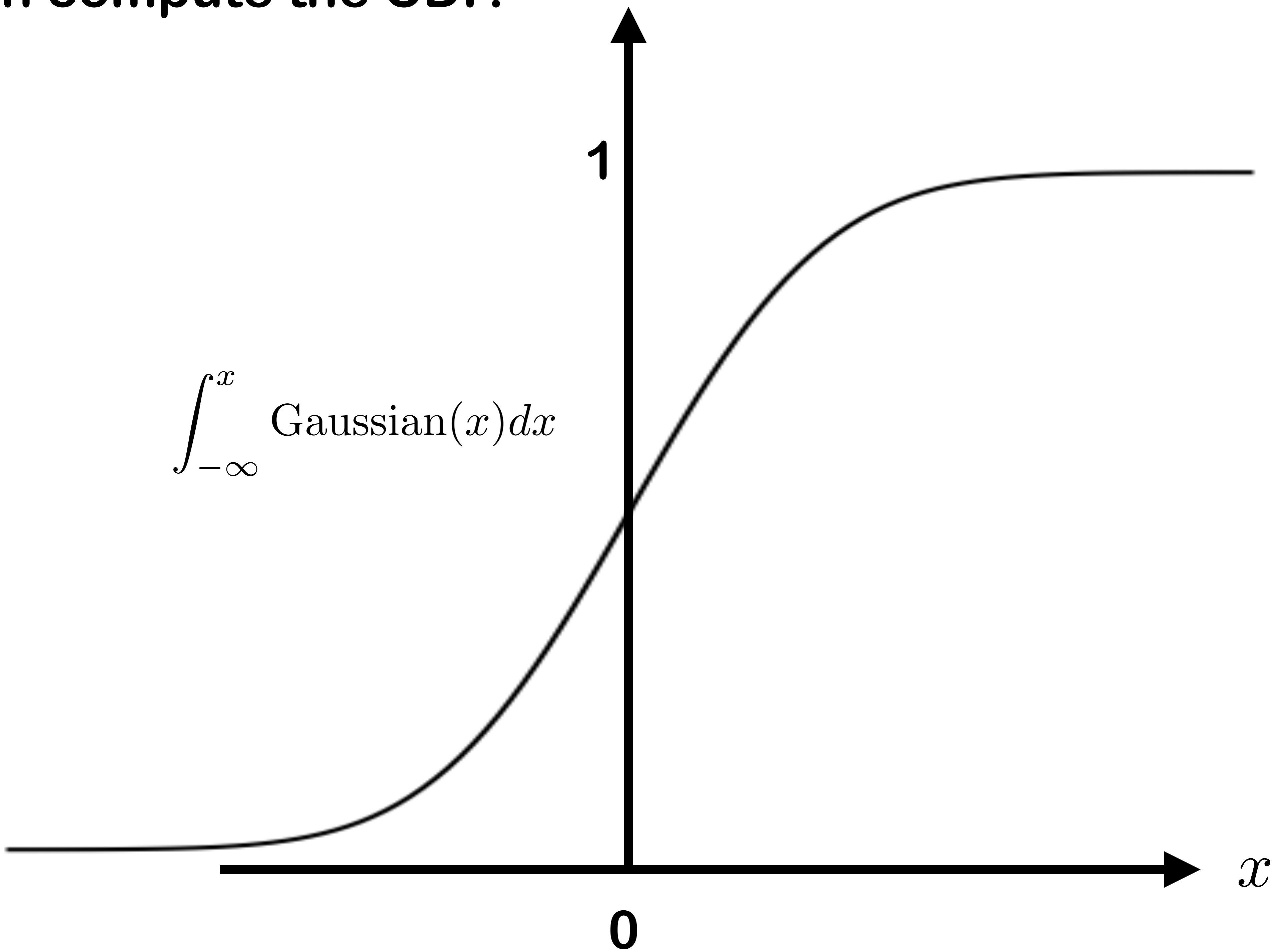


Number drawn between [0,1] was 0.21. Select -3.4!

This method is sometimes called the "CDF" (cumulative distribution function) method for drawing samples from distributions. It only works when you can compute the CDF.



Most of the time, calculating the CDF is not possible. In that case we use a completely different method called Monte Carlo to draw samples from complicated distributions.

In many cases we use Gaussians for forces from which Maxwell-Boltzmann can be derived. Gaussians can be sampled directly.

Why Gaussian?

Why Gaussian?

Tautological answer: Gaussians appear everywhere.

The following are approximately Gaussian:

Test scores, human heights, planet sizes, number of photons emitted by excited atoms, kick magnitudes on a protein, …

Why Gaussian?

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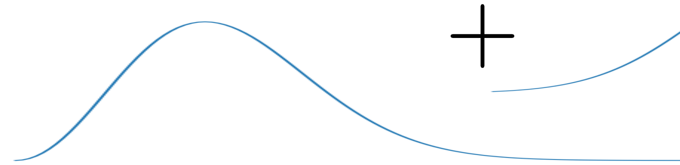
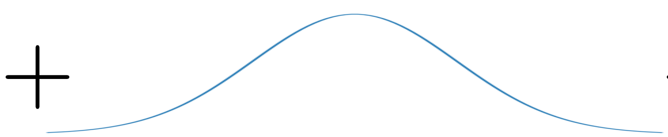
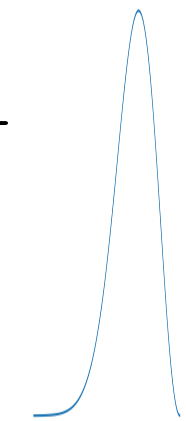
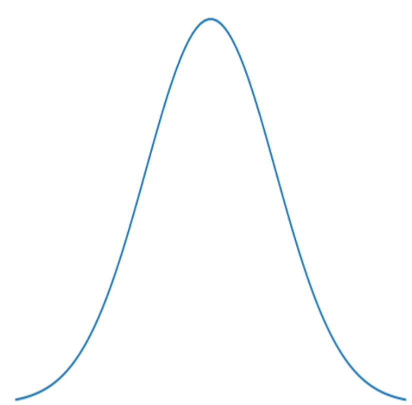
$$\text{Net effect} = \text{first cause} + \text{second cause} + \cdots$$

$=$  $+$  $+$ 

$=$ 

Why Gaussian?

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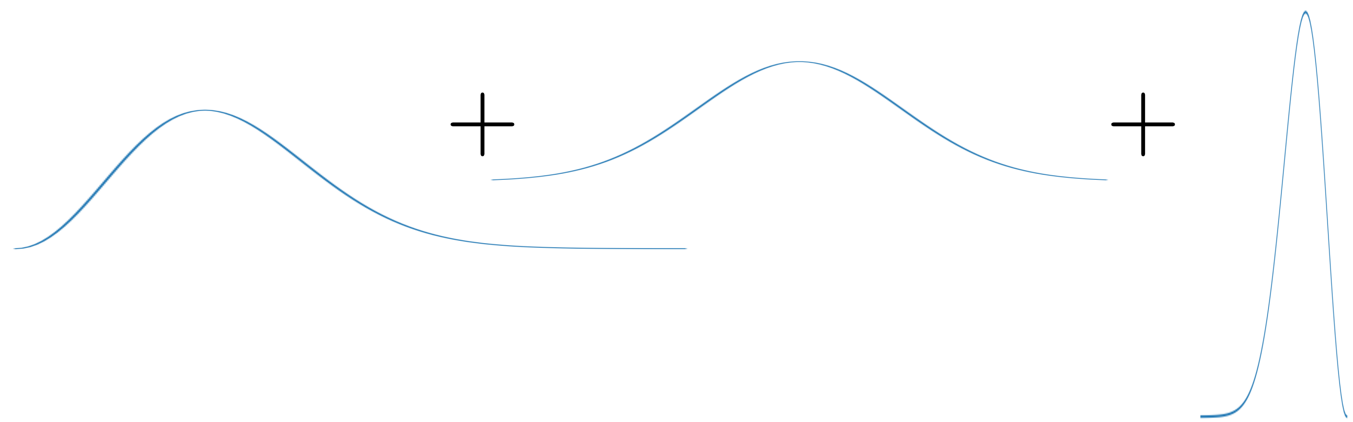
$=$



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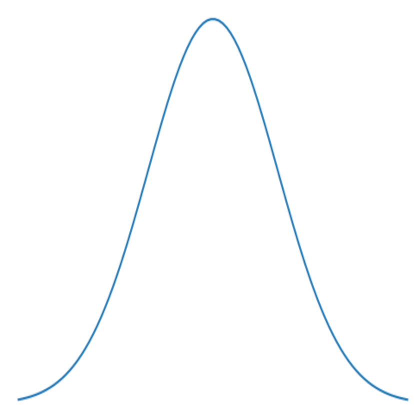

Central limit theorem

(the most important result of applied mathematics)