Modelling of Complex Systems

Random Walks

A Random Walk is the path of a particle (in some space) defined by a **random sequence of displacements**.

The displacements of a Random Walk are generated by a Markov process, i.e., the next state (i.e., position of the particle) depends only on the current state (the particle *has no memory*), which implies that **displacements are independent**.

A long history

The Roman philosopher Lucretius (60 BC) observed motion of dust particles as evidence of the existence of atoms.

In 1785, Jan Ingenhousz (physiologist, biologist) observed coal dust particles moving on the surface of alcohol.

In 1827, Robert Brown (botanist) observed pollen particles floating on water.

In 1863, Jules Regnault (French mathematician and stockbroker) applied ideas of randomness and Random Walks to the analysis of the stock market.

In 1905, Einstein found a relationship between diffusion coefficient *D,* the mobility μ, and the temperature T

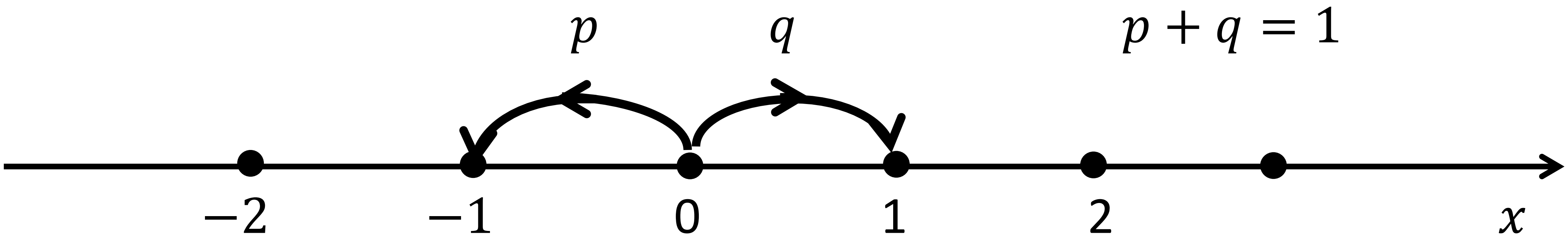
$$D = \mu k_B T.$$

Applications of the ideas of Random Walks:

- diffusion of particles
- ecology and biology (animals searching a food)
- computer science (Google ranking)
- folding of polymer particles and molecules
- economics (fluctuations in the stock market)
- neuroscience (activation of neurons)

One-dimensional Random Walks

We consider the following process of random *jumps* (displacements) on a one-dimensional periodic lattice:



A particle jumps with probability p on the left and with probability q on the right:

$p + q = 1$

First let us study the symmetrical case

$$p = q = 1/2$$

Each time step the particle jumps either on the left or on the right.

Where will be the particle after t jumps: $x(t)$?

What is the probability of finding particle at x after t jumps?

We introduce a random variable

$$S = \pm 1 = \begin{cases} +1, & \text{jump to the right} \\ -1, & \text{jump to the left} \end{cases}$$

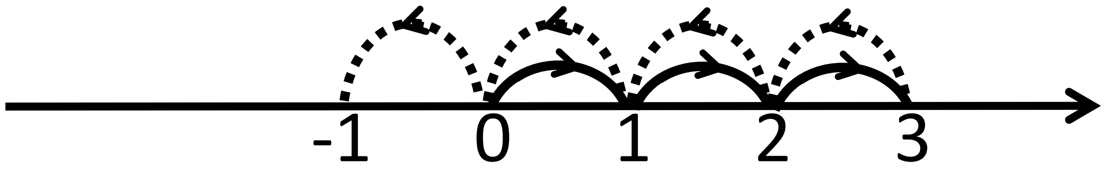
The probability distribution function of S:

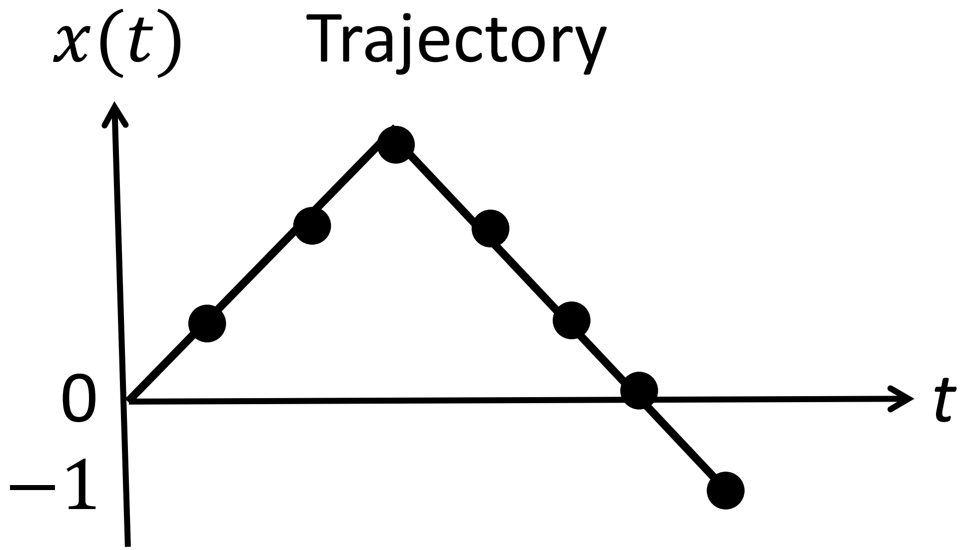
$$P(S) = \frac{1}{2}\delta(S-1) + \frac{1}{2}\delta(S+1), \quad \sum_{S=\pm1} P(S) = 1, \quad \sum_{S=\pm1} P(S)S = 0.$$

Here $\delta(S \pm 1)$ is the Kronecker delta. After t jumps the particle is at the point

$$x(t) = S_1 + S_2 + \ldots S_t = \sum_{i=1}^{t} S_i \equiv x(S_1, S_2, \ldots S_t)$$

where $S_i = \pm 1$ for the i-th jump.





Every Random Walk is characterized by a trajectory.

The number of possible trajectories after t random jumps is 2^t.
In symmetrical RWs, all trajectories have the same probability $1/2^t$.

The mean value of $x(t)$ after t jumps is

$$\langle x(t)\rangle = \langle x(S_1, S_2,\ldots S_t)\rangle = \sum_{trajectories} \frac{1}{2^t} x(S_1, S_2,\ldots S_t)$$

$$= \sum_{\{S_1,S_2,\ldots S_t\}} \prod_{i=1}^{t} P(S_i) x(S_1, S_2, \ldots S_t) = \sum_{\{S_1,S_2,\ldots S_t\}} \prod_{i=1}^{t} P(S_i) \sum_{j=1}^{t} S_j$$

$$= \sum_{j=1}^{t} \sum_{\{S_1,S_2,\ldots S_t\}} \prod_{i=1}^{t} P(S_i)\, S_j = \sum_{j=1}^{t} \langle S_j\rangle = 0\,.$$

Therefore, the mean position of a particle is

$$\langle x(t)\rangle = 0.$$

The variance is

$$\langle (x(t) - \langle x(t)\rangle)^2\rangle = \langle x^2(t)\rangle - \cancelto{0}{\langle x(t)\rangle^2} = \langle x^2(t)\rangle =$$

$$= \left\langle \left(\sum_{i=1}^{t} S_i\right)^2 \right\rangle = \sum_{i=1}^{t}\sum_{j=1}^{t} \langle S_i S_j\rangle = \sum_{i=1}^{t} \langle S_i^2\rangle + \sum_{i\neq j}^{t} \langle S_i S_j\rangle$$

Furthermore, we assume that jumps are independent (the Markovian property), i.e., there are no correlations between S_i's (no memory). Therefore,

$$\langle S_i S_j\rangle = \langle S_i\rangle\langle S_j\rangle = 0$$

We get

$$\langle x^2(t)\rangle = \sum_{i=1}^{t} \langle S_i^2\rangle = \sum_{i=1}^{t} 1 = t$$

$$\Rightarrow \langle x^2(t)\rangle = t,$$

where we use $S_i^2 = 1$ since $S_i = \pm 1$.

Then the standard deviation is

$$\sigma = \sqrt{\langle x^2(t) \rangle} = \sqrt{t}$$

These results agree with the Central Limit Theorem.

To see this, we introduce a variable

$$X = \frac{1}{t}\sum_{i=1}^{t} S_i = \frac{x(t)}{t}$$

According to the Central Limit Theorem, at $t \gg 1$, the mean value and variance of X are

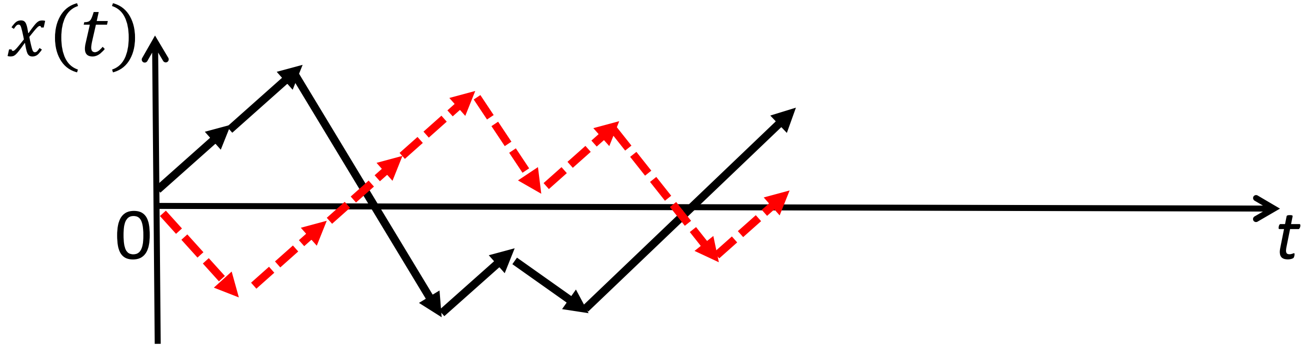
$$\langle X \rangle = \langle S \rangle = 0, \qquad \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle = \frac{\langle S^2 \rangle}{t} = \frac{1}{t}$$

Therefore,

$$\langle X^2 \rangle = \frac{\langle x^2(t) \rangle}{t^2} = \frac{1}{t} \quad \Longrightarrow \quad \langle x^2(t) \rangle = t$$

An explicit solution of 1D Random Walks

At $t = 0$ the particle is at $x = 0$, then it makes a random walk.
We repeat this process N times and get N trajectories ($N \gg 1$).
That there are exactly 2^t possible trajectories of t steps, and all of them have the same probability 2^{-t} to be chosen by the particle.



We count how many of the N trajectories end up at point x; call it $N(x,t)$.
The probability $P(x,t)$ to observe the particle at a point x after t steps equals

$$P(x,t) = \frac{\text{number of trajectories that end up at point x after t jumps}}{\text{total number of trajectories after t jumps}}$$

$$\Rightarrow P(x,t) = \frac{N(x,t)}{N}$$

Another definition of $P(x,t)$. At $t=0$ we have $N \gg 1$ particles at $x=0$. Then they start randomly walking simultaneously. Let us count the number of particles that reach a point x after t steps. We denote this number as $n(x,t)$.

Then
$$P(x,t) = \frac{n(x,t)}{N}.$$

This approach is convenient for simulations. The first approach is convenient for analytical calculations.

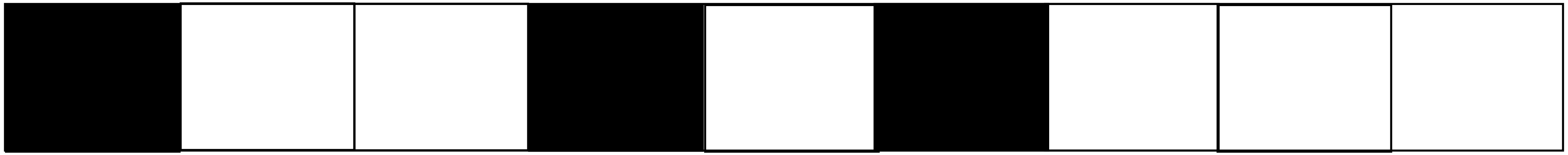
Let us assume the particle made n_+ jumps to the right and n_- jumps to the left. We have equalities:

$$\begin{cases} t = n_+ + n_- \\ x = n_+ - n_- \end{cases} \Longrightarrow \begin{cases} n_+ = \frac{t+x}{2} \\ n_- = \frac{t-x}{2} \end{cases}$$

It is obvious that

$$-t \leq x \leq t$$

We represent a trajectory as a sequence of white and black boxes:



$-1 \quad 1 \quad 1 \quad -1 \quad 1 \quad -1 \quad 1 \quad 1 \quad 1$

White boxes represent jumps to the right ($S = +1$). Black boxes represent jumps to the left ($S = -1$).

The number of ways we can distribute n_- black boxes among $t = n_+ + n_-$ boxes equals the numbers of trajectories that end up at point $x = n_+ - n_-$:

$$C_{n_-}^t = \frac{t!}{(t - n_-)!\, n_-!} = \frac{t!}{n_-!\, n_+!} = \frac{t!}{\left(\frac{t-x}{2}\right)!\left(\frac{t+x}{2}\right)!}$$

Here we used the fact that $n_- = \frac{t-x}{2}, n_+ = \frac{t+x}{2}$. We get the probability

$$P(x,t) = \frac{C_{n_-}^t}{2^t} = \frac{1}{2^t}\frac{t!}{\left(\frac{t-x}{2}\right)!\left(\frac{t+x}{2}\right)!}.$$

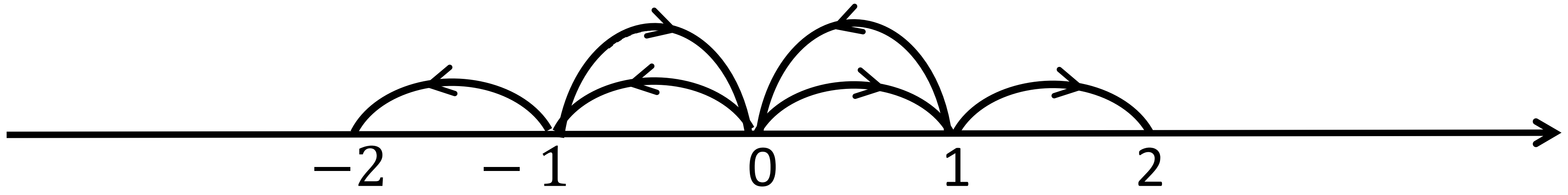
$P(x,t) = C^t_{n_-} 2^{-t}$ is the explicit probability distribution function.

Normalization: $$\sum_{x=-t}^{t} P(x,t) = 1$$

To see this, notice that the summation over x is equivalent to summation over n_-

$$\sum_{x=-t}^{t} P(x,t) = \sum_{n_-=0}^{t} C^t_{n_-} \left(\frac{1}{2}\right)^{n_-} \left(\frac{1}{2}\right)^{t-n_-} = \left(\frac{1}{2}+\frac{1}{2}\right)^t = 1$$

Note that if t is even ($t = 2m$) we only can reach sites with even coordinates, i.e., $x = 2l$ where $l = 0, \pm 1, \dots \pm m$. If t is odd ($t = 2m+1$) we only can reach sites with odd coordinates, i.e., $x = 2l+1$ where $l = 0, \pm 1, \dots \pm m$. For example, at $t = 2$ we only can reach $x = 0, \pm 2$.



Particular cases:

$$x = 0 \qquad P(0,t) = \frac{1}{2^t}\frac{t!}{\left(\frac{t-x}{2}\right)!\left(\frac{t+x}{2}\right)!} = \frac{1}{2^t}\frac{t!}{\left(\frac{t}{2}\right)!\left(\frac{t}{2}\right)!} =$$

$$x = \pm t \qquad P(\pm t, t) = \frac{1}{2^t} = e^{-t\ln 2}$$

Approximate equation for $P(x,t)$

In the case $t \gg 1, |x| \ll t$, we can use Stirling's approximation

$$t! \approx \sqrt{2\pi t}\, t^t e^{-t}$$

$$\left(\frac{t+x}{2}\right)! \approx \sqrt{2\pi\left(\frac{t+x}{2}\right)}\left(\frac{t+x}{2}\right)^{\frac{t+x}{2}} e^{-\left(\frac{t+x}{2}\right)}$$

$$= \sqrt{2\pi}\left(\frac{t}{2}\right)^{\frac{1}{2}+\frac{t+x}{2}} \exp\left[-\left(\frac{t+x}{2}\right) + \left(\frac{1}{2}+\frac{t+x}{2}\right)\ln\left(1+\frac{x}{t}\right)\right]$$

Then we use the Taylor expansion: $\ln\left(1+\frac{x}{t}\right) \approx \frac{x}{t} - \frac{x^2}{2t^2}$. We get

$$\exp\left[-\left(\frac{t+x}{2}\right)+\left(\frac{1}{2}+\frac{t+x}{2}\right)\ln\left(1+\frac{x}{t}\right)\right] \approx \exp\left[-\frac{t}{2}+\frac{x}{2t}+\frac{x^2}{4t}\right]$$

Which gives

$$\left(\frac{t+x}{2}\right)! \approx \sqrt{2\pi}\left(\frac{t}{2}\right)^{\frac{t+x+1}{2}} \exp\left[-\frac{t}{2}+\frac{x}{2t}+\frac{x^2}{4t}\right]$$

Therefore

$$\left(\frac{t+x}{2}\right)!\left(\frac{t-x}{2}\right)! \approx 2\pi\left(\frac{t}{2}\right)^{t+1} \exp\left[-t+\frac{x^2}{2t}\right]$$

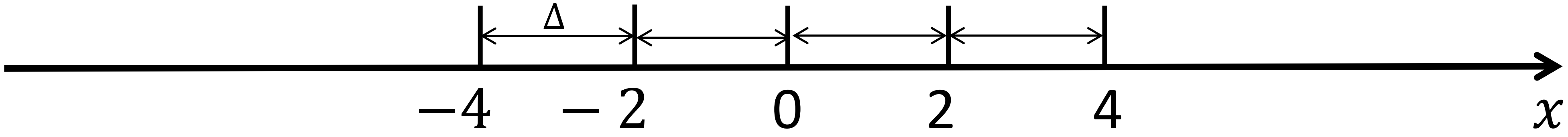
Finally,

$$P(x,t) = \frac{1}{2^t}\frac{t!}{\left(\frac{t-x}{2}\right)!\left(\frac{t+x}{2}\right)!} \approx \frac{1}{2^t}\frac{\sqrt{2\pi t}\, t^t e^{-t}}{2\pi\left(\frac{t}{2}\right)^{t+1} \exp\left[-t+\frac{x^2}{2t}\right]} = \frac{2}{\sqrt{2\pi t}}e^{-\frac{x^2}{2t}}$$

We get

$$P(x,t) \approx \frac{2}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}}$$

Recall that in this formula x is even if t is even (and x is odd if t is odd).
Let us generalize this formula for an arbitrary x and t.



The width of the bin equals $\Delta = 2$.

Normalization

$$1 = \sum_{l=-m}^{m} P(x = 2l, t = 2m) = \sum_{l=-m}^{m} \frac{P(x = 2l, t = 2m)}{\Delta} \Delta$$

The probability density is

$$P(x,t) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}}$$

Let us check the normalization:

$$\int_{-\infty}^{\infty} P(x,t)dx = \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2t}} dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{y^2}{2}} dy = 1$$

where $y = x/\sqrt{t}$.

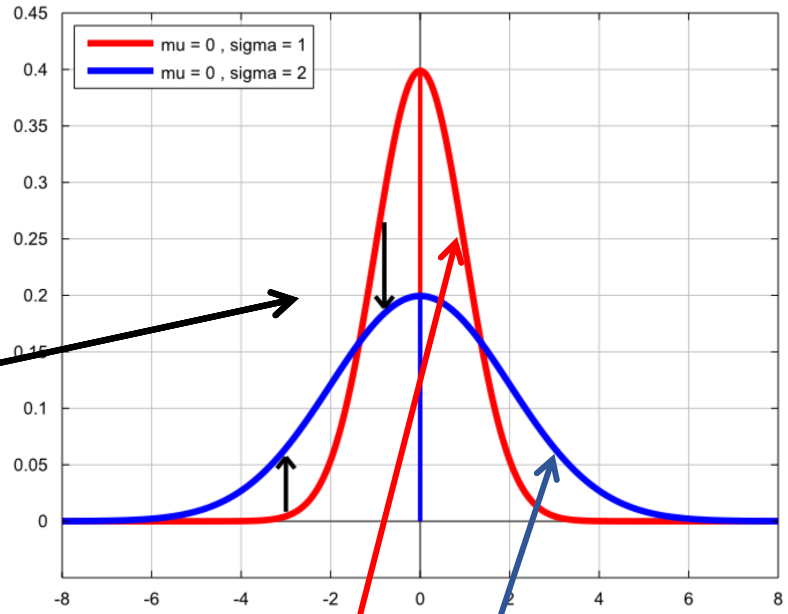
Probability to (density) observe particle at initial point $x = 0$ is $P(0,t) = \frac{1}{\sqrt{2\pi t}}$.

This probability decreases with increasing time t.

The mean value $\langle x \rangle = \int_{-\infty}^{\infty} xP(x,t)dx = 0$

The variance is

$$\sigma^2 = \int_{-\infty}^{\infty} x^2 P(x,t)dx = \int_{-\infty}^{\infty} e^{-\frac{x^2}{2t}} \frac{x^2 dx}{\sqrt{2\pi t}} = t$$



$t_1 < t_2$

If at $t = 0$ we have N particles at $x = 0$, then $NP(x,t)$ is the density of particles at time t.