Diffusion and Random Walks

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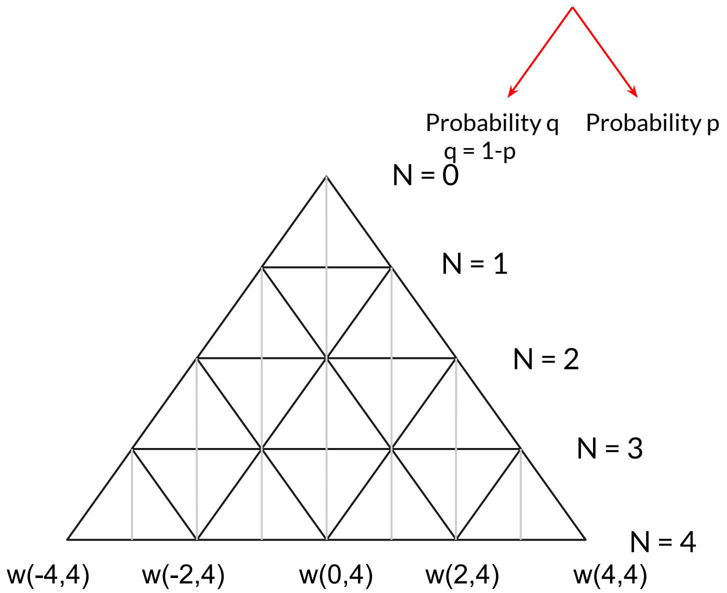
1-D Random Walk

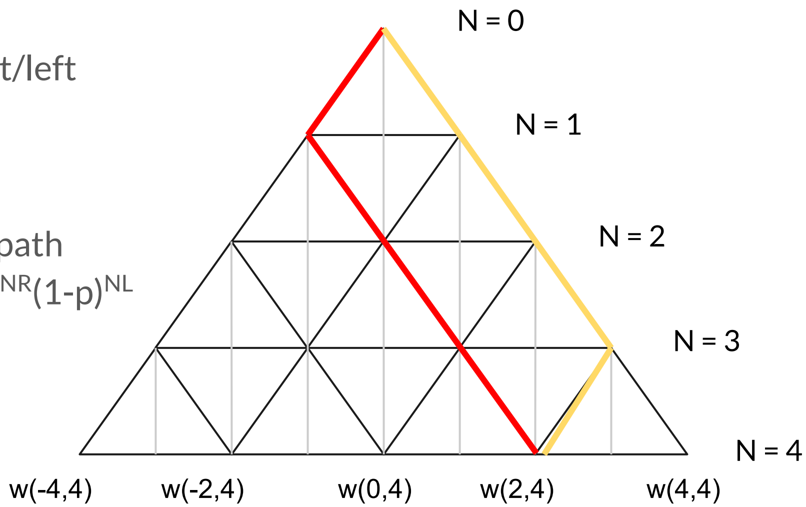
Generally characterized by: time step Δx, spacial step Δt, probability of going left or right

- Let p be chance of going right, q = 1- p be the chance of going left
- Let m = x/Δx be cumulative number of spacial steps
- Let N = t/Δt be variable for time steps passed
- Let w(m,N) be the probability of being at position m at time N



Finding the probability w(m,N) for a 1-D walk

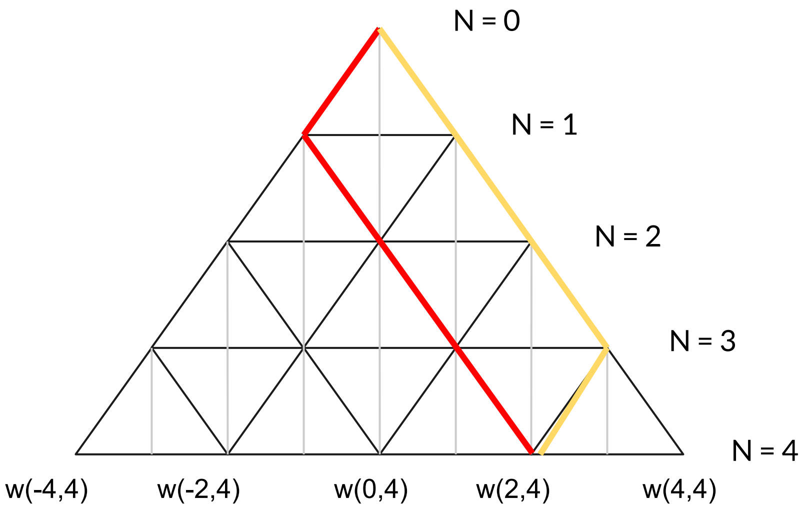
- For some N, only certain m are possible
  - I.e. at N = 2, m is either -2, 0, or 2
- For some m and N, there is only 1 combination of right/left paths that lead to that point:
  - $m = N_R - N_L$ and $N = N_R + N_L$
  - $N_R = (N+m)/2$ and $N_L = (N-m)/2$
- Since we know the probability of each step, for some path there is a probability that exactly that path is taken: $p^{NR}(1-p)^{NL}$



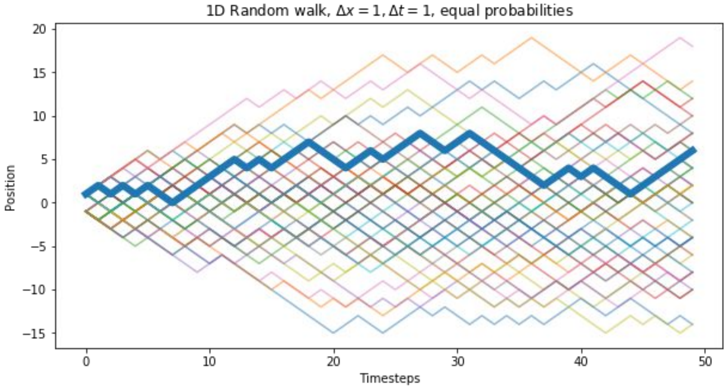
Finding the probability w(m,N) for a 1-D walk

- To get total probability for all paths leading to some m, N, multiply by the number of possible paths:

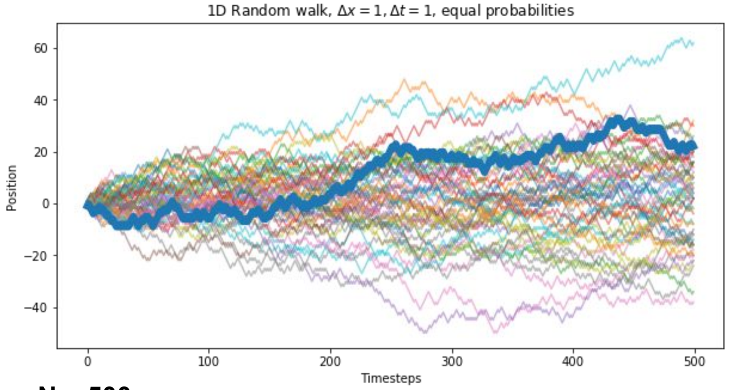
$$w(m,N) = p^{NR}(1-p)^{NL} * (N!/N_R!N_L!)$$



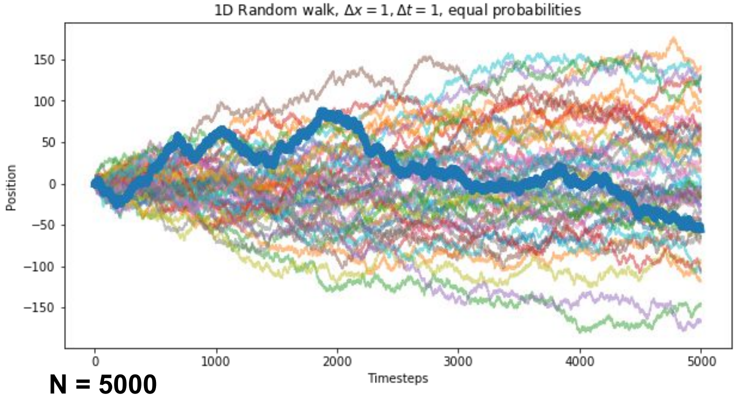
Simulating a random walk



N = 50
max m ~ 15



N = 500
max m ~ 40

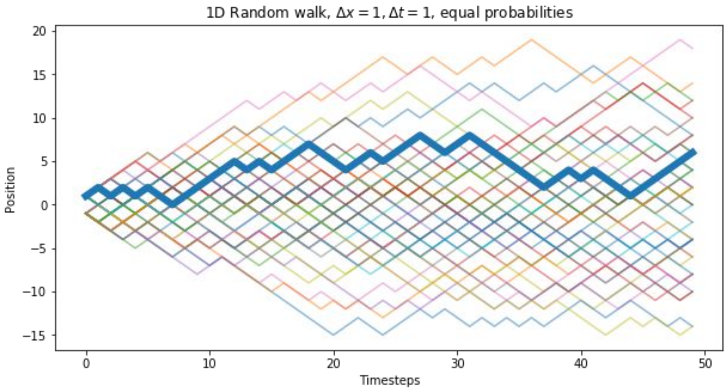


N = 5000
max m ~ 150

Plotted with p = 0.5

Note that the fluctuations have the same "structure" at any N - relative size of the variations in the path

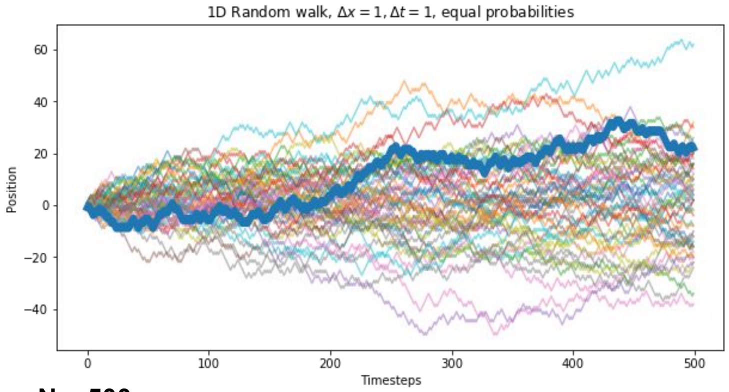
Simulating a random walk



N = 50
max m ~ 15

Note that the spread of the random walks increases as roughly the square root of N

This is a consequence of the Central Limit Theorem → σ proportional to √N



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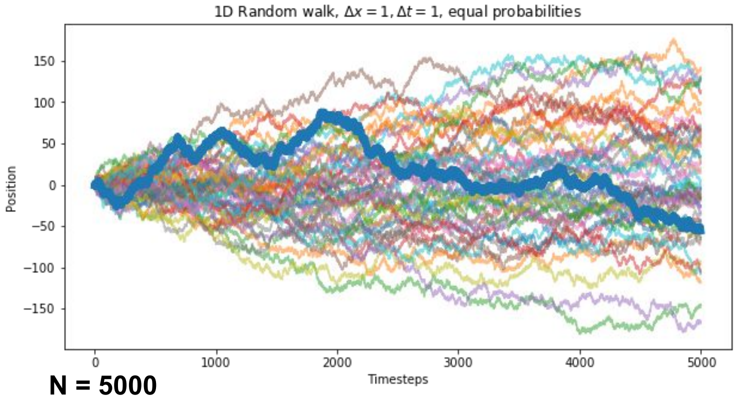

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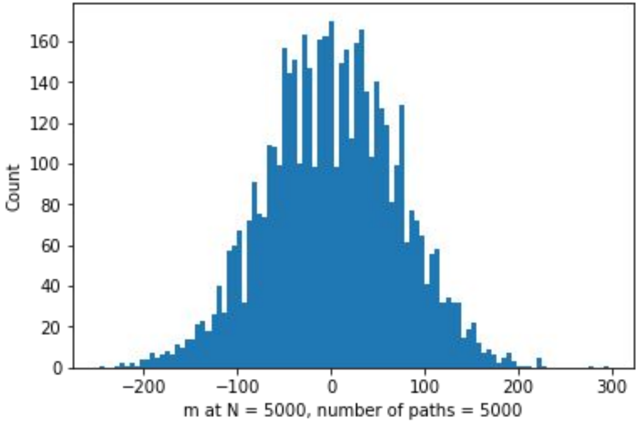
Simulating a random walk

Gaussian distribution of end points
(5000 trials, N = 5000 timesteps)



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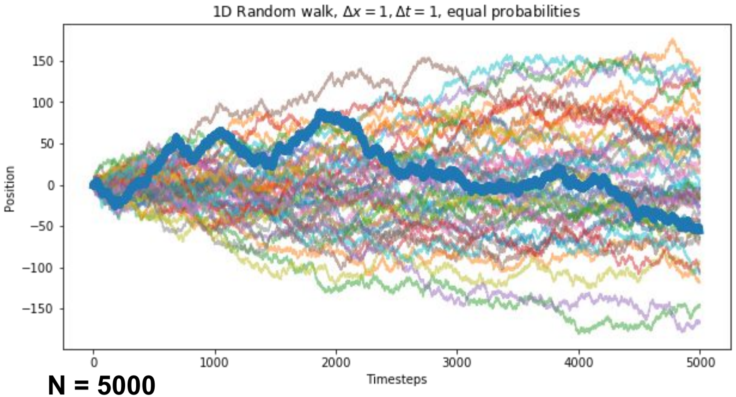


N = 5000
max m ~ 150

Taking the continuous limit for a 1-D walk

- Use a non-drifting walk, i.e. $p = ½$
- Probability of arriving at some (m, N) is ½ the probability of arriving at (m-1,N-1) + ½ the probability of arriving at (m+1,N-1), at the previous timestep
  - i.e. **$w(m,N) = ½\, w(m-1,N-1) + ½\, w(m+1,N-1)$**

- Switching from m,N to x,t : $m = x/\Delta x$ and $N = t/\Delta t$. Let u = continuous probability function.
  - **$2u(x,t) = u(x-\Delta x, t-\Delta t) + u(x+\Delta x, t-\Delta t)$**

Taking the continuous limit for a 1-D walk

- Take the Taylor expansion around x and t with the variables Δx and Δt.
  - $2u = u - \Delta t^* u_t - \Delta x^* u_x + ½ (\Delta x^2 u_{xx} + 2\Delta x \Delta t\, u_{xt} + \Delta t^2 u_{tt}) + ...$
    $+ u - \Delta t^* u_t + \Delta x^* u_x + ½ (\Delta x^2 u_{xx} - 2\Delta x \Delta t\, u_{xt} + \Delta t^2 u_{tt}) + ...$
  - $0 = 2\,\Delta t^* u_t + \Delta x^2 u_{xx} + \Delta t^2 u_{tt} + ...$

$$\frac{\partial u}{\partial t} = \frac{(\Delta x)^2}{2\Delta t}\frac{\partial^2 u}{\partial t^2}$$

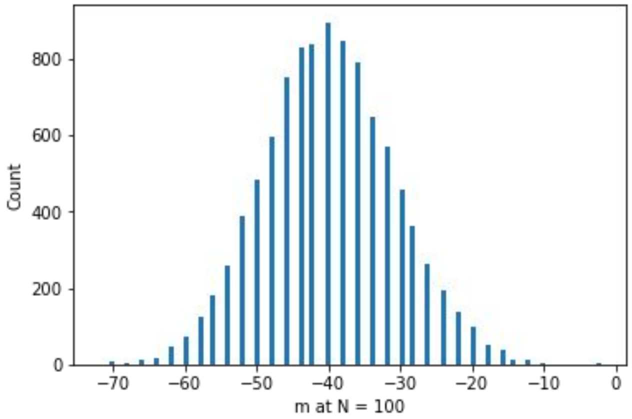
D

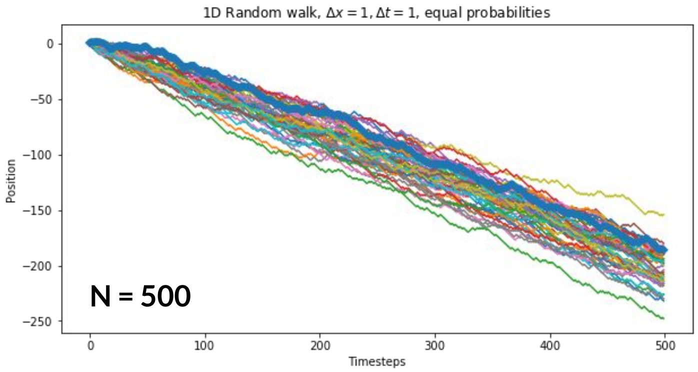
- At small Δt and Δx, we get the following:
  - **$u_t = (\Delta x^2/2\Delta t)\, u_{xx}$**, also stated →
  - Constant is the diffusion coefficient D
  - Higher D → faster diffusion due to larger typical spacial step in a random walk
  - Only linearly varying distributions are stable
- In 1-D, solutions look like linear connections between any boundary conditions

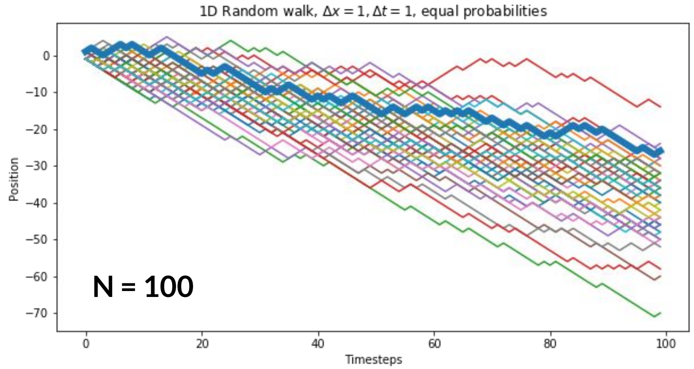
The diffusion equation describes changes in distributions where motion is governed by random walks

Other walks - drifting 1-D walk

- Unequal p and q
- Final positions still obey Gaussian distribution:





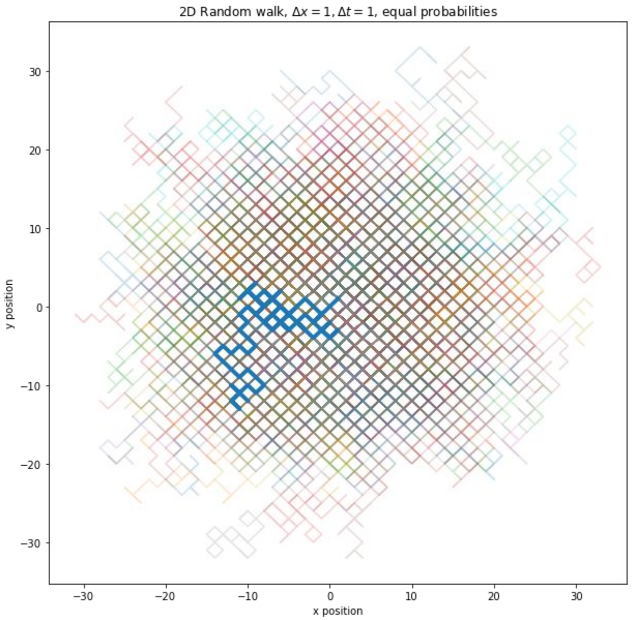


p = 0.3, and q = 0.7

Other walks - higher dimensions (2D)

- Different probabilities for (up, left), (up, right), (down, left), (down, right)
- For equal probabilities, is essentially two random walks in different directions superimposed
- Can make it drift diagonally, or create some correlation between different choices for up/down and right/left
- Creates the diffusion equation as follows:
- Rate of change depends on curvature - configurations that solve Laplace's equation are stable

$$\frac{\partial \phi(\mathbf{r},t)}{\partial t} = D\nabla^2\phi(\mathbf{r},t),$$



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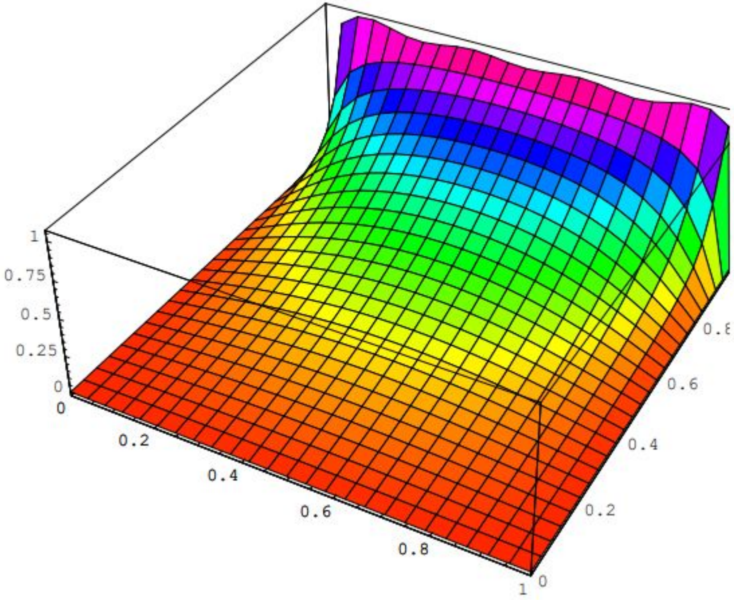
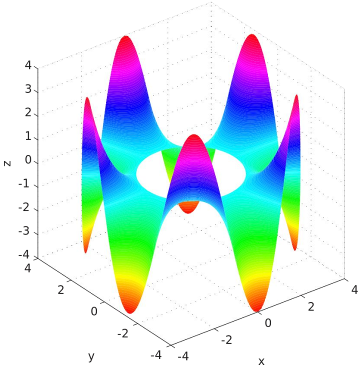
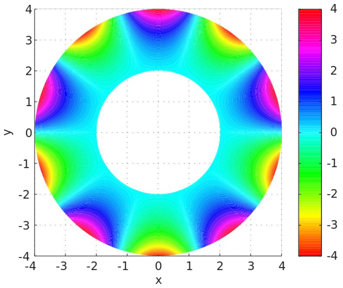


Solutions for various boundary conditions can be solved with Laplace's equation





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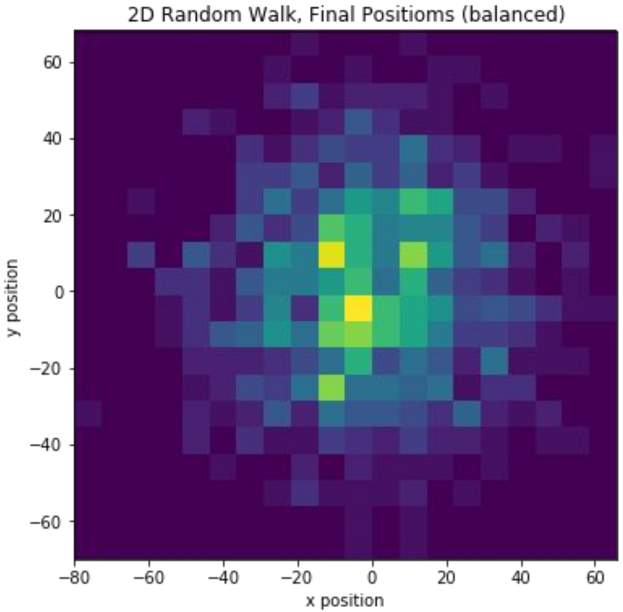

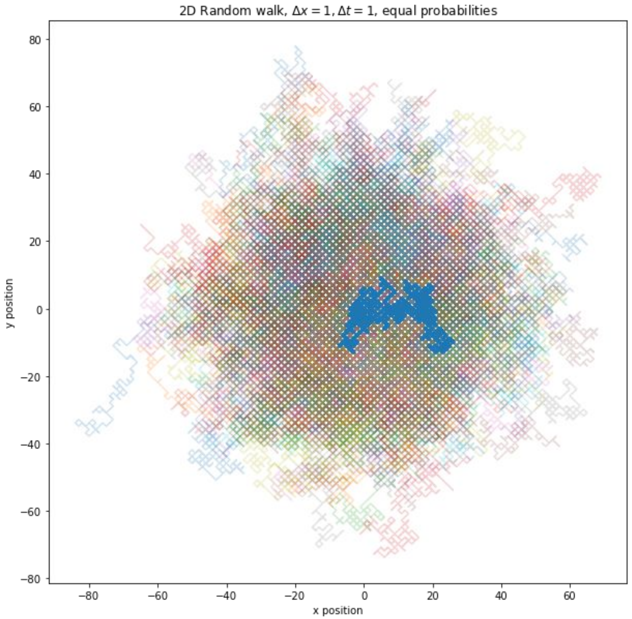

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