

In class - Diffusion by coin flips

Thursday, February 22, 2024 1:55 PM

calculate the probabilities of different outcomes

time $t=0$ $t=a$ $t=2a$ $t=3a$

probability $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{4}$ $\frac{1}{4}$ $\frac{1}{2}$ $\frac{1}{4}$ $\frac{1}{4}$ $\frac{1}{8}$ $\frac{1}{8}$ $\frac{1}{4}$ $\frac{1}{4}$ $\frac{1}{8}$ $\frac{1}{8}$ $\frac{1}{4}$

$\langle x \rangle$ $\langle x^2 \rangle$

$\frac{1}{2}(-a) + \frac{1}{2}(+a) = 0$ $\frac{1}{2}(-a)^2 + \frac{1}{2}(+a)^2 = a^2$

$\frac{1}{4}(-2a) + \frac{1}{2}(0) + \frac{1}{4}(2a) = 0$ $\frac{1}{4}(-2a)^2 + \frac{1}{2}(0)^2 + \frac{1}{4}(2a)^2 = \frac{1}{4} \cdot 4a^2 + \frac{1}{4} \cdot 4a^2 = 2a^2$

$\frac{1}{8}(-3a) + \frac{1}{4}(-a) + \frac{1}{4}(a) + \frac{1}{8}(3a) = 0$ $\frac{1}{8}(-3a)^2 + \frac{1}{4}(-a)^2 + \frac{1}{4}(a)^2 + \frac{1}{8}(3a)^2 = \frac{1}{8} \cdot 9a^2 + \frac{1}{4} \cdot a^2 + \frac{1}{4} \cdot a^2 + \frac{1}{8} \cdot 9a^2 = 3a^2$

$\rightarrow x$

$\sqrt{\langle x^2 \rangle}$
= RMS
root mean square

We conclude:

$\langle x^2 \rangle = N a^2 = \frac{T}{\Delta t} a^2 = \frac{a^2}{\Delta t} \cdot T$

of coin flips
= $\frac{T}{\Delta t}$ → total time
 Δt → time step

ESTIMATING THE DIFFUSION TIME BY DIMENSIONAL ANALYSIS

unknown exponents
 $t_{diff} = L^\alpha D^\beta$
 $T = L^\alpha \left(\frac{L^2}{T}\right)^\beta$

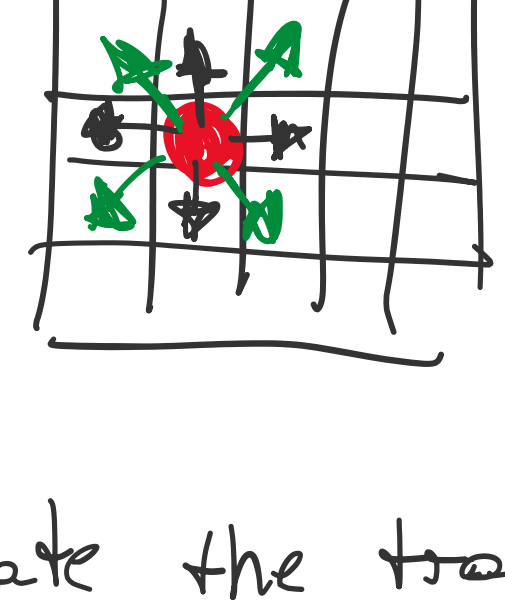
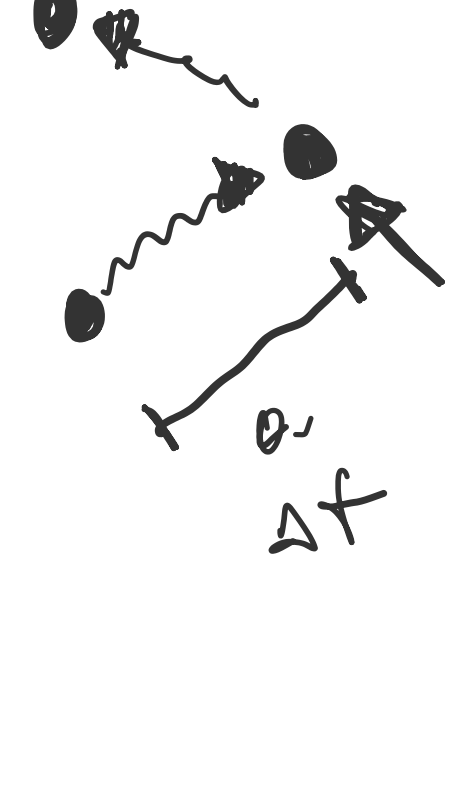
only D includes time, so $\beta = -1$
 $t_{diff} = L^\alpha D^{-1}$

to balance units $\alpha = 2$
 $t_{diff} = \frac{L^2}{D}$

$l^2 = D t_{diff}$

$\langle x^2 \rangle = D \cdot T$
 $= \frac{l^2}{\Delta t} \cdot T$

size of jump
 $D = \frac{a^2}{\Delta t}$
time between jumps



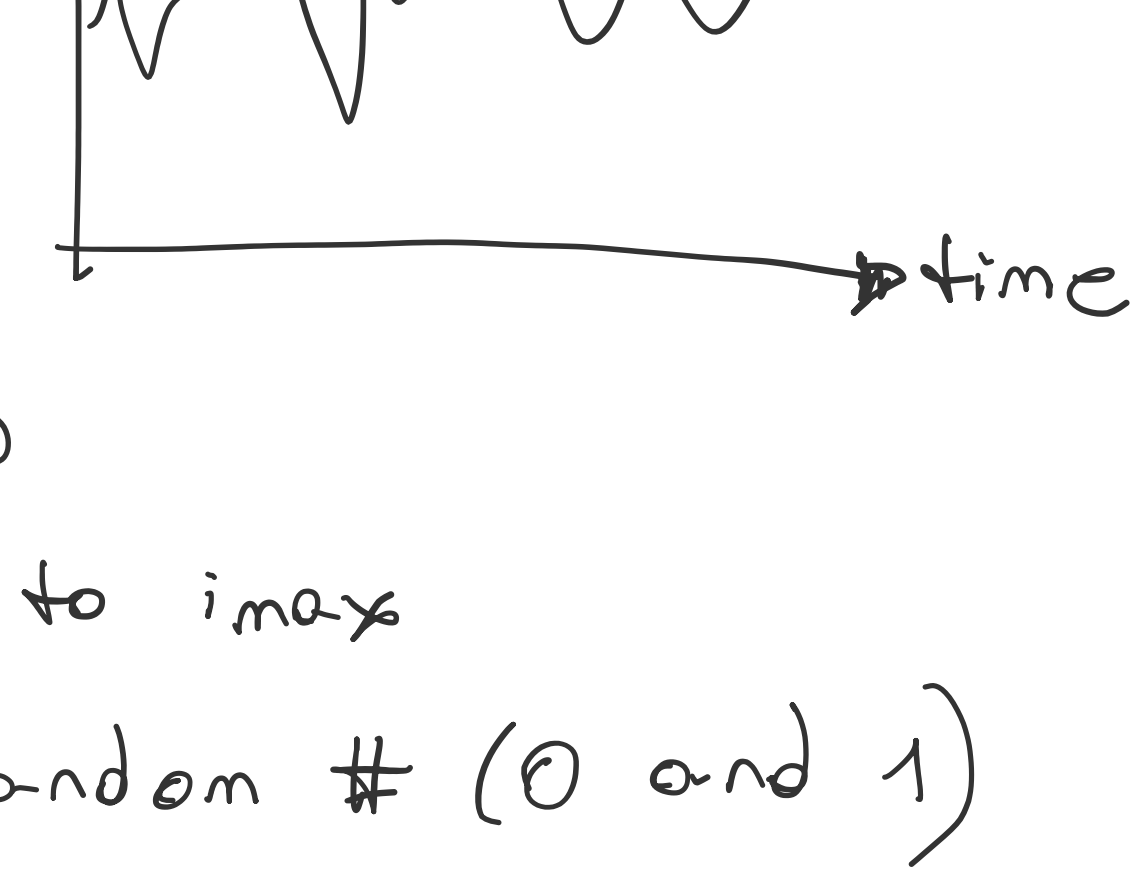
Next to simulate the trajectory of a random walker

$x = [x_0, x_1, \dots, x_{N-1}]$ = position of random walker
of coin flips

At every time step \rightarrow right: $N[i] = N[i-1] + 1$
or \rightarrow left



$D_{prot} = 10 \frac{m^2}{s} = \frac{a^2}{\Delta t}$



$N[i=0] = 0$

for $i=1$ to i_{max}

rand = random # (0 and 1)

if rand > 0.5 (move to the right)

$N[i] = N[i-1] + 1$

else (move to the left)

$N[i] = N[i-1] - 1$

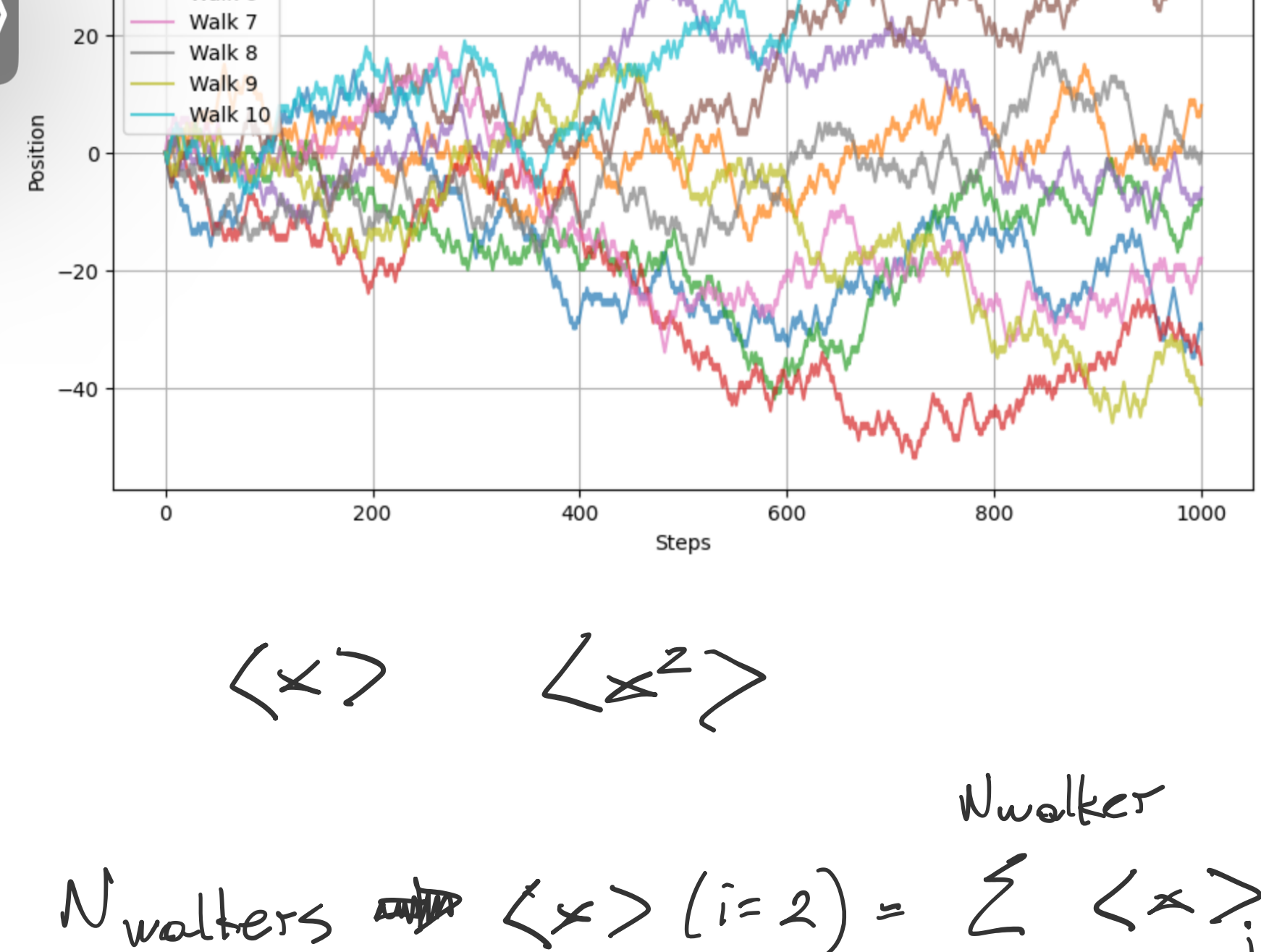
end if

end for loop

Now do the simulation for 1000 walkers

walkers

Daniel Camilo Pineda Rodriguez
02:58 PM



$\langle x \rangle$ $\langle x^2 \rangle$

$N_{walkers} \langle x \rangle (i=2) = \sum_{j=1}^{N_{walker}} \langle x \rangle_j (i=2) \cdot \frac{1}{N_{walkers}}$
walker j

$x = [x_0, x_1, \dots, x_{N-1}]$ (for 1 walker)

walker # \uparrow time point # \uparrow

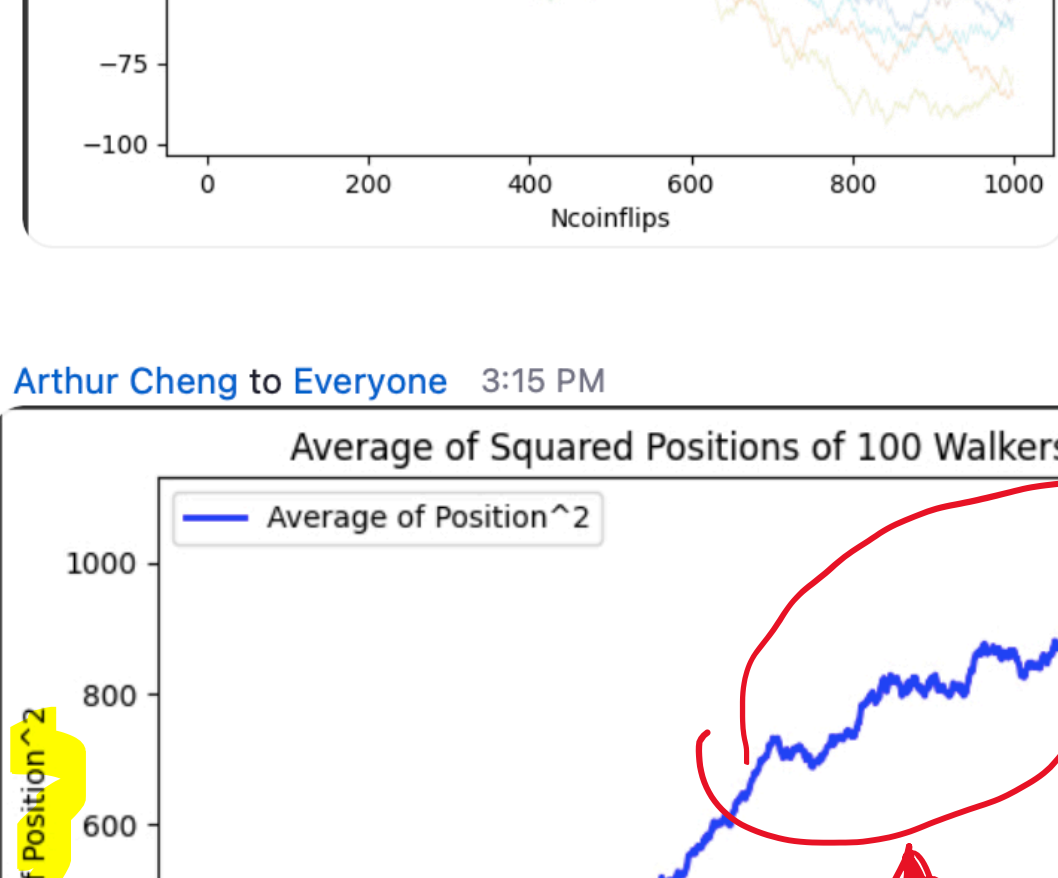
$X = \begin{bmatrix} x_{00} & x_{01} & \dots & x_{0N-1} \\ x_{10} & & & \\ \vdots & & & \\ x_{Nwalker,0} & \dots & \dots & x_{Nwalker,N-1} \end{bmatrix}$

$\langle x \rangle$ $\langle x^2 \rangle$

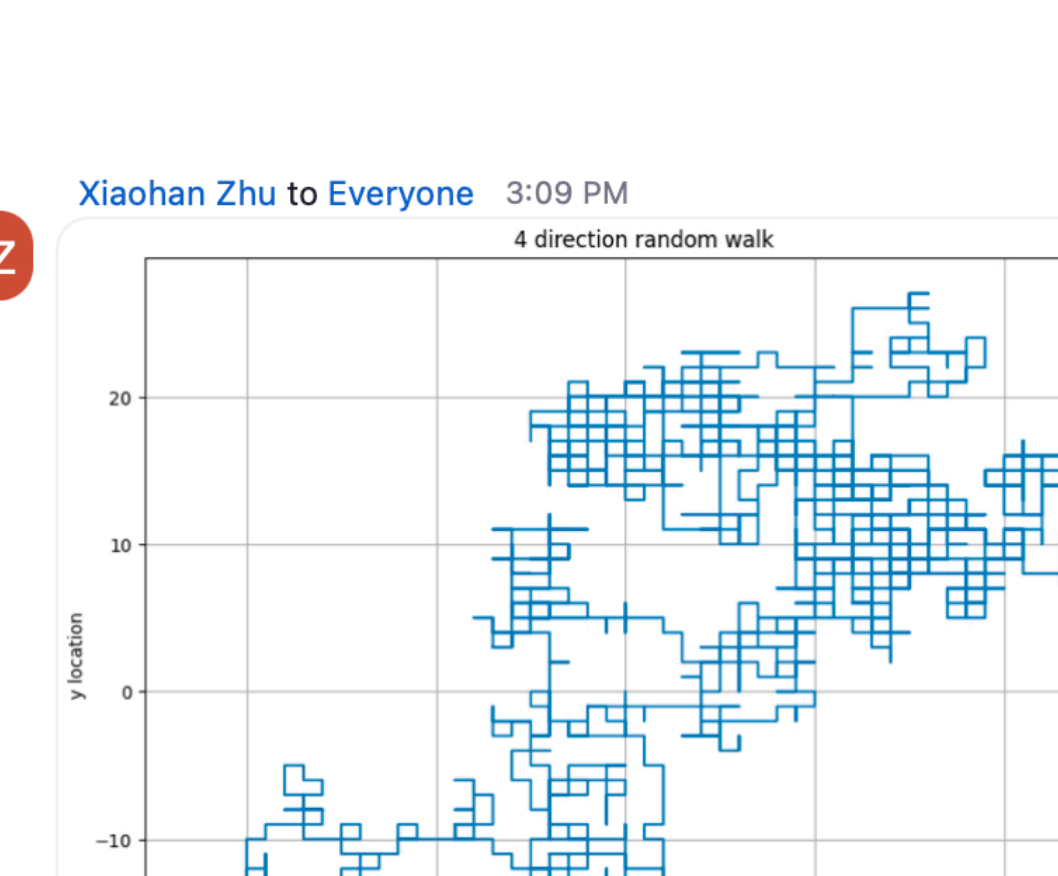
\uparrow \uparrow

i i

Average Position of 100 Walkers

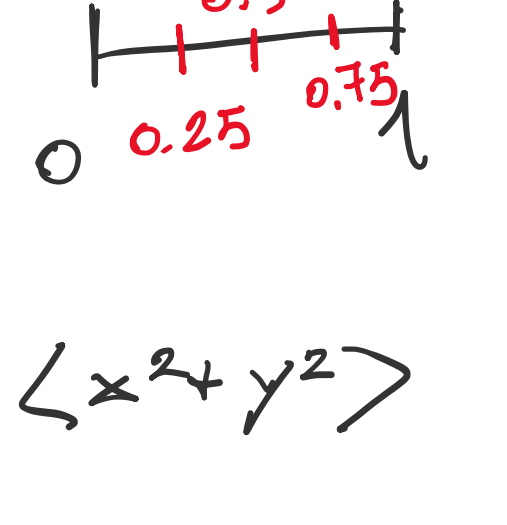


Average of Squared Positions of 100 Walkers



$\langle x^2 \rangle = a^2 N$
 $= N$

4 direction random walk



$\langle x^2 + y^2 \rangle$