

Origin Assignment 1 Answers - Simulation of a 2-D Random Walk

1. Write a brief explanation of operation of the script for the 2-d random walk.
2. Plot 'Data1' with a 'Line + Symbol' plot to display the final random walk.
3. Plot 'Data2' with a 'Scatter' plot to display the distribution of the final positions in the x-y plane.
4. Change Column A in the worksheet Data3 from an array of X-values to an array of Y-values (Click on Data 3 to select it; the navigate Column:Set as Y). Plot both Column A and B in a scatter plot. Fit them both to a Gaussian Amp function.
5. Note the value for w , which is related to the root mean square deviation. Repeat the simulation for *several* different values of the total number of steps in a walk. (You will need to modify the script to introduce different numbers of steps, *e.g.* 10, 25, 50, *etc.*). Save the data for these different simulations, and fit them to Gaussian functions as in part 4. Calculate the root mean square deviation, and plot the root mean square deviation as a function of the step number. What is this function? (What should it be?)
6. **Extra Cr.** Reformulate the script to generate a random walk, where each step length is the same, but the direction of each successive step can be in *any* direction in the x-y plane, independent of the previous step. (Hint: Use the random number generator with trigonometric functions, *e.g.* sine and/or cosine. Plot out representative data akin to parts 1, 2 and 3 above. Include a printout of the script.

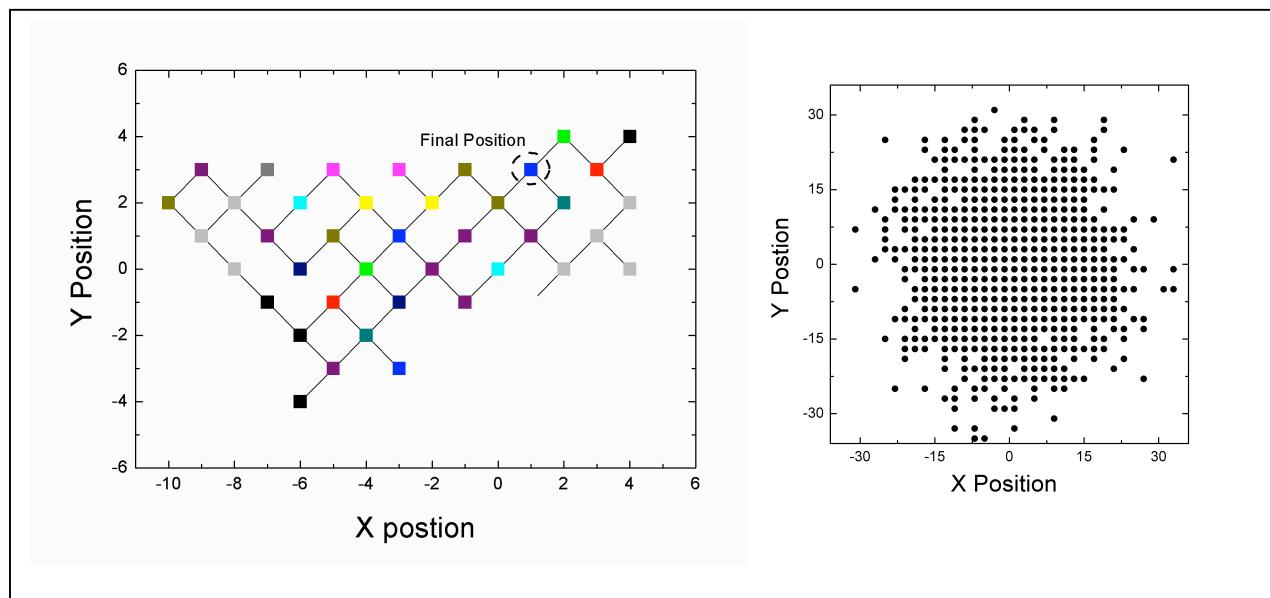
Answers

1. The annotated script describes how the random walk algorithm works:

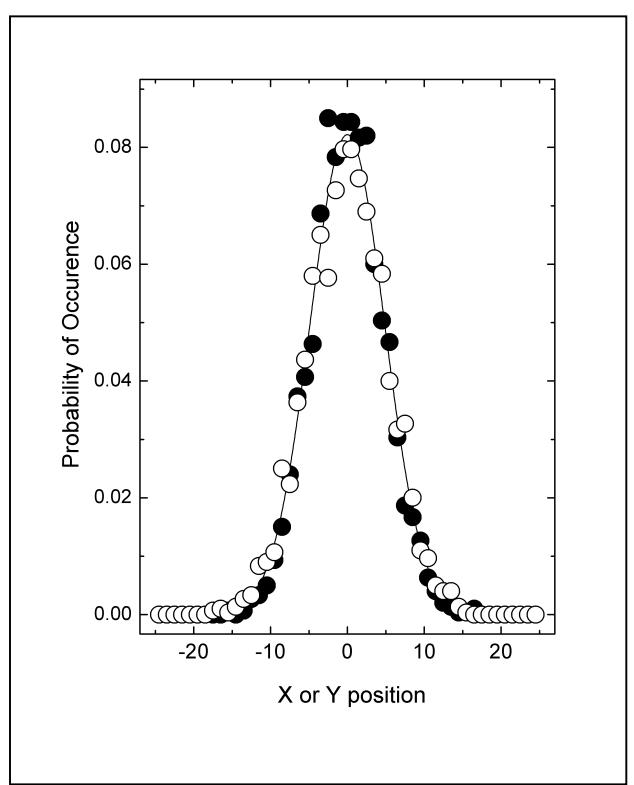
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for (jj = 1; jj <=3000; jj++)
    //This for loop specifies 3000 random walks
{
    data1_a[1] = 0;
    data1_b[1] = 0;
    for (ii = 2; ii <= 100; ii++)
        //Nested for loop starts random walk
    {
        xsteptemp = rnd(0) - 0.5;
        if (xsteptemp > 0) xstep=1; else xstep=-1;
        data1_a[ii] = data1_a[ii-1] + xstep;
        ysteptemp = rnd(0) - 0.5;
        if (ysteptemp > 0) ystep=1; else ystep=-1;
        data1_b[ii] = data1_b[ii-1] + ystep;
    };
    data2_a[jj]=data1_a[100];
    data2_b[jj]=data1_b[100];
};
Data3_a = histogram(Data2_a,2,-50,50);
Data3_b = histogram(Data2_b,2,-50,50);
    //records final x & y positions of jjth walker
    //resorts the final x and the final y positions
    //according to the distance from the origin
  
```

2 & 3. Plots of the 3000th random walker (Q2) and the x-y distribution of the 3,000 walkers (Q3) are shown below



4. Change column A in the worksheet Data3 from an array of X-values to an array of Y-values (Click on Data 3 to select it; the navigate Column:Set as Y). Plot both Column A and B in a scatter plot. Fit them both to a Gaussian Amp function.



Data: Data3_A,Data3_B
Model: GaussAmp

$$y = y_0 + Ae^{-(x-x_c)/2w^2}$$

$$y_0 = 0.00 \text{ (fixed)}$$

$$x_c = -0.01 \pm 0.06$$

$$w = 4.85 \pm 0.06$$

$$A = 0.0822 \pm 0.0009$$

The width of the Gaussian distribution (w) is proportional to the root mean square deviation of a particle after a certain period of time, or equivalently after a certain number of steps. In fact, $w^2 = 2Dt$, and thus $w = (2Dt)^{1/2}$. In this case the root mean square deviation (4.85) does not have physically meaningful units, because the steps (' t ') are simulation cycles. The diffusion coefficient also has no meaningful units.

5. Simulations that differ in the numbers of steps (lengths of times) are expected to yield root mean square deviations (Gaussian widths) that grow in proportion to the number of steps. The data in the table and graph support this idea. Net movement away from the origin ($x_c \sim 0$) is not significant in all the simulations, thus the ensemble averages of the random walkers' position remains unchanged. On the other hand, the population spreads about the origin as the number of steps increases. This is reflected in the decrease in the probability of finding the walker at the origin (A) as the number of steps increases, and an increase in the width of the distribution (w). This root mean square deviation increases as the square root of the number of steps taken, as the fit of the data to the function $y = ax^{1/2}$ demonstrates.

Number of Steps	x_c	A	w
5	0.507 ± 0.008	0.374 ± 0.002	1.09 ± 0.01
10	0.008 ± 0.009	0.262 ± 0.001	1.53 ± 0.01
25	0.51 ± 0.02	0.161 ± 0.001	2.49 ± 0.02
50	0.04 ± 0.04	0.114 ± 0.001	3.54 ± 0.04
100	-0.01 ± 0.06	0.082 ± 0.001	4.85 ± 0.06
150	-0.05 ± 0.07	0.0677 ± 0.0007	5.89 ± 0.07
200	0.04 ± 0.10	0.0582 ± 0.0007	6.83 ± 0.10
300	0.1 ± 0.10	0.0500 ± 0.0006	7.98 ± 0.12

