

University of Hull

600093 - Computational Science

Cellular Automata

Nathan Rignall

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1 | Introduction

This report shall show the steps taken to simulate the growth of cancer cells in a tissue using the Gompertz Equation to model growth.

Growth for individual cells can be modelled using a differential equation so that the number of cells is a function of time. The Gompertz Model of Cell Growth works well in this application because it can accurately model the non exponential nature of cell growth (Tatro n.d.). Once an area has reached it's capacity no more tumour cells can form, hence the cells must begin to move through a tissue. This movement can be simulated using simple random walk algorithm or more complex genetic algorithms.

This paper specifically shall analyse the computational complexity of such models and evaluate the differences between simulation techniques. The underlying implementation shall be investigated, including random algorithms and accuracy of simulations on computer systems.

2 | Methodology

2.1 Cell Movement

The random movement of cells should be modelled using a probability distribution

There are several probability distributions that can be classified as discrete or continuous, we will analyse uniform, bernoulli and beta.

The uniform distribution is usually regarded as a continuous distribution but can also be used to model discrete variables.

Area under the graph is one

$$f(x) = \begin{cases} a & \text{if } x = 1 \\ b & \text{if } x = 0 \end{cases}$$

$$f(x) = \begin{cases} 1 & \text{for } 0 \leq x \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

Uniform distribution Definition of distributions Uniform distributions Bernoulli Distribution

Bias introduced with different distributions

When all directions are equally probable a uniform distribution could be used.

If a Bernoulli distribution was selected, it would introduce a bias to the direction of movement This could be desired in a complex model where factors such as surface tension affect the direction of movement

Both directions have bias

Square goes to right, diagonal goes down

This is because it is a single step run, the number generation is random, hence direction is random

100 steps, diagonal moves further than square

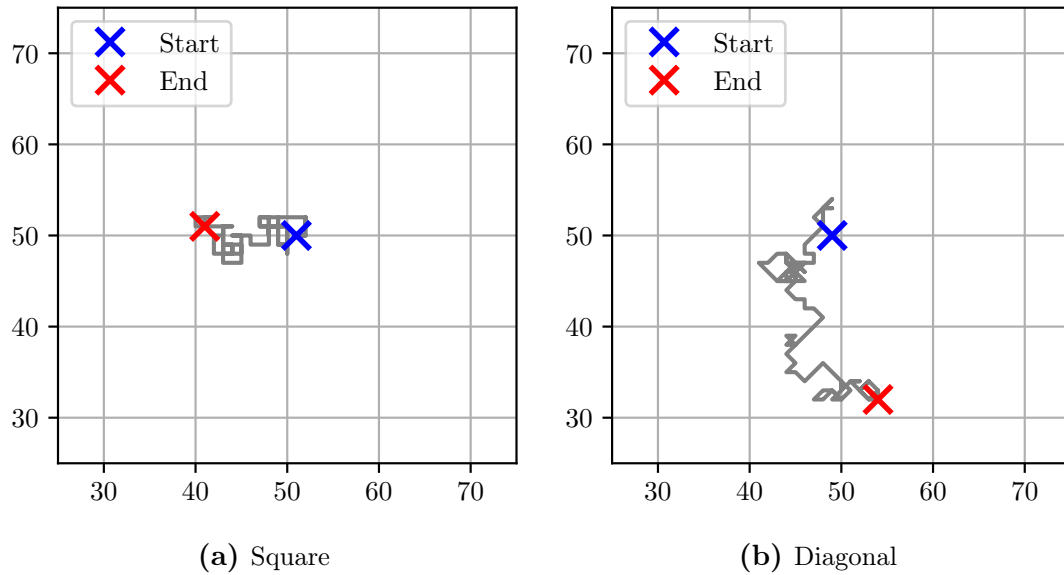


Figure 2.1: Cell movement plots

2 Methodology

By mapping the visited cells, we can see the difference in the movement of the cells across thousands of steps to validate the evenness of the uniform distribution.

Select random start and end points using a uniform distribution, iterate until end point is reached

Small hotspots, but overall even distribution

With more iterations, the distribution will be more even

Validates the uniform distribution of both the square and diagonal movements

And validates the uniform distribution of the random start and end points

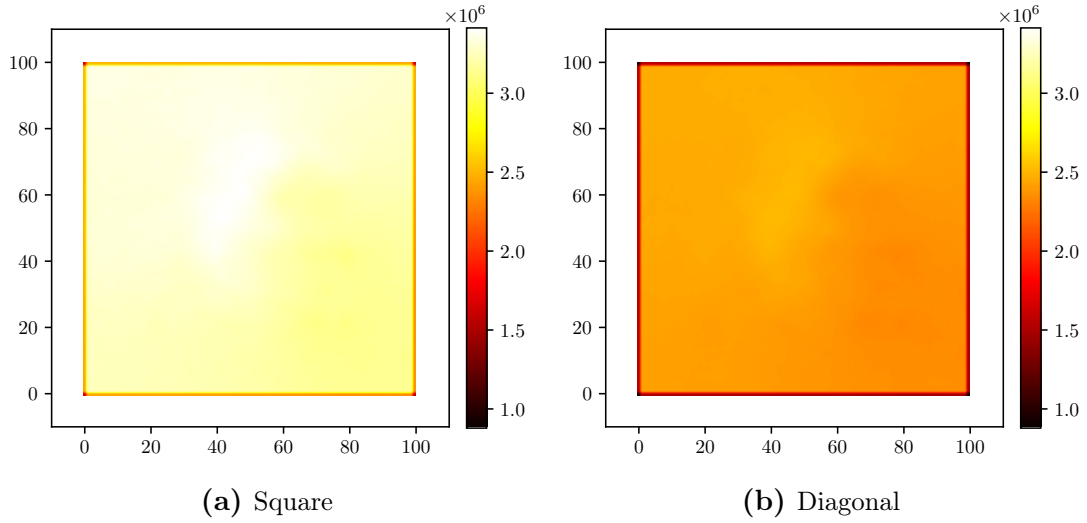


Figure 2.2: Visited cells simulation heatmap

There is a significant difference in the number of visited cells between the square and diagonal movements.

This is because the diagonal movement can move further in a single step than the square movement.

The square can perform one step to the left, right, up or down.

The diagonal can perform one step to the left, right, up, down, up-left, up-right, down-left or down-right. Any diagonal movement is equivalent to two square movements.

Hence square movement is on average $(1 \times 4)/4 = 1$ steps

The diagonal movement is on average $(\sqrt{2} \times 4 + 1 \times 4)/8 = 1.2071$ steps

Square is factor of $1/1.2071 = 0.8284$ compared to diagonal

Hence in the scene of moving from one point to another, the diagonal movement is more efficient than the square movement.

However, this is different from computational complexity, where the square movement is more efficient than the diagonal movement.

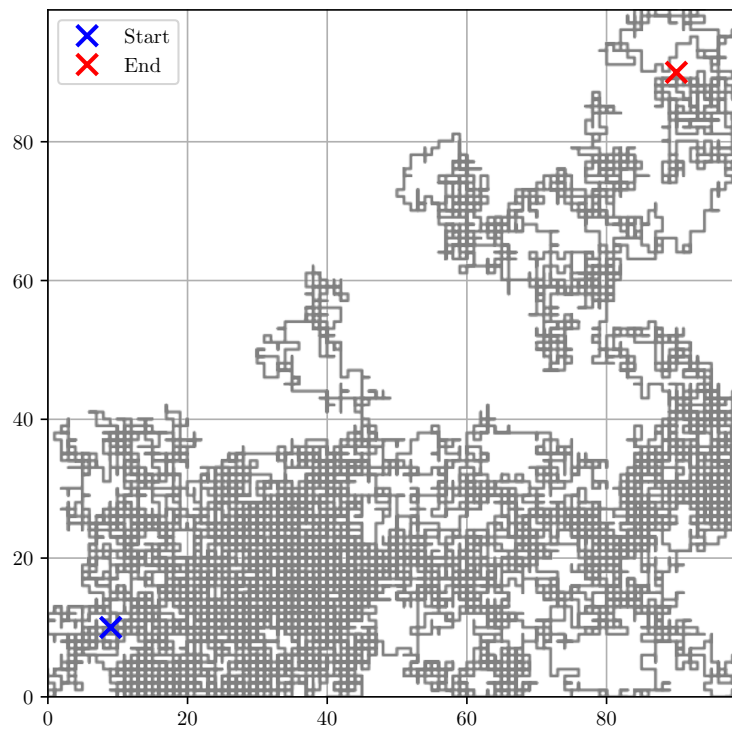


Figure 2.3: Square cell movement plot with fill

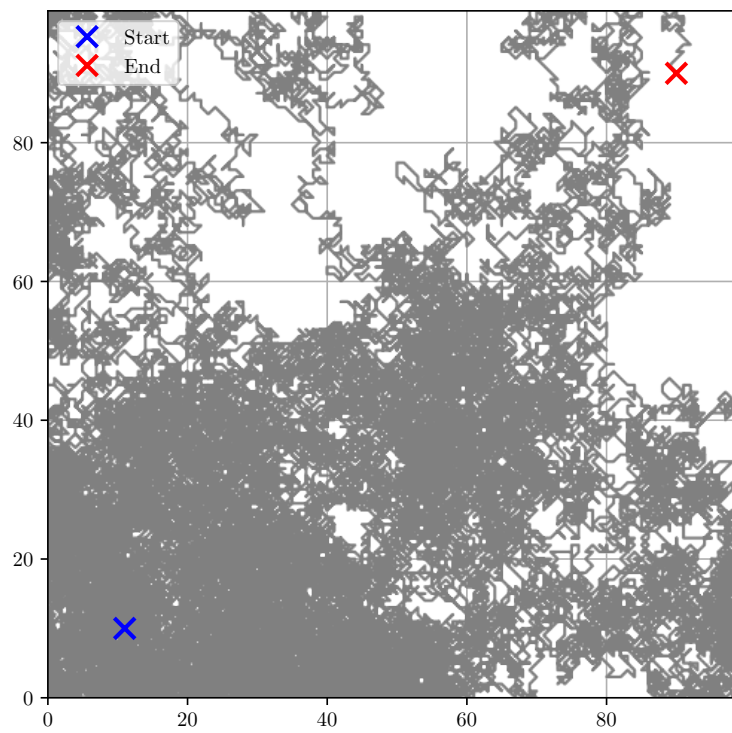


Figure 2.4: Diagonal cell movement plot with fill

2 Methodology

Measure the computational complexity of the different movements.

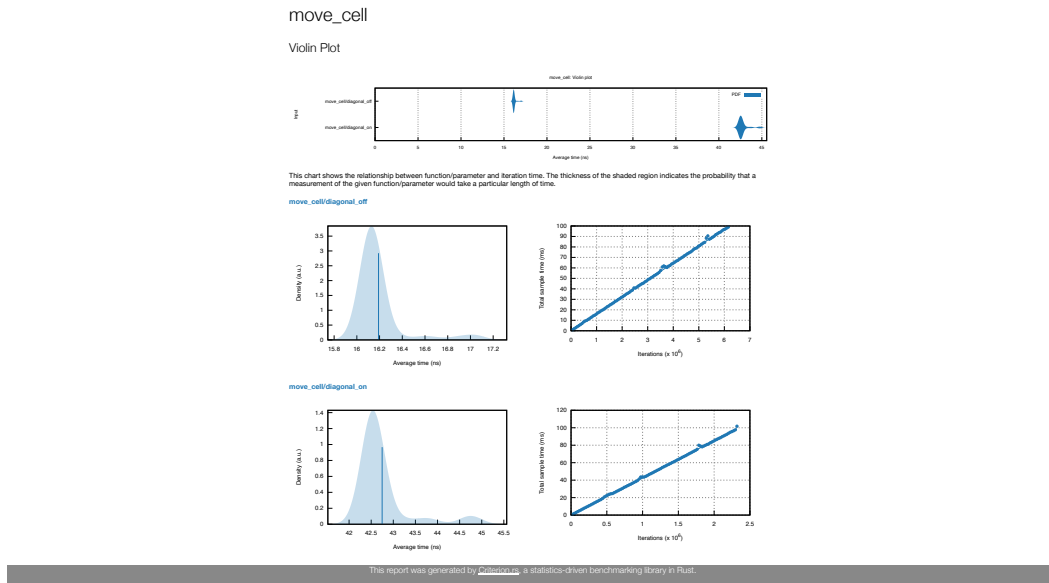


Figure 2.5: Cell movement criterion

Square takes 16.2ns

Diagonal takes 42.7ns

This is a ratio of 0.3794

Diagonal movement is more computationally complex than square movement.

This is because the diagonal movement requires more checks to ensure the cell does not move off the grid.

The act of generating a random number is the same for both movements as a single random number is generated to determine the direction of movement, regardless of the movement method.

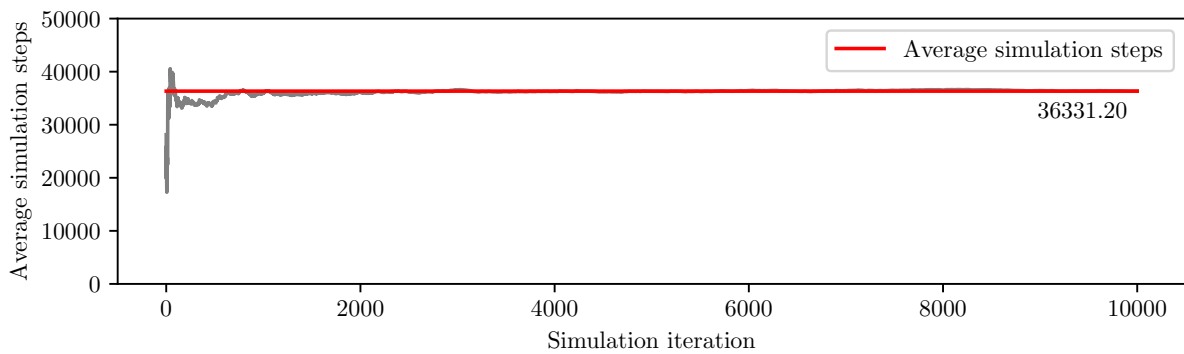
By selecting a random start and end point, we can compare the number of steps taken by the square and diagonal movements.

If this movement simulation is performed multiple times, the average number of steps taken by the square and diagonal movements can be compared.

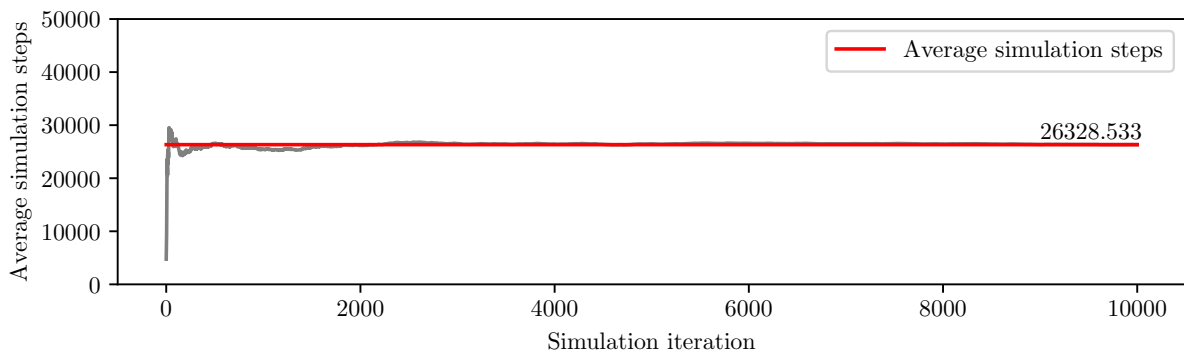
Given enough iterations, the average should stabilise and the difference in the number of steps taken by the square and diagonal movements can be calculated.

Non Diagonal - (74, 67) - (55, 40) - 32534.4086

Diagonal - (74, 67) - (55, 40) - 23247.6747



(a) Square



(b) Diagonal

Figure 2.6: Comparison of square and diagonal simulation steps

Plotting on to the same graph...

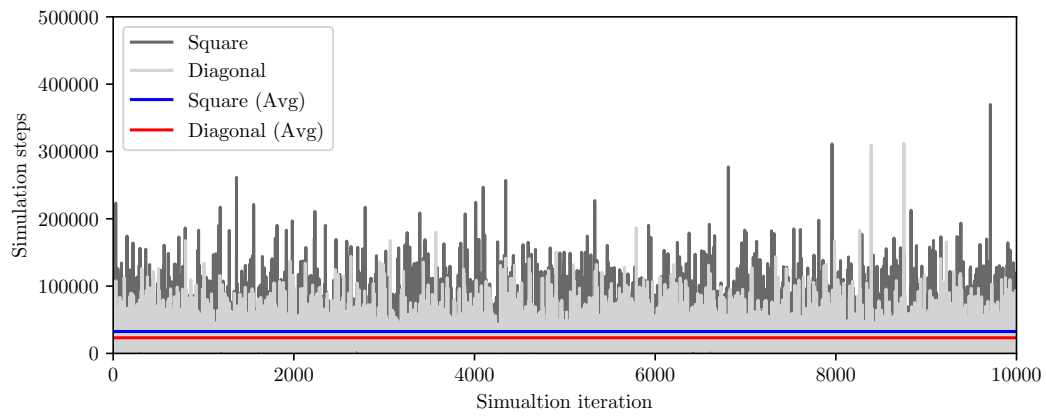


Figure 2.7: Comparison of square and diagonal simulation steps

Taking the same process and applying it to multiple different start and end points

Measure the average number of steps taken by the square and diagonal movements for a given distance between the start and end points.

Also measure the average time taken by the movements.

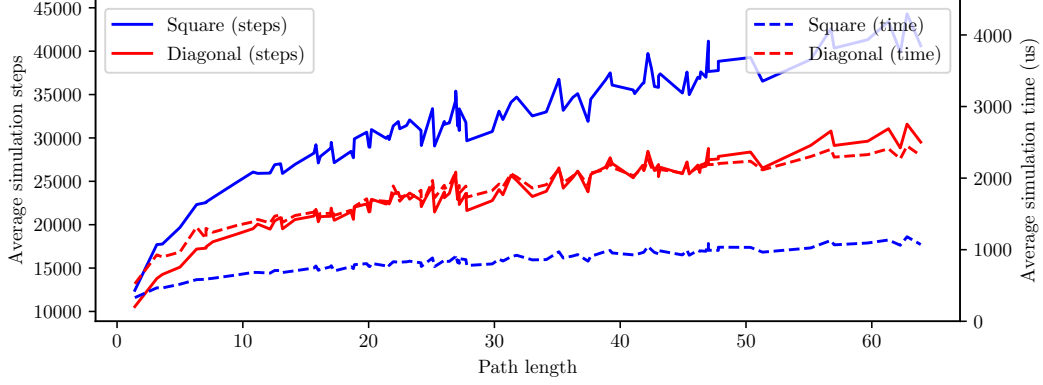


Figure 2.8: Comparison of multiple square and diagonal simulation steps

Next, by plotting the ratio of the average number of steps taken by the square and diagonal movements we can establish a factor by which the diagonal movement is more efficient than the square movement.

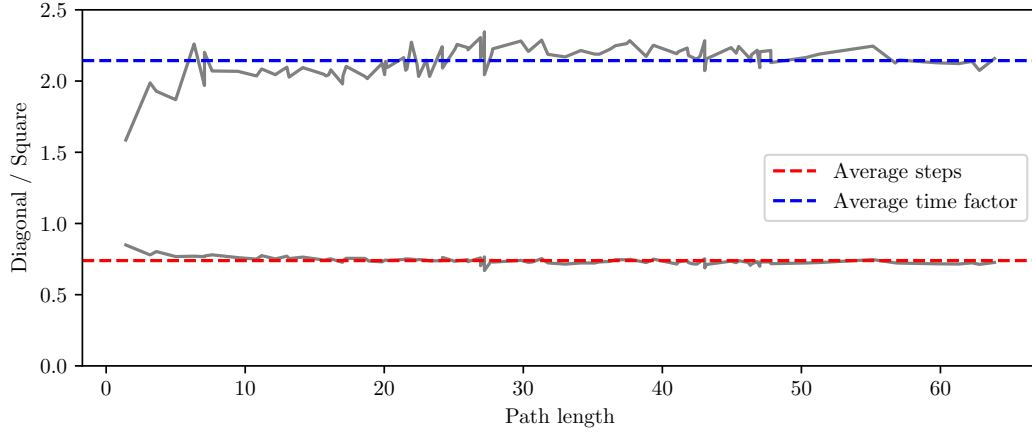


Figure 2.9: Comparison of multiple square and diagonal simulation steps (factor length)

The average factor for simulation steps is 0.7393 which is within the order of magnitude of the expected factor of 0.8284.

The discrepancy is ilkey due to additional factors such as the size of the grid and the number of iterations. Non linear behaviour from the interactions at the edge of the grid to prevent the cells from moving off the grid.

The average factor for simulation time is 2.1436

2 Methodology

Given the square movement is 0.3794 times faster than the diagonal movement, and the diagonal movement takes 0.8284 times as many steps as the square movement, the expected factor for simulation time is $0.3794 \times 0.8284 = 2.184$.

This is exceptionally close to the measured factor of 2.1436.

In conclusion, the diagonal movement is more efficient than the square movement in terms of the number of steps taken, but less efficient in terms of computational complexity. The computational complexity is significantly higher for the diagonal movement than the square movement, this overwhelms the number of steps taken. Hence, the square movement is more efficient than the diagonal movement overall.

2.2 Cell Growth

$$\frac{dN}{dt} = kN \ln\left(\frac{M}{n}\right)$$

$$N = \frac{M}{10^{4e^{-kt}}}$$

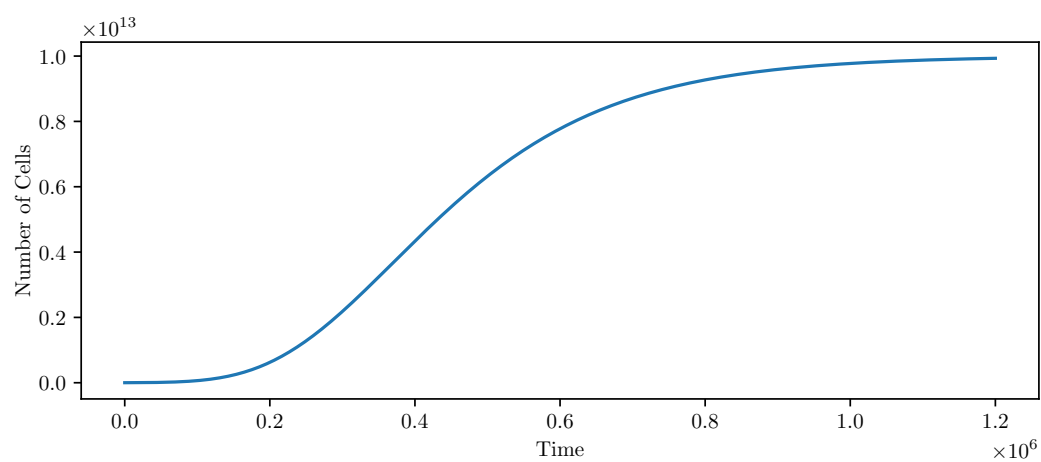


Figure 2.10: Cell growth simulation

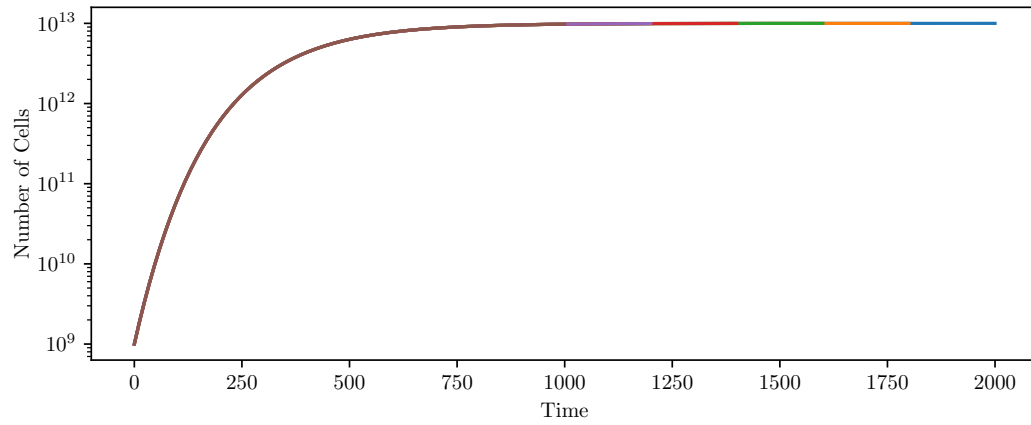


Figure 2.11: Cell growth simulation with different T values

| T | Cells | Full |
|------|----------|---------|
| 2000 | 1.00e+13 | 0.9999% |
| 1800 | 1.00e+13 | 0.9998% |
| 1600 | 9.99e+12 | 0.9994% |
| 1400 | 9.98e+12 | 0.9979% |
| 1200 | 9.93e+12 | 0.9931% |
| 1000 | 9.77e+12 | 0.9774% |

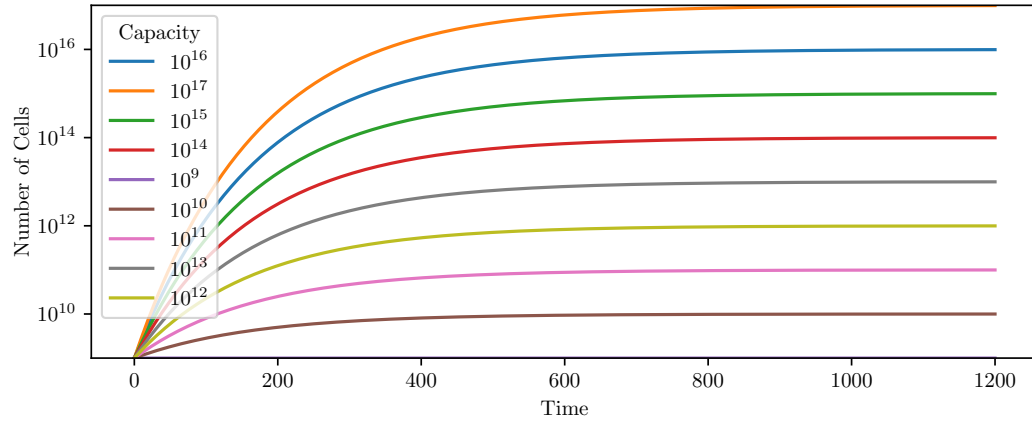


Figure 2.12: Cell growth simulation with different capacity values

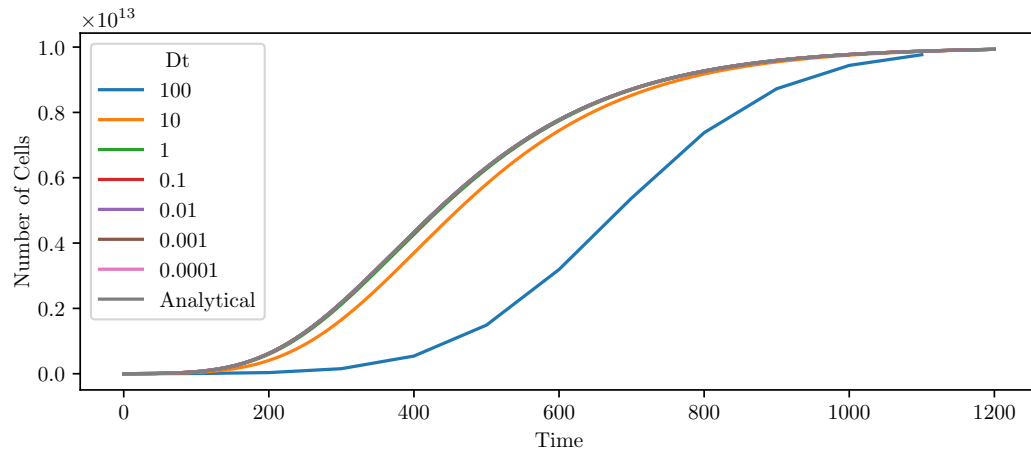


Figure 2.13: Cell growth simulation with different dt values

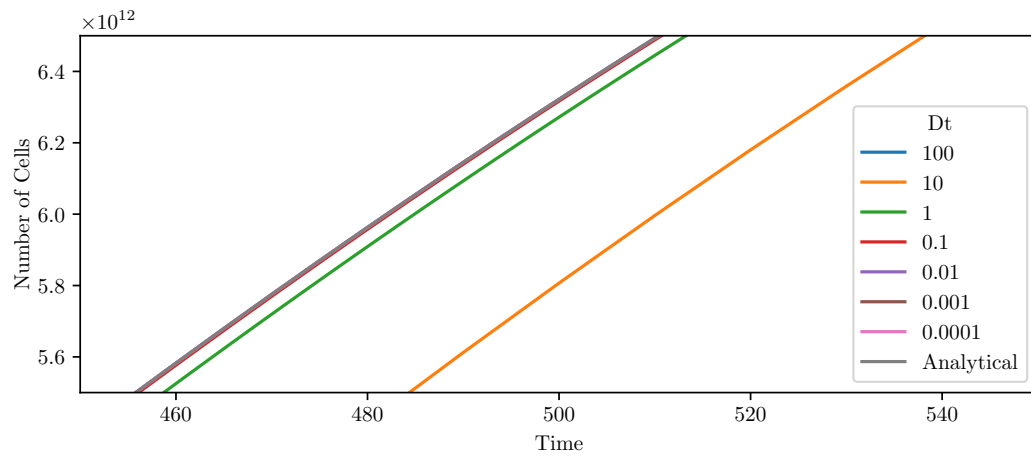
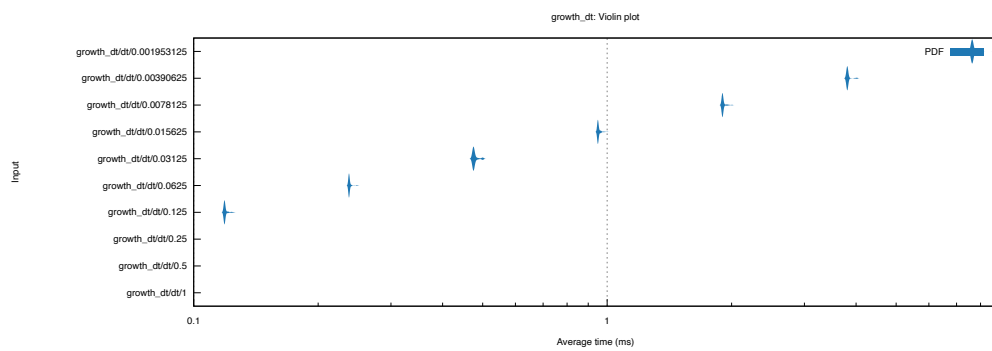


Figure 2.14: Cell growth simulation with different dt values (zoomed)

| h | Error |
|------------|------------|
| 100 | 66.69% |
| 10 | 5.296% |
| 1 | 0.5238% |
| 0.1 | 0.05233% |
| 0.01 | 0.005233% |
| 0.001 | 0.0005239% |
| 0.0001 | 5.82e-05% |
| Analytical | 0.0 |

growth_dt

Violin Plot



This chart shows the relationship between function/parameter and iteration time. The thickness of the shaded region indicates the probability that a measurement of the given function/parameter would take a particular length of time.

Line Chart

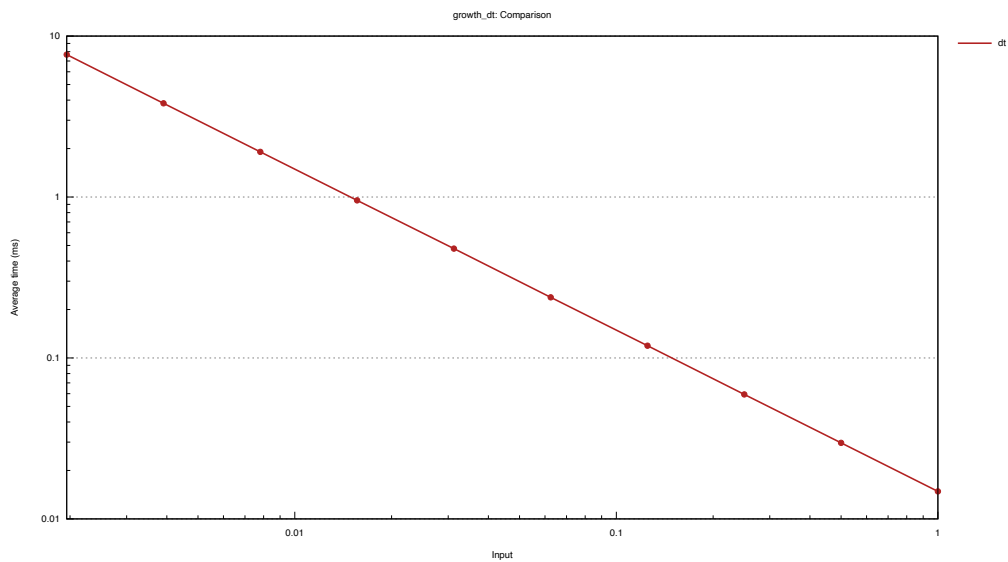


Figure 2.15: Cell growth criterion

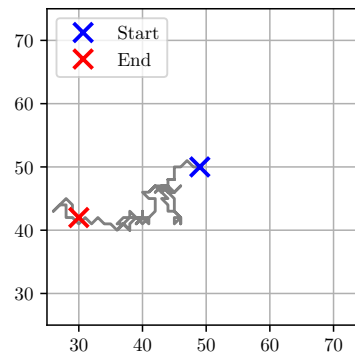


Figure 2.16: Cell growth simulation with diagonal movement

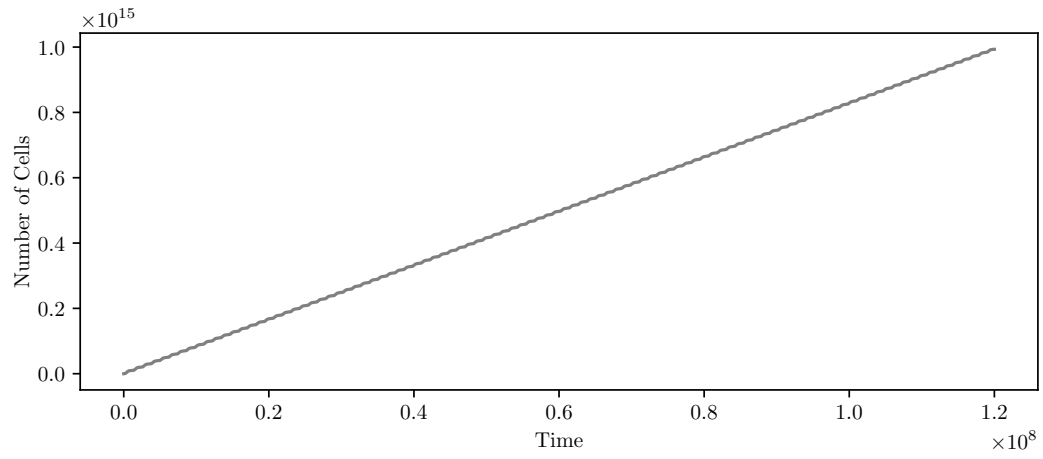


Figure 2.17: Cell growth simulation with diagonal movement (total cells)

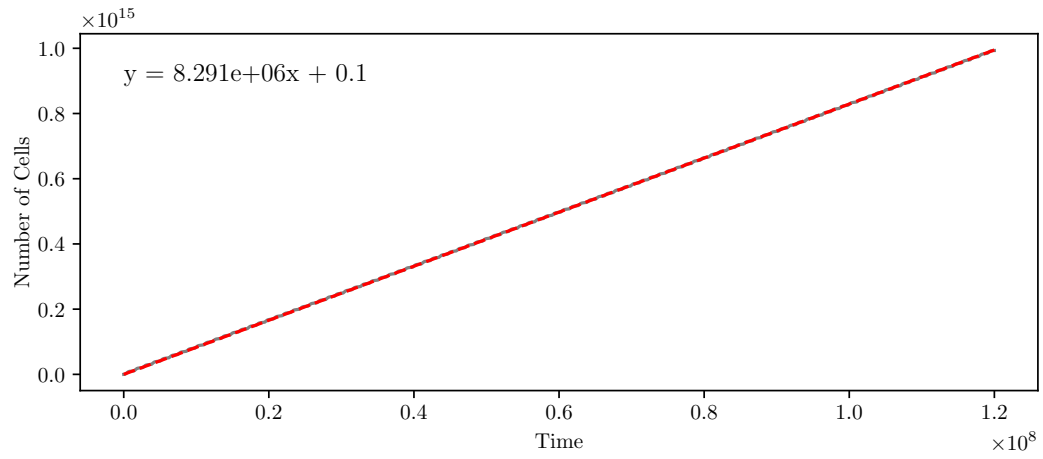


Figure 2.18: Cell growth simulation with diagonal movement (total cells) linear estimation

Appendix

Integration using substitution

$$\begin{aligned}\frac{dN}{dt} &= kN \ln\left(\frac{M}{N}\right) \\ \frac{dN}{N \ln\left(\frac{M}{N}\right)} &= k dt \\ \int \frac{dN}{N \ln\left(\frac{M}{N}\right)} &= \int k dt\end{aligned}$$

$$\text{with } u = \ln\left(\frac{M}{N}\right) \qquad \text{and} \qquad \frac{du}{dN} = -\frac{1}{N}$$

$$\begin{aligned}\int \frac{-N du}{Nu} &= \int k dt \\ \int -\frac{1}{u} du &= \int k dt \\ -\ln(|u|) &= kt + c \\ \ln(|u|) &= -kt - c \\ \ln\left(\left|\ln\left(\frac{M}{N}\right)\right|\right) &= -kt - c \\ \ln\left(\frac{M}{N}\right) &= e^{-kt-c} \\ \frac{M}{N} &= e^{e^{-kt-c}} \\ N &= \frac{M}{e^{e^{-kt-c}}}\end{aligned}$$

2 Methodology

Calculate c using the initial values

$$M = 10^{13}$$

$$k = 0.06$$

$$N = 10^9$$

$$t = 0$$

$$\begin{aligned}10^9 &= \frac{10^{13}}{e^{e^{-0.006(0)-c}}} \\e^{e^{-c}} &= \frac{10^{13}}{10^9} \\e^{e^{-c}} &= 10^4 \\-c &= \ln(|\ln(10^4)|) \\c &= -\ln(|\ln(10^4)|)\end{aligned}$$

Substitute c back in and simplify

$$\begin{aligned}N &= \frac{M}{e^{e^{-kt+\ln(|\ln(10^4)|)}}} \\&= \frac{M}{e^{e^{-kt}}e^{e^{\ln(|\ln(10^4)|)}}} \\&= \frac{M}{e^{e^{-kt}\ln(10^4)}} \\&= \frac{M}{(e^{\ln(10^4)})e^{-kt}} \\N &= \frac{M}{10^4e^{-kt}}\end{aligned}$$

3 | Conclusion

Some text

Also talk about edge processing and limited requirements

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Tatro, Dyjuan (n.d.). “The Mathematics of Cancer: Fitting the Gompertz Equation to Tumor Growth”. In: ().