

Scent of Attraction: Exploring Random Walk Algorithms as a Tool for Studying E. coli Chemotaxis

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Abstract- A report investigating the effect of periodically placed obstacles in two-dimensional random walk simulations and their relationship to E. coli chemotaxis and the complexities of life.

I. INTRODUCTION

The 1992 American drama *Scent of a Woman* explores the unexpected beauty that is fostered by life's contradictions. The film follows a blossoming friendship between an honest student, Charlie, and a waspish Vietnam veteran, Colonel Slade. Slade—played by none other than Al Pacino—is blind, yet finds direction in his life through both his interactions with Charlie and his attraction towards beautiful women. As the unlikely duo spends more time together, their random wandering leads them to a path of integrity. As Charlie puts it, “If you’re tangled up, just tango on” [1].

Although the list of similarities between award-winning actor Al Pacino in *Scent of a Woman* and microorganisms is by no means long, both Colonel Slade and E. coli lack inert directionality. As a blind vet flounders to find his purpose in life, E. coli bacteria stochastically tumble through chemical fluid. However, both subjects are guided by their ability to move towards fragrance, as observed by Slade's affinity for female perfume, and in the case of E. coli, chemical attractants [2]. Though seemingly unrelated, both Colonel Slade and E. coli are united by their movements, either through the turbulent waters of middle-aged alcoholism, or through concentration gradients.

E. coli bacteria use flagella to propel themselves through space. The flagella act as multi-directional motors controlling the movement of E. coli. The bacteria move in phases dictated by linear movement and punctuated by tumbles which alter the orientation of the unit cell [3]. Tumbles are variable in length, but effectively randomize the direction in which the E. coli travel. The flagellar motor rotates, meaning the ambient chemical surroundings act to further guide the swimming of the bacteria [4]. In areas where chemical attractant is present, the tumbling phase is stifled. When cells detect a greater amount of attractant, the bacteria run up the chemical gradient [2]. This detection-travel relationship is known as chemotaxis and is utilized by many different types of bacteria to travel through air, water, chemical solutions, and beings [5].

The process of chemotaxis provides fundamental insight into the evolution of bacterial species. Although studies have been done to analyze the tumbling phase of E. coli movement, the purpose of the tumbling mechanism is still widely questioned. In addition, the cause for variations in the tumbling phase are unknown [6]. Ultimately, however, the chemotactic behavior of E. coli allows for cell adjustment based on ambient factors.

Chemotaxis presents a contradiction: despite the primitiveness of this bacteria's capability for travel, a complex stratagem exists which enables a simple microorganism to interact with its macroscopic environment.

Random walk simulations offer an algorithmic representation of chemotaxis and E. coli movement; these simulations can be used to investigate the systematic trends which arise from unsystematic movement. The run and tumble nature of bacteria makes the random walk a strong candidate for modeling the stochastic wandering of cells towards attractant. While this mathematical theory may assign a generalized shape to the frolicking of E. coli, it is important to note that the frequency at which tumbling occurs is variable. In other words, random walks are limited in their ability to identify the distinctive phase that categorizes the cell movement [6].

The distance in which E. coli cells travel is directly proportional to the concentration of attractive solute present in chemical solution [4]. The greater the concentration of solute, the more likely it is for the microorganism to find its path. While the abundance of favorable environmental conditions may fluctuate over time, these characteristics are represented by random walking simulations with variable obstacle sizes.

In my tests, I investigated the trends of random movement through square matrices with the existence of obstacles of varying sizes. Through my experiment, I wanted to determine whether increased tumbling led to increased travel. Furthermore, I sought to determine not only whether obstacles influenced the path traveled by a microorganism, but also how differing concentrations of solute would impact the distance that cells could cover over time. I wanted to discover a set of conditions which would enable E. coli to move the furthest from the origin, and whether these conditions held true over multiple trials. I predicted that increased tumbling would result in greater distance traveled, since there would be a higher amount of potential “steps” taken by the cell. I predicted that increased obstacles would reduce the total distance traveled by the cell, since avoiding the barriers in the way of the random walk would require a more linear, less randomized path. Moreover, I predicted that conditions with no obstacles would result in the largest distances traveled since the random walk would not be inhibited by any restrictions.

II. METHODOLOGY

A. Analyzing a Tumble-Distance Relationship.

My first tests were conducted to determine whether there exists a relationship between the number of tumbles performed by the bacteria and the distance the bacteria travels from its starting location. A random walking simulation was

performed on a 501x501 lattice with the origin centered at (250,250). The test was performed with a non-self-avoiding walk. A random step function was used to determine the location of the object's travel, and consisted of a random number generator which would create a number between 0-100. The values 0-25 were sorted to increment in the positive x-direction, 25-50 in the negative x-direction, 50-75 in the positive y-direction, and 75-100 in the negative y-direction. At the start of every trial, a single, random step was taken 1000 times from the same starting point, and the distance from the current location of the walker to the origin was stored. The distances across equal step numbers were then averaged to determine how far away from the origin the random walker would travel approximately at a given step. A total of 1,000,000 steps were taken on the 501x501 grid.

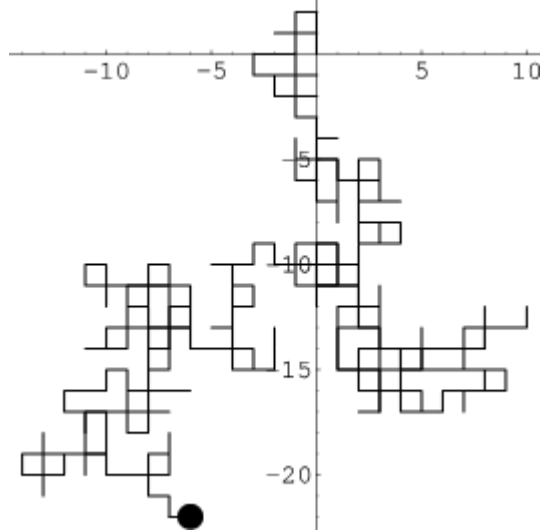


Fig. 1 A random walker traveling in a 2D lattice.

Image taken from Wolfram MathWorld:

<https://mathworld.wolfram.com/RandomWalk2-Dimensional.html>

B. Determining the Impact of Obstacles on Cell Travel

Using the same lattice size and random walking function as described in A, I tested whether the implementation of 1x1 obstacles would limit the distance traveled by the random walker. Single unit obstacles were periodically placed throughout the grid, equally spaced five units apart in both the vertical and horizontal directions. If the random direction that was chosen caused the walker to collide with an obstacle, the randomizing function was repeated to generate a new direction for the walker to travel in. The average distances travelled per step were stored and graphed against the average distances travelled with no obstacles.

Fig. 2 displays the sample conditions in which the random walker travelled. Due to scaling, obstacles were placed four units apart in the figure, though a standard length of five units was utilized for all tests. In the figure, the drunken walker is represented by the "1" at the origin, and obstacles are denoted by "5" colored in red. With the implementation of obstacles, data collected within the first 200 steps was truncated since the walker's radius of travel was inherently limited. The primary purpose of this experiment was to determine the

general trend of the walker's movement with obstacles, so the loss of 200 steps out of 1,000,000 total steps had no significant impact on the data collection process.

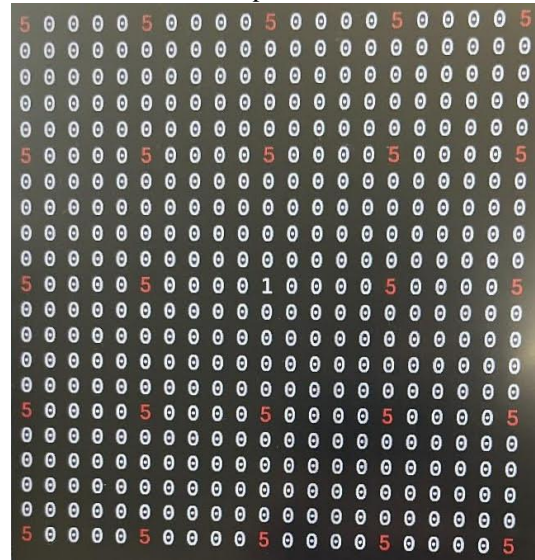


Fig. 2 1x1 obstacles placed in square matrix with walker centered at the origin. Sample generation, not the scale of experiment conditions.

C. Varying Obstacle Size to Find Ideal Travel Conditions

Varying obstacle size required more computational power, so lattice size was reduced to 301x301 with 1000 trials run at each step for 15,000 steps. Once again, average distances were recorded at each step taken. Obstacle generation increased for each experiment run. The obstacles were placed five units apart, and included sizes of 1x1, 2x2, 3x3, 4x4, and 5x5. The first 100 steps were truncated in graphical representations, and a linear fit was applied to the distance traveled throughout varying conditions to determine the obstacle size that would result in the furthest distance traveled from the origin.

III. RESULTS

A. Random Walks in the 1001x1001 Grid

Based upon the data collected, increasing step values result in increased distance traveled by the cell. It is important to note that the raw graphs of the distance to step relationship



Fig. 3 Graph of the natural log of distance traveled over the natural log of steps taken in a 1001x1001 lattice at 1,000,000 steps with no obstacles present.

demonstrate an exponential relationship, so the natural log was taken of both axes to display a linear relationship. All graphs presented utilize the natural log to project a linear relationship. As clearly shown in **Fig. 3**, more steps resulted in further distances travelled. Surprisingly, the graph remained noisy despite the use of averages for all distances. This variation is likely due to the natural tendency of the walker to stochastically trace over previous steps taken, repeatedly reducing, and increasing the distance from the origin.

B. 1x1 Obstacles in the 1001x1001 Grid

The distance traveled by the random walker in the 1x1 obstacle grid did not significantly differ from the empty grid, though the graphs show considerable variation in noise levels. While the distance of the 1x1 walker deviates slightly from the control walker, both lines show an increasing distance with more steps. For the 1x1 distances, there exists significant drops in distance as steps increase. These valleys are likely due to the walker getting trapped around a single object or around a small series of objects, repeatedly crossing over previous steps rather than venturing further into the grid.

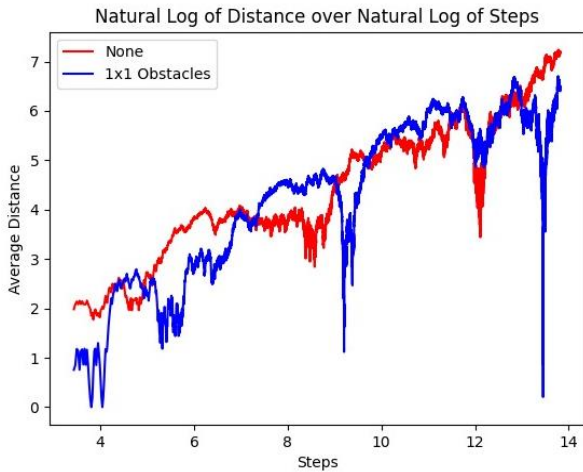


Fig. 4 Graph showing distance traveled by walker in empty grid (red) as well as distance traveled by walker in grid periodically filled with 1x1 obstacles (blue). X-axis does not start at zero due to truncation.

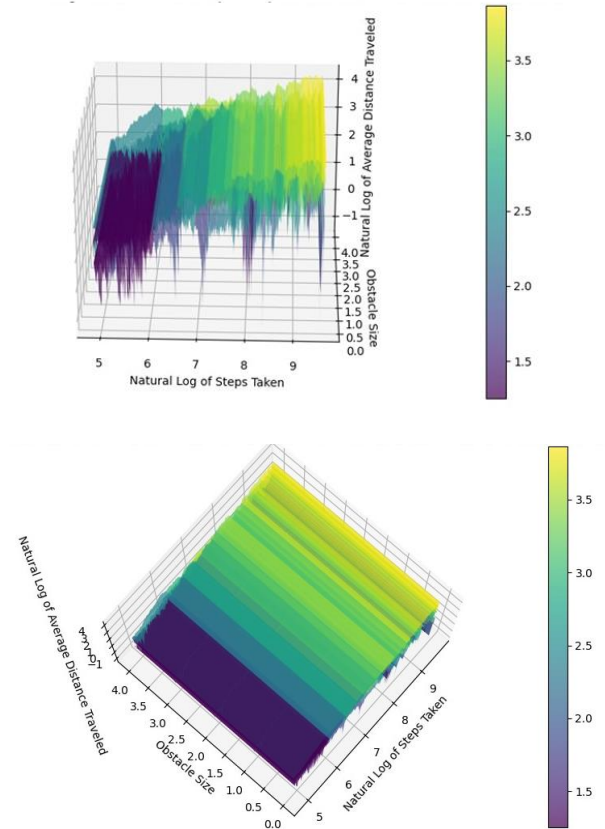
C. Increasing Obstacle Size in a 301x301 Grid

Regardless of obstacle size, all data shows that increasing steps effectively increases the distance between the origin and the walker. All conditions tested support that more tumbles result in further distances traveled. Both views of **Fig. 5** show a substantial increase in distance traveled as denoted by the yellow gradient peaks near the upper bounds of the x and z-axis.

The linear fit of the distances traveled by the empty grid, 1x1, 3x3, and 5x5 conditions all denote a steady increase in distance. Given enough steps, the 1x1 and 5x5 conditions both exceed the distance traveled compared to that of the obstacle-less grid. Surprisingly, the 3x3 obstacle trial falls below that of the control walker, though the slope of the 3x3 line appears to be able to surpass that of the control with increased steps.

Fig. 5 Side (upper) and top (lower) views surface plot with natural log of distance traveled plotted over both steps taken and

Surface Plot of Natural Log of Average Distance Traveled per Step in Varying Conditions (No Obstacles, 1x1, 2x2, 3x3, 4x4)



obstacle size. X-axis does not start at zero due to truncation.

The 5x5 conditions report the greatest slope, or the furthest distance traveled per step at the fastest rate. Although this result seems contradictory, it seems that obstacles help to guide the path of the walker. Rather than inhibiting the outward movement of the drunken walk, 5x5 obstacles act as funnels to create linear paths for the walker to travel up the grid. With smaller concentrations of open grid space, the walker is forced to move in a more controlled manner.

In cases where the concentration of obstacles is sparser—as seen in the 1x1 and 3x3 trials—it appears that the walker has more difficulty navigating further throughout the grid in lower step quantities. As the number of steps increases, the walker in obstacle-filled conditions has a higher likelihood of travelling further distances given that more steps are taken. Comparing only the first half of **Fig. 6** shows that the control walker travels more in the first 7,500 steps than that of 1x1 and 3x3 walkers in the same step range. This fact may stand true across trials of small step quantities, but the generalized behavior of the walker in obstacle filled conditions depicts that of increased travel with larger obstacles present.

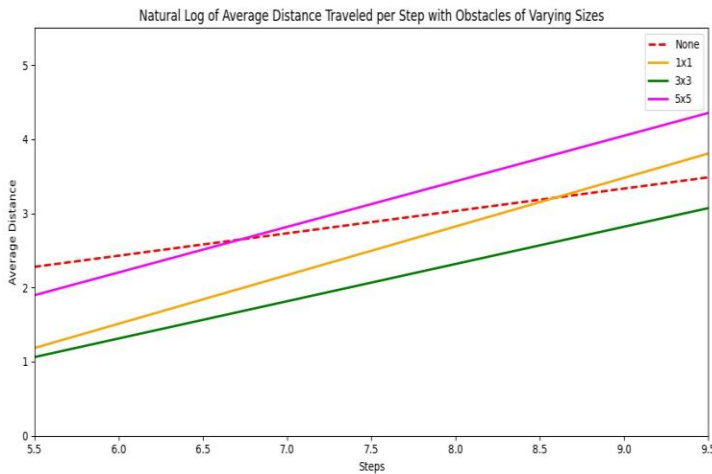


Fig. 6 Linear fit of average distance traveled per step taken for empty grid, 1x1, 3x3, and 5x5 obstacles in the 301x301 grid. X-axis does not start at zero due to truncation.

IV. CONCLUSION

An intricate balance exists between directed movement towards chemical stimuli and the apparent randomness of microbiological motion. These findings resonate with the poignant moral of *Scent of a Woman*, where Colonel Slade navigates life's anomalies with a blend of both intuitive and non-intuitive solutions. Through an exploration of chemotaxis and random walk algorithms, we are forced to confront the unpredictability of nature. Living things must adapt to both environmental factors and internal randomness to thrive.

My results align with the fundamentals of chemotaxis: as the concentration of favorable solute attractants increases, the concentration of traversable chemical solvent decreases. Thus, the bacteria are capable of suppressing tumbling to move towards the attractant. Likewise, as the size of evenly generated obstacles increased in my experiments, the grid availability decreased, resulting in further travel by the bacteria. This result is outrageously counterintuitive—with increased barriers it is easy to expect reduced travel. However, by framing these conditions as the abatement of empty space rather than the augmentation of obstacles, these conclusions appear more reasonable.

Despite the validity of these results, inherent errors exist within my simulation. Foremost, the noisiness of my distance data is likely due to the logic utilized in the random walking function. When an obstacle was detected, the random walk function was recalled within itself. Within my code exists the potential for the direction generated to become stuck within this loop. This structure may account for the substantial divots in distance as seen in **Fig. 4**. Additionally, in a more holistic sense, my simulation is that of a misrepresented scale for the movement of a microorganism. In practicality, *E. coli* bacteria are miniscule and have infinite space to roam. Through the confines of computational strength, I modeled a non-microscopic particle moving in captivity. While these errors may limit the realism of my simulation, they do not substantially undermine my conclusions.

Much like Colonel Slade's journey, this study underscores the essential process of life's complexities and contradictions, intuition, and navigating through them. Just as Colonel Slade discovers that sometimes the most effective solutions are not always the most obvious, our understanding of chemotaxis and random walking *E. coli* behavior highlights the significance of considering non-intuitive explanations in research.

Life's contradictions lead us to unexpected insights, echoing the timeless message of *Scent of a Woman* and reinforcing the importance of the unknown in the continual attempt to better understand the natural world. As screenplay writer Bo Goldman puts it, "If there is a moral to the film, it is that if we leave ourselves open and available to the surprising contradictions in life, we will find the strength to go on" [7].

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