



Modeling SARS-CoV-2 with Stochastic Simulations

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Abstract

The COVID-19 pandemic of 2020 has caused both immense political and social upheaval on local and global scales. To mitigate the spread, health officials around the world have suggested wearing masks, social distancing, and minimizing social gatherings such as attending parties or even going to the workplace. By designing, running, and collecting data from stochastic simulations, we analyze and draw conclusions from trends in the results of those simulation runs. In addition to intuitively and mathematically confirming guidelines put forth by organizations like the CDC and the WHO, our data and analysis indicate the existence of the so-called “2/3 Phenomenon” - that when 2/3 of the population complies with regulations such as social distancing, the population is able to create a herd immunity-like state, and disease spread becomes much easier to contain.

Keywords

stochastic, COVID-19, compliance, distancing, mitigation, simulation

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Introduction

The global SARS-CoV-2 pandemic has sparked intense debate regarding safety guidelines, their effectiveness, and their feasibility while also maintaining economic stability. The recent uptick in infections in the United States attests to how persistent the virus can be, even when large portions of the population are generally complying with guidelines such as wearing masks, washing their hands, and social distancing. As of today, in the United States alone, there have been over 400,000 deaths due to SARS-CoV-2 [2].

In the United States, daily recorded cases of COVID-19 initially peaked in early April, and started to decline steadily well into late May. However, with large-scale state reopenings as well as mass protests in major cities during the last week of May, the country saw a spike in cases just two to three weeks later, eventually reaching more than 78,000 recorded cases in one day on July 24th [2]. In more recent weeks, the United States has shattered previous records, reaching more than 200,000 cases on November 20th alone. Analyzing situations not only like these, in which people can be clustered together, but also situations involving commuting, such as the workplace, can help shed light on the specific circumstances that cause the spread of SARS-CoV-2.

Preventing new outbreaks from occurring on a local scale will help stop exponential-like growth of cases. General scientific consensus argues that so-called “super-spreaders” are responsible for a large portion of cases due to their large range of movement, infecting people wherever they go [6]. For example, if a super-spreader were to go to a crowded place, they would likely infect multiple people at that location, who in turn would infect several others. This triggers an exponential growth in local

cases, and the majority of these will not be detected without a test or until the incubation period has passed, at which point many people will already be infected. Paired with people who frequently commute, each of these hotspots can, in principle, trigger an outbreak [6]. Indeed, countries have struggled to contain the spread of SARS-CoV-2, and it is for this reason that understanding how commuting affects the spread of the virus could be crucial to preventing further outbreaks.

There are several reasons why SARS-CoV-2 is difficult to contain. The incubation period can cause difficulty in identifying carriers early on and allows each carrier to expose other individuals to the pathogen for an extended period of time [1]. In addition, the prevalence of asymptomatic carriers makes it difficult to know, without testing, if someone is infected and contagious [14]. To better understand how the disease spreads in local clusters and derive techniques to mitigate the spread, we turn to stochastic simulations, which provide a safe yet robust alternative to model the spread of disease. Specifically, we wish to simulate social interaction at the workplace and at home, which will help uncover details behind the spread of SARS-CoV-2 in more crowded environments and on a local scale.

Stochastic modeling has been previously used to model local outbreaks and epidemics. For example, stochastic simulations have been used to predict the dynamics and “probabilistic infection routes” of dengue fever outbreaks in Australia [12]. In another example, authors examined outbreaks of swine flu in Hong Kong and found that their simulation “achieves high accuracy in parameter estimation (less than 10.0 % mean absolute percentage error)” [11]. These two examples together show that stochastic sim-

ulations can approximate real-world simulated data pertaining to the spread of disease. Thus, we decided to leverage this tool to better understand the dynamics of SARS-CoV-2 virus during the global pandemic of 2020.

Here, we use stochastic simulations to tease out the factors related to commuting and the workplace that contribute to the spread of SARS-CoV-2. We can also visualize and measure the

general spread of the disease with stochastic simulations and mathematically derive a value for optimal amounts of social compliance and an optimal amount of social interaction. Combining information from the CDC, data on the number of cases we see, and results from stochastic simulations, we can create a robust set of guidelines to mitigate the spread of SARS-CoV-2.

Materials and Methods

To simulate the movement of people throughout their daily lives, we implemented a random walk - a collection of random movements that simulates the motion of particles, bacteria, or

people in a simulation, over a certain period of time [7]. This average distance traveled, x , can be calculated as:

$$x = \sqrt{2Dt} \quad (\text{Equation 1})$$

where x is the total displacement, D is the diffusion coefficient, in units of area per time, and t is the time-scale, in units of time. Multiplying this movement by a value sampled from a standard normal distribution yields a subject's displacement - along one axis - for a simulated test subject. This calculation can be done for each axis along which simulated subjects move.

A blank "slate" was defined as an area to be populated with people, which are simulated as a set of Cartesian coordinates (x , y). Each simulation starts with one person infected and a set distance threshold that determines which nearby people will get infected. This threshold was set at 2 meters, which is the prevalent international standard for social distancing [3]. Additional features include recovery time and immunity retention time, which control how long the person remains sick and how long the person stays immune after recovery, respectively. These values are normally distributed to produce realistic results, with means set to 10 days and 75 days, respectively, as derived from the literature [3,13].

To simulate commuting and the increased risk of infection in the workplace - or any social gathering - people are placed into their "home positions" in a ring around a central point. After setting up a clock system, each commuter is nudged towards the center, i.e. the workplace. They are then nudged back to their home positions at the end of the workday. These nudges are calculated by taking the distance from the person to their desired destination and moving them halfway towards the location. When people arrive near the coordinates of the workplace, their commute mechanics are disabled to let random walk mechanics control their movement. While random walk mechanics are important to use during the work period, to effectively simulate people staying in their homes, we need to make sure that they stay close to their assigned home spot. For this reason, commute mechanics are not disabled on the way back home. This ensures that any movement too far away from their home will be counteracted by the commute mechanic since it stays in effect as long as people are not at work. At the beginning of the simulation, approximately 50% of people are randomly chosen to be commuters. The first

infected person is then selected randomly from the pool of commuters.

Two additional hyper-parameters are explored in the simulation - the length of the workday, and the “mean social compliance”. The length of the workday corresponds to how long people stay away from home. The mean social compliance is a hyperparameter that works as part of the function to calculate the value of the mean diffusion coefficient (Equation 2). The compliance ranges from 0% to 100%, with 0% not modifying the mean diffusion coefficient at all, and 100% making it zero. The compliance value

for each person is selected from a normal distribution with a mean determined by the mean social compliance hyper-parameter. Compliances less than 0% are set to 0% while compliances greater than 100% are set to 100%. As a real-world connection, one could think of social compliance as how well people follow regulations such as keeping two meters away from others. To better simulate realistic movement, the diffusion coefficient varies with the time of day as well as the mean social compliance. Thus, the mean diffusion coefficient is calculated as follows:

$$D_{mean} = \begin{cases} 0 & 0 \leq h \leq 5 \\ 50 * (1 - \frac{sc}{100}) * (\sin(\pi * \frac{h-5}{19}))^4 & 5 < h < 24 \end{cases} \quad (\text{Equation 2})$$

where D_{mean} is in meters squared per hour, h is the time of day, in hours, and sc is the mean social compliance in percentage, from 0% to 100%. Since the goal of this function was to simulate activity peaking in one part of the day and going down in others in a cyclic manner, a sine function was used. People are simply inactive for large stretches during the night, which made a piecewise function necessary. After setting hours zero to five as zero, to signify limited to no activity during the night, the sine wave was used to model the remaining 19 hours in the day. To create a sine wave with an initial output value of zero at five hours and a final output value of 0 at 24 hours, we modified the input by first subtracting five, and then scaling by the factor $\pi/19$.

Then, the result is multiplied by a factor scaled by the mean 19 social compliance. This results in the function outputting zero for all hours

when the mean social compliance is 100 and outputting the unmodified sine wave values when the mean social compliance is zero. The scale factor of 50 is intended to be the maximum mean diffusion coefficient calculated by the function.

Finally, the sine is smoothened by raising it to the fourth power to avoid a sudden increase in the mean diffusion coefficient when the simulation reaches 5 a.m. and an analogous abrupt decrease at midnight. The function also constrains the majority of movement to the late morning and afternoon hours of the day, when people are outside and most active. Thus, higher social compliance corresponds to a lower D_{mean} and values closer to $h = 14$ correspond to a higher D_{mean} with the exception of values of h between 0 and 5, as those are set to 0. The values at various h and sc can be found in Table 1.

Table 1: Values of Social Compliance obtained from the function in equation 2

Social Compliance (%)	Time of day (h)							
	0	6	10	14	14.5	15	19	23
0	0	0.037	14.65	49.32	50	49.32	14.65	0.037
20	0	0.029	11.72	39.456	40	39.456	11.72	0.029
40	0	0.022	8.79	29.592	30	29.592	8.79	0.022
60	0	0.015	5.86	19.728	20	19.728	5.86	0.015
80	0	0.007	2.93	9.864	10	9.864	2.93	0.007
100	0	0	0	0	0	0	0	0

This table shows values of D_{mean} for various h and sc . The values of sc were chosen to be evenly spaced, and the values of h were chosen to highlight the sinusoidal nature of the diffusion coefficient function as well as the inactivity period at the beginning of the day.

The D_{mean} is added to a value sampled from a standard normal distribution for each person in the simulation, which creates individual diffu-

sion coefficient values for each person. Each of those resulting diffusion coefficients are plugged into Equation 1 to calculate the movement for each person along the x- and y-axes.

Results

Stochastic simulations are consistent with expected behaviors as explained by the CDC

In order to analyze the dynamics of the spread of SARS-CoV-2, we created a simulation as described in Materials and Methods. Video 1 shows the simulation running for approximately 48 hours, which shows the dynamics and tracking methods employed. During the hours 00:00 to 05:00, there is no movement at all, and there are no spikes in the basic reproduction number. The basic reproduction number is defined as the ratio of the number of new infections to the number of people previously infected. So, if two

people were to infect a total of four people, the basic reproduction number would be two. There are also no spikes in the increase in cases, and no increase in the active cases graph. This is around the time when people are simulated to be immobile due to the early time of the day. After 05:00, movement begins to increase consistently into the late afternoon. At 09:00, the commute mechanic kicks in, causing commuters to move to work. The spread of infections is visible during these hours at the workplace. After the workday has elapsed, people move back to their homes, and movement decreases until 00:00, at which point the cycle repeats. Screenshots from another simulation run are shown in Figure 1.

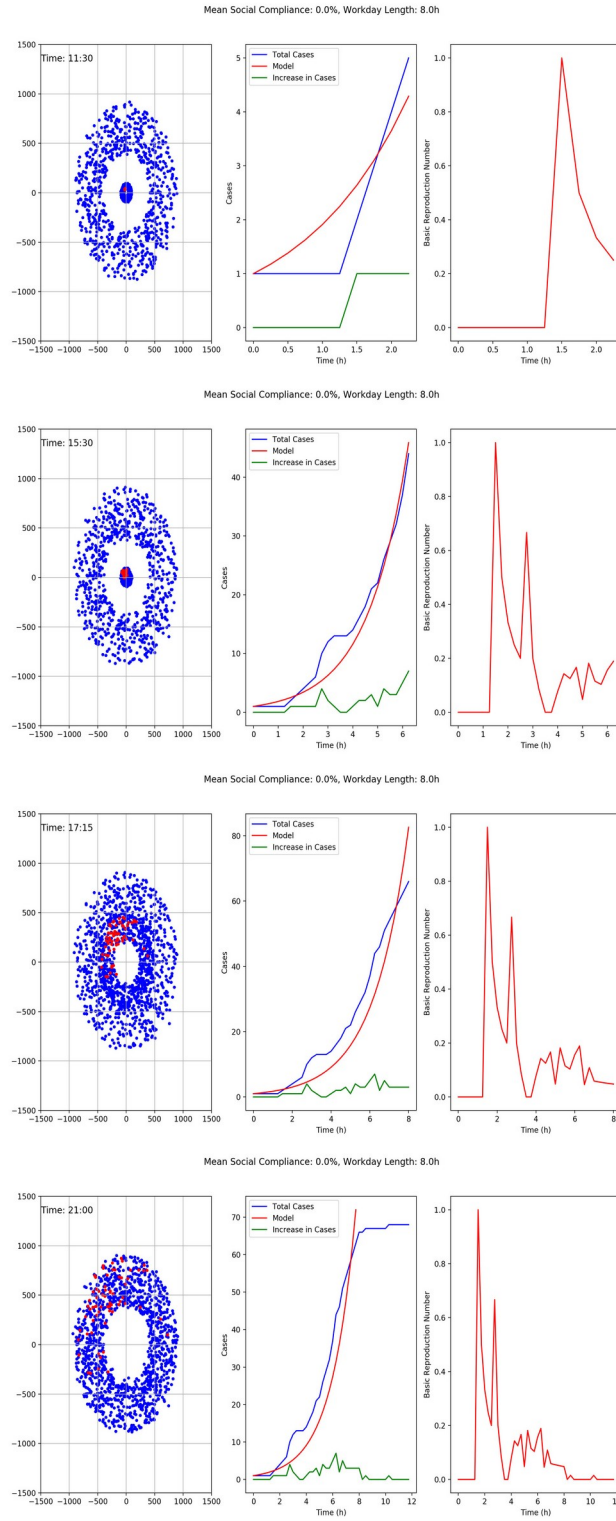


Figure 1: These images show the cycle of the simulation, run with an 8 hour workday and a 0% mean social compliance. The first shows the beginning of the workday, where 4 new people have been infected by the first infected commuter. The next image shows the exponential increase in infections. The third shows people commuting back home - they are midway between the workplace and their home positions. Finally, we see people at their homes, and the corresponding decrease in infections over time.

Video 1: Video of simulation run

<https://www.youtube.com/watch?v=lSms2uwIPO4>

also available as a supplementary file mp4 video

This video shows the progression of a simulation. On the left, you see the actual simulation slate, with each blue dot representing a healthy person, and each red one representing an infected one. The units of position are in meters. In the center is a graph of the current total cases, the increase in cases, and an exponential model of the total active cases during the first workday. On the right is a measure of the basic reproduction number over time. We calculate this by taking the number of sick people in any iteration of the simulation and dividing it by the number of sick people in the previous iteration.

If we examine the times at which infections take place, we can get a better understanding of where infections spread. For example, in Video 1, during the first workday, the simulation

shows a total of 49 cases. After people return home, one more person becomes infected, meaning that during that day, 98% of the infections occurred at the workplace. On the second day, roughly 260 new infections take place, about 20 of which happen away from the workplace, which means about 93.3% of infections occurred at the workplace. In addition, these at-home infections take place exclusively in areas where people are very close to each other. This helps simulate the concept that those who live with people who frequently commute are also at high risk of infection, which is also consistent with CDC guidelines which suggest that those who are living in close quarters should minimize their outside exposure. [4] However, we

can more rigorously show that our tool effectively and accurately models the spread of SARS-CoV-2 by introducing a control group.

Since the primary mechanic of the simulation is commuting, we created a control condition without a workday - in other words, a simulation without any commuting. Since CDC guidelines state that staying home and minimizing close contact prevent the spread of SARS-CoV-2 [5], we expect very few if any infections during the simulation runs. The control group was run at a zero hour workday for mean social compliances from 0% to 100%, with intervals of 5%, and 50 times for each combination - which totals to 1,050 simulation runs. The hyperparameter of mean social compliance determines the simulated people's degree of movement, as described in Materials and Methods. The results of these runs are shown in Figure 2.

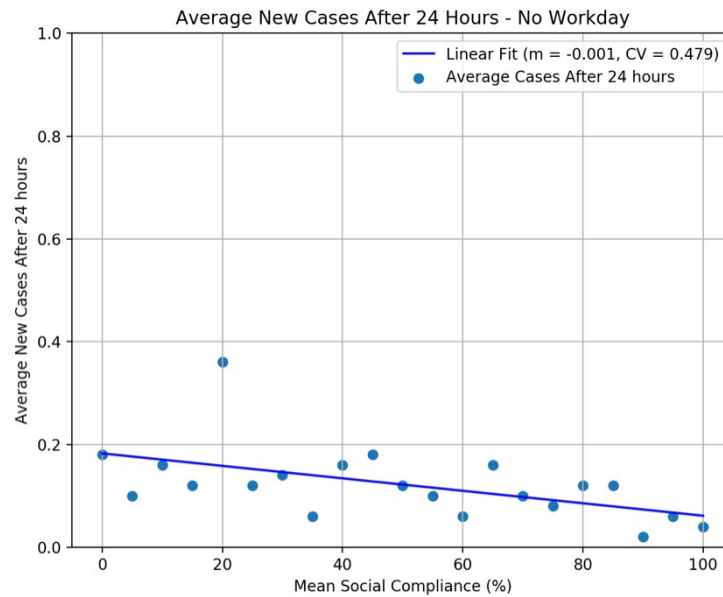


Figure 2: comparison of the mean social compliance to the average number of cases in the simulation after 24 hours, without any workday. Each data point represents the average of 50 simulation runs. The blue line shows a best-fit line to the data, and the slope m and coefficient of variation (CV, i.e. RMSE / mean) are displayed in the legend. The vertical axis is scaled from 0 to 1 to display the values corresponding to no infections and the threshold for an un-contained outbreak, respectively.

The data show that the average number of cases was consistently below 1, which means, on average, there were no new infections at all. Given that each data point is the average of 50 simulations, this means that in the overwhelming majority of simulation runs, the number of transmissions was zero. This shows that the majority of infections are likely to take place at social gatherings - and in the case of our simulation, the workplace. Thus, we have demonstrated that our simulation models the expected behavior of the disease when CDC guidelines of staying home and minimizing interpersonal contact are followed.

Outbreak cases are dependent on social compliance and workday length

To look into the effect that social gatherings and commuting would have on the rise of new COVID-19 cases, we varied workday length and mean social compliances. We varied mean social compliance from 0% to 100%, in intervals of 5%, and workday length from 0 hours to 8 hours, in intervals of 0.5 hours. This creates a total of 357 unique possible combinations, each of which was run 50 times to avoid susceptibility to random outliers - a total of 17,850 simulation runs. We then averaged all 50 runs for each individual combination as described above (Figure 3).

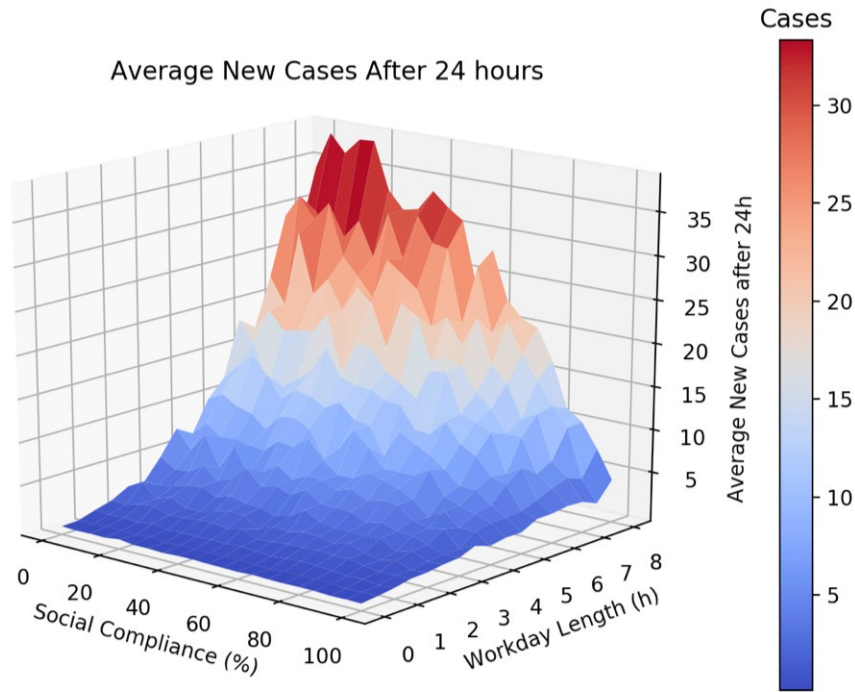


Figure 3: the effect that social compliance and workday length have on the total cases after 24 hours. The color gradient represents the number of cases after 24 hours, with blue being the lowest value in the data and red being the highest. Each value on this graph represents the average of 50 simulation runs.

Based on the data in Figure 3, we show that increased workday lengths - or the time spent at a social gathering - are directly related to the severity of a local outbreak in terms of active cases. Along the social compliance axis, we see that the values at lower workdays are always “more blue” than values at higher workdays, which suggests a positive, or direct, correlation between workday length and active cases. The opposite is true for mean social compliance. The average number of cases at the lowest social compliances are always higher (less blue / more red) than at higher social compliances. This shows that there is an inverse correlation between social compliance and active cases. These data offer a sharp contrast to the control condition, in which the average number of cases was always below 1. We also noticed a change in the slope of the graph when social compliance passed roughly 60%. However, to more carefully examine the slopes, we decided to reduce the 3D data into a format more conducive to in-depth analysis.

Social compliance rules become more effective when enough people abide by them

In order to better understand the change in slope observed in Figure 3, we averaged the data over workday length to collapse the data into a 2D array. The result is a new dataset that shows the generalized relationship between mean social compliance and the active cases after 24 hours,

and this is shown in Figure 4. Given our initial observation that the inflection point in Figure 3 was at approximately 60% mean social compliance, we split the data into two subsets: one from 0-60% and the other from 65-100% social compliance. We then fit an independent linear model to the entire dataset as well as to each subset.

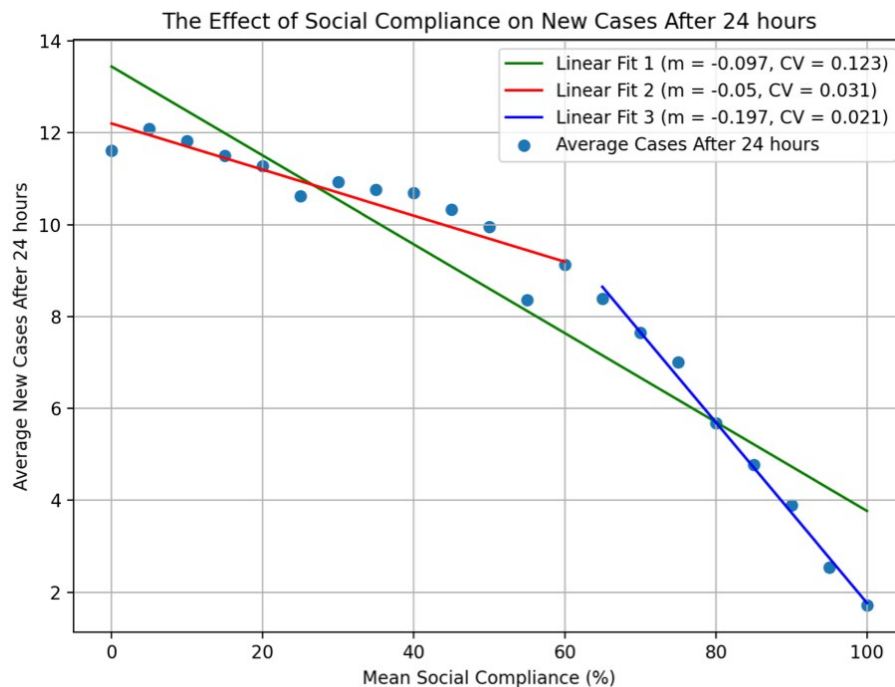


Figure 4: the general relationship between mean social compliance and average new cases after 24 hours. Each data point is representative of 850 simulation runs. The green line is a linear fit to all of the data. The blue line is the linear fit for the subset of the data at social compliances less than or equal to 60%, and the red line is the linear fit for the subset of the data at social compliances greater than or equal to 65%. The values of m - the slope - of each linear fit, as well as the coefficients of variation, are listed on the graph.

Both from visual inspection and the values of the coefficients of variation, we observe that the individual fits for each subset are better than the overall fit to the entire range of 0-100% social compliance - Linear Fit 1. Thus, we can see that the two individual linear fits are better at modeling the data than the original line. We found that the slopes of the lines fit to the individual sub-

sets differed by a factor of four, implying that when mean social compliance reaches roughly 65%, each incremental increase is more effective at preventing new infections than the same increase with a lower compliance. For example, an increase in mean social compliance from 30% to 50% on the graph reduced the average cases after 24 hours by about 0.98. However, a

change from 60% to 80% caused a decrease of 3.44 cases, more than 3.5 times the magnitude of the change from 30% to 50%. This mathematically shows that mean social compliance begins to work better and better when enough people begin to adhere to it, and that threshold is around 65%, or $2/3$.

We next averaged the average number of cases over the social compliance axis. This yielded data that would show the relationship between workday length and average cases after 24 hours. Based on Figure 3, we expected these

data to show a strong positive relationship between workday length and average cases after 24 hours. The graph produced from the resulting data is shown in Figure 5. As expected, Figure 5 shows a direct relationship between workday length and the average cases after 24 hours. After examining the data, we fit an exponential model and found that the coefficient of variation was 0.134, indicative of a good fit. In addition to being consistent with previous knowledge from CDC guidelines, these data further validate our simulation as an effective tool for modeling disease spread.

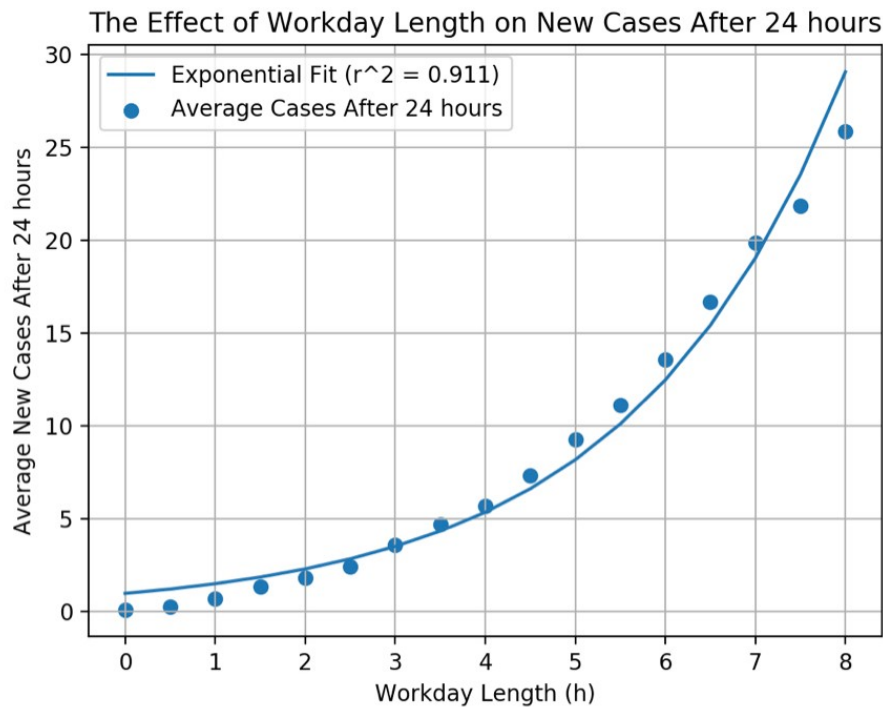


Figure 5: the general relationship between workday length and new cases after 24 hours. Each data point is representative of 1,050 simulation runs. An exponential model was fitted to these data, and the coefficient of variation is listed in the legend.

Discussion

The 2/3 Phenomena

Initial predictions for our simulated results supported the idea that shorter workdays and higher social compliance would better minimize the number of infections. Note that there were two distinct best-fit lines for the data comparing mean social compliance to the number of active cases after 24 hours. The slope increased by a factor of roughly four when the mean social compliance exceeded 65%, or about 2/3. This seems to indicate that when enough members of a population comply with guidelines, or when each member of the population complies with guidelines at a certain level, disease spread is significantly easier to contain.

Interestingly, our data suggesting that 2/3 is an important number for the containment of disease is consistent with the public health concept of herd immunity [10]. When enough members of a population are inoculated against a disease, each infected individual will more often come into contact with inoculated individuals, who are not susceptible to becoming carriers. Thus, the disease does not spread. Similarly, if enough people follow guidelines, then infected individuals will not be able to pass the virus onto others, as they will be protected by their guideline-following - whether that be social distancing or mask-wearing. Thus, via the method of stochastic simulations, we have confirmed that we can indeed begin to approach a herd immunity-like state purely based on approximately 2/3 of people adhering to CDC guidelines like social distancing. Once this state is achieved, mitigating spread with further adherence to guidelines becomes much easier.

However, we do not yet have much insight into the reasoning behind this phenomena's occurrence. We know from various studies that at the root of a large portion of disease spread are su-

per-spreaders [6]. This means that a large amount of infection transmission is driven by a small portion of the population. From surveys of interpersonal contacts, we can see that very small percentages - approximately 6% - of the population interact with more than 6 or 7 people [9] - therefore, it is likely that these people behave as super-spreaders. This implies that social compliance does not mainly target single person-to-person transmission, but works as a way to prevent a super-spreader from infecting large numbers of people at once. If a large portion of the population is not susceptible to being infected, then it would become much harder for a super-spreader to pass on the pathogen to enough people to sustain an outbreak, and we have determined this number to be 2/3 of the population. Effectively, we believe that the reason behind the appearance of the number 2/3 is that it is a tipping point at which it starts to become significantly more difficult for super-spreaders to spread the pathogen to large numbers of people - difficult enough that the rate at which they infect people is stifled by their limited interpersonal interaction.

A complicating factor is that the number 2/3 could also be interpreted as an average - for example, if half the population was 71% compliant and the other half was 61% compliant, the average would still be around 2/3. Different combinations of population portions complying at different levels could lead to the number 2/3. However, we do not have experimental data to support that this interpretation is valid and would lead to similar results. Given the practical implications of different averages leading to a 2/3 social compliance, it would be unwise to draw such conclusions without further data. This question opens avenues for further research on the topic.

Thus, the phenomenology and appearance of the works in the interest of all parties involved. Number $2/3$ yields two major findings. First, that once the portion of the population complying with guidelines exceeds $2/3$, each increase in compliance after that is more effective than if fewer than $2/3$ of people were complying with guidelines. This conclusion is derived by looking at the slopes of linear fits 2 and 3 in Figure 4. Since the slope of Linear Fit 3 is roughly four times that of Linear Fit 2, the rate of case decrease with respect to social compliance at compliances above 65%, or roughly $2/3$, is four times greater in magnitude. Second, that by increasing social compliance, we can make it much more difficult for any person to be a super-spreader, because more people are coming into contact less often, decreasing the chances of large gatherings and super-spreader events. Because these super-spreaders can single-handedly cause large-scale local outbreaks, increasing mean social compliance beyond $2/3$ will help create a herd immunity-like state, which will prevent not only single person-to-person transmissions, but also epidemics caused by super-spreaders.

Workday Length Recommendations

The results of the simulation runs show that shorter workdays are linked to lower case numbers, with an absence of workdays causing an average of zero new infections. The direct exponential relationship between workday length and average cases after 24 hours suggests that minimizing the workday as much as possible

Many companies face the problem of maintaining social distancing - they may not be able to rent more space, but will need to keep people distanced from each other. However, given the shorter workdays, it would be easier to divide employees into shifts. This provides an additional safety measure, as employees will be in separate groups at different times. So, if an employee becomes infected, the chance that they pose a risk to everyone in the workplace is reduced since only a fraction of the company's workforce is coming in close contact with them. This also mitigates the risk of infection for people who are staying at home. From our description and analysis of Video 1, we know that the risk for people at home is greater if they live with someone who is a frequent commuter. By decreasing the risk of infections for those who must be in a physical workplace, we would also help those who live in the homes of commuters stay safe. Combined with guidelines regarding wiping down surfaces to prevent the virus from spreading through surface-to-person contact, shorter workdays and breaking up employees into shifts would increase productivity and keep employees, their families and communities safe from infection.

Software

The software that was used to run these simulations can be seen and downloaded at: <https://github.com/gsingh-0-0-1/covid-simulations>
Please make sure to follow the instructions on the homepage of the repository - or in the README.md file - in order to download and install of the dependencies to correctly run the software.

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