DATA 604 HW6 Magnus Skonberg These exercises and their solutions were made with reference to Modeling and Simulation in Python (version 3) authored by Allen B. Downey. This week's exercises focused on **Optimization**, chapters 12 and 13 of the text. # Configure Jupyter so figures appear in the notebook %matplotlib inline # Configure Jupyter to display the assigned value after an assignment %config InteractiveShell.ast_node_interactivity='last_expr_or_assign' # import functions from the modsim.py module from modsim import * Chapter 12 **Previous Code** def make system(beta, gamma): """Make a system object for the SIR model. beta: contact rate in days gamma: recovery rate in days returns: System object init = State(S=89, I=1, R=0) init /= sum(init) t0 = 0t end = 7 * 14return System(init=init, t0=t0, t_end=t_end, beta=beta, gamma=gamma) def update_func(state, t, system): """Update the SIR model. state: State with variables S, I, R t: time step system: System with beta and gamma returns: State object s, i, r = stateinfected = system.beta * i * s recovered = system.gamma * i s -= infected i += infected - recovered r += recovered return State(S=s, I=i, R=r) def run_simulation(system, update_func): """Runs a simulation of the system. system: System object update_func: function that updates state returns: TimeFrame frame = TimeFrame(columns=system.init.index) frame.row[system.t0] = system.init for t in linrange(system.t0, system.t_end): frame.row[t+1] = update_func(frame.row[t], t, system) return frame **Metrics** We can compute metrics to quantify what we're interested in, like the total number of sick students, for example. def calc total infected(results): """Fraction of population infected during the simulation. results: DataFrame with columns S, I, R returns: fraction of population return get_first_value(results.S) - get_last_value(results.S) In [4]: beta = 0.333gamma = 0.25system = make system(beta, gamma) results = run simulation(system, update func) print(beta, gamma, calc total infected(results)) 0.333 0.25 0.46716293183605073 **Exercise** Write functions that take a TimeFrame object as a parameter and compute the other metrics mentioned in the book: 1. The fraction of students who are sick at the peak of the outbreak. 2. The day the outbreak peaks. 3. The fraction of students who are sick at the end of the semester. Note: Not all of these functions require the System object, but when you write a set of related functions, it is often convenient if they all take the same parameters. Hint: If you have a TimeSeries called I, you can compute the largest value of the series like this: I.max() And the index of the largest value like this: I.idxmax() You can read about these functions in the Series documentation. # 1. The fraction of students who are sick at the peak of the outbreak. def frac sick peak(results): return results.I.max() # 2. The day the outbreak peaks. def peak day(results): return results.I.idxmax() # 3. The fraction of students who are sick at the end of the semester. def frac sick end(results): return get last value(results.I) #verify that they work print(frac_sick_peak(results), peak_day(results), frac_sick_end(results)) 0.043536202687592354 30 0.0006741943156034474 From above we could extend that: • the fraction of students who are sick at the peak of the outbreak: 0.0435 • the day the outbreak peaks: 30 the fraction of students who are sick at the end of the semester: 0.000674 What if? Now we account for the impact of immunization: def add immunization(system, fraction): """Immunize a fraction of the population. Moves the given fraction from S to R. system: System object fraction: number from 0 to 1 system.init.S -= fraction system.init.R += fraction #initialize variables tc = 3 # time between contacts in days # recovery time in days beta = 1 / tc # contact rate in per day gamma = 1 / tr# recovery rate in per day system = make system(beta, gamma) #run model without immunization results = run simulation(system, update func) calc total infected(results) #run model with 10% immunization system2 = make system(beta, gamma) add immunization(system2, 0.1) results2 = run simulation(system2, update func) calc total infected(results2) #plot results / difference plot(results.S, '-', label='No immunization') plot(results2.S, '--', label='10% immunization') decorate(xlabel='Time (days)', ylabel='Fraction susceptible') savefig('figs/chap12-fig01.pdf') Saving figure to file figs/chap12-fig01.pdf 1.0 No immunization --- 10% immunization 0.9 Fraction susceptible 8.0 0.7 0.6 0.5 20 0 40 60 80 100 Time (days) #Define sweep immunization function def sweep_immunity(immunize_array): """Sweeps a range of values for immunity. immunize array: array of fraction immunized returns: Sweep object sweep = SweepSeries() for fraction in immunize array: system = make_system(beta, gamma) add_immunization(system, fraction) results = run_simulation(system, update_func) sweep[fraction] = calc_total_infected(results) return sweep #Sweep through range of values for the fraction of the population who are immunized. immunize array = linspace(0, 1, 21) infected_sweep = sweep_immunity(immunize_array) #Plot results plot(infected_sweep) decorate(xlabel='Fraction immunized', ylabel='Total fraction infected', title='Fraction infected vs. immunization rate', legend=False) savefig('figs/chap12-fig02.pdf') Saving figure to file figs/chap12-fig02.pdf Fraction infected vs. immunization rate 0.4 Total fraction infected 0.3 0.2 0.1 0.0 0.2 0.4 0.6 1.0 0.0 8.0 Fraction immunized **Logistic Function** def logistic(x, A=0, B=1, C=1, M=0, K=1, Q=1, nu=1): """Computes the generalize logistic function. A: controls the lower bound B: controls the steepness of the transition C: not all that useful, AFAIK M: controls the location of the transition K: controls the upper bound Q: shift the transition left or right nu: affects the symmetry of the transition returns: float or array exponent = $-B \star (x - M)$ denom = C + Q * exp(exponent)return A + (K-A) / denom ** (1/nu) spending = linspace(0, 1200, 21) #range of possible spending def compute factor(spending): """Reduction factor as a function of spending. spending: dollars from 0 to 1200 returns: fractional reduction in beta return logistic(spending, M=500, K=0.2, B=0.01) percent reduction = compute factor(spending) * 100 plot(spending, percent reduction) decorate(xlabel='Hand-washing campaign spending (USD)', ylabel='Percent reduction in infection rate', title='Effect of hand washing on infection rate', legend=False) Effect of hand washing on infection rate 20.0 Percent reduction in infection rate 17.5 15.0 12.5 10.0 7.5 5.0 2.5 0.0 0 200 400 600 800 1200 1000 Hand-washing campaign spending (USD) **Exercise** Modify the parameters M, K, and B, and see what effect they have on the shape of the curve. Modify the other parameters and see what effect they have. Notes on modifying parameters: • **M**: being that 'M' controls the location of the transition, when we increase it the sigmoid shifts right along the X axis and when we reduce it the sigmoid shifts left along the X axis with the midpoint (of the sigmoid) being situated over the specified value. • K: being that 'K' controls the upper bound, when we increase it the maximum value of the Y axis shifts ip and when we reduce it the maximum value shifts down, with the sigmoid reaching its apex at the specified value. • **B**: being that 'B' controls the steepness of the transition, when we increase it the transition is quicker from the minimum Y value to maximum Y value (fewer increments of X) and when we decrease it the transition is slower from minimum Y value to maximum Y value (more increments of X). • Other values: when we vary 'A' the lower bound follows, when we vary 'C' the Y value is impacted, when we vary 'Q' the X value is impacted, and when we vary 'nu' the location of transition and slope vary. Handwashing We'll explore the effect hand-washing has on our model and then put it all together: def add hand washing(system, spending): """Modifies system to model the effect of hand washing. system: System object spending: campaign spending in USD factor = compute factor(spending) system.beta *= (1 - factor) # time between contacts in days tr = 4# recovery time in days beta = 1 / tc # contact rate in per day gamma = 1 / tr # recovery rate in per day beta, gamma spending_array = linspace(0, 1200, 13) for spending in spending array: system = make system(beta, gamma) add_hand_washing(system, spending) results = run_simulation(system, update_func) print(spending, system.beta, calc total infected(results)) def sweep hand washing(spending array): """Run simulations with a range of spending. spending array: array of dollars from 0 to 1200 returns: Sweep object sweep = SweepSeries() for spending in spending_array: system = make system(beta, gamma) add_hand_washing(system, spending) results = run_simulation(system, update_func) sweep[spending] = calc_total_infected(results) return sweep spending array = linspace(0, 1200, 20) infected_sweep = sweep_hand_washing(spending_array) plot(infected sweep) decorate(xlabel='Hand-washing campaign spending (USD)', ylabel='Total fraction infected', title='Effect of hand washing on total infections', legend=False) savefig('figs/chap12-fig03.pdf') 0.0 0.3328871432717143 0.4667702312363652 100.0 0.3321342526691939 0.46414165040064037 200.0 0.33017160845482885 0.4572170063132055 300.0 0.32538647186519215 0.4398872029120663 400.0 0.3154039052420003 0.40163064627138245 500.0 0.3 0.3370342594898199 600.0 0.28459609475799963 0.26731703056804546 700.0 0.2746135281348078 0.22184699045990752 800.0 0.26982839154517113 0.20079159841614402 900.0 0.2678657473308061 0.1923921833925878 1000.0 0.26711285672828566 0.18921320781833872 1100.0 0.26683150821044227 0.18803175228016467 1200.0 0.26672740341296003 0.1875955039953746 Saving figure to file figs/chap12-fig03.pdf Effect of hand washing on total infections 0.45 0.40 Total fraction infected 0.35 0.30 0.25 0.20 0 200 400 600 800 1000 1200 Hand-washing campaign spending (USD) **Optimization** num students = 90 budget = 1200price_per_dose = 100 max doses = int(budget / price per dose) dose_array = linrange(max_doses, endpoint=True) max doses for doses in dose_array: fraction = doses / num_students spending = budget - doses * price_per_dose system = make_system(beta, gamma) add immunization(system, fraction) add_hand_washing(system, spending) results = run_simulation(system, update_func) print(doses, system.init.S, system.beta, calc_total_infected(results)) def sweep_doses(dose_array): """Runs simulations with different doses and campaign spending. dose array: range of values for number of vaccinations return: Sweep object with total number of infections sweep = SweepSeries() for doses in dose array: fraction = doses / num students spending = budget - doses * price_per_dose system = make_system(beta, gamma) add immunization(system, fraction) add_hand_washing(system, spending) results = run simulation(system, update func) sweep[doses] = calc_total_infected(results) return sweep infected_sweep = sweep_doses(dose_array) plot(infected sweep) decorate(xlabel='Doses of vaccine', ylabel='Total fraction infected', title='Total infections vs. doses', legend=False) savefig('figs/chap12-fig04.pdf') $0\ 0.9888888888888889\ 0.26672740341296003\ 0.1875955039953746$ $1\ 0.977777777777779\ 0.26683150821044227\ 0.17458071882622528$ $2\;\; 0.96666666666666667\;\; 0.26711285672828566\;\; 0.16290983834857686$ $3 \ 0.9555555555555556 \ 0.2678657473308061 \ 0.15350834947768177$ $4 \quad 0.944444444444445 \quad 0.26982839154517113 \quad 0.1485650923152827$ 5 0.933333333333333 0.2746135281348078 0.15294595061102179 6 0.922222222222 0.28459609475799963 0.1749644150235239 7 0.91111111111111 0.3 0.21734316168444845 8 0.9 0.3154039052420003 0.2590710444883414 9 0.8888888888888 0.32538647186519215 0.27840288410342784 10 0.87777777777778 0.33017160845482885 0.2779145346228302 $11 \ 0.8666666666666667 \ 0.3321342526691939 \ 0.2673574966927026$ 12 0.855555555555556 0.3328871432717143 0.25279694563572175 Saving figure to file figs/chap12-fig04.pdf Total infections vs. doses 0.28 0.26 Total fraction infected 0.240.22 0.20 0.18 0.16 2 6 0 10 12 Doses of vaccine **Exercises** 1. Suppose the price of the vaccine drops to \$50 per dose. How does that affect the optimal allocation of the spending? 2. Suppose we have the option to quarantine infected students. For example, a student who feels ill might be moved to an infirmary, or a private dorm room, until they are no longer infectious. How might you incorporate the effect of quarantine in the SIR model? In [34]: price per dose = 50 max_doses = int(budget / price_per_dose) dose array = linrange(max doses, endpoint=True) for doses in dose array: fraction = doses / num students spending = budget - doses * price per dose system = make system(beta, gamma) add immunization(system, fraction) add hand washing(system, spending) results = run simulation(system, update func) infected sweep = sweep doses(dose array) plot(infected sweep) decorate(xlabel='Doses of vaccine', ylabel='Total fraction infected', title='Total infections vs. doses (\$50)', legend=False) savefig('figs/chap12-fig05.pdf') Saving figure to file figs/chap12-fig05.pdf Total infections vs. doses (\$50) 0.18 Total fraction infected 0.16 0.14 0.120.10 5 10 15 0 20 25 Doses of vaccine 1. answer When the price of the vaccine drops to 50 dollars per dose, doses of the vaccine become more economical. With that said, rather than 4 doses of the vaccine at 100 dollars for a total of 400 dollars and a total fraction infected of 0.16, we now allocate 500 dollars for 10 doses of the vaccine for a total fraction infected of 0.10. 2. answer When quarantine is an option for infected students, we have to make assumptions. For example, we could assume that all infected students that are put into quarantine, obey orders, do not break quarantine, and so the virus has little-to-no opportunity to spread or we can assume that a certain percent of students will break quarantine regardless and so we perform a sweep on percent of students that break quarantine (ie. midpoint of 20%) and observe the impact on total infected. Unless we assume that no students obey quarantine orders, the total percent infected will go down in proportion to the percent of students that obey orders. For modeling this, I would create an add_quarantine as well as a sweep_quarantine function to be incorporated in the overall model. Quarantine would reduce the percent that trickle forward from the state of S (susceptible) into the state of I (infected) and down the line into a state of R (recovered). Chapter 13 Sweeping beta #make a range of values for beta with a constant gamma beta_array = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0 , 1.1] gamma = 0.2#wrap a loop in a function and return SweepSeries object def sweep beta(beta array, gamma): """Sweep a range of values for beta. beta_array: array of beta values gamma: recovery rate returns: SweepSeries that maps from beta to total infected sweep = SweepSeries() for beta in beta array: system = make system(beta, gamma) results = run_simulation(system, update_func) sweep[system.beta] = calc_total_infected(results) infected_sweep = sweep_beta(beta_array, gamma) label = 'gamma = ' + str(gamma) plot(infected_sweep, label=label) decorate(xlabel='Contact rate (beta)', ylabel='Fraction infected') savefig('figs/chap13-fig01.pdf') Saving figure to file figs/chap13-fig01.pdf 1.0 gamma = 0.2 0.8 Fraction infected 0.6 0.4 0.2 0.0 0.2 1.0 0.4 0.6 8.0 Contact rate (beta) Sweeping gamma #create an array of values for gamma $gamma_array = [0.2, 0.4, 0.6, 0.8]$ plt.figure(figsize=(7, 4)) for gamma in gamma array: infected_sweep = sweep_beta(beta_array, gamma) label = 'gamma = ' + str(gamma) plot(infected sweep, label=label) decorate(xlabel='Contact rate (beta)', ylabel='Fraction infected', loc='upper left') plt.legend(bbox to anchor=(1.02, 1.02)) plt.tight layout() savefig('figs/chap13-fig02.pdf') Saving figure to file figs/chap13-fig02.pdf 1.0 gamma = 0.2 gamma = 0.4 8.0 gamma = 0.6 Fraction infected gamma = 0.8 0.6 0.4 0.2 0.0 0.2 0.4 1.0 0.6 8.0 Contact rate (beta) **Exercise** Suppose the infectious period for the Freshman Plague is known to be 2 days on average, and suppose during one particularly bad year, 40% of the class is infected at some point. Estimate the time between contacts. In [41]: #make a range of values for beta with a constant gamma beta array = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1]gamma = 0.5#wrap a loop in a function and return SweepSeries object def sweep beta(beta array, gamma): """Sweep a range of values for beta. beta array: array of beta values gamma: recovery rate returns: SweepSeries that maps from beta to total infected sweep = SweepSeries() for beta in beta array: system = make_system(beta, gamma) results = run simulation(system, update func) sweep[system.beta] = calc_total_infected(results) return sweep infected sweep = sweep beta(beta array, gamma) label = 'gamma = ' + str(gamma) plot(infected sweep, label=label) decorate(xlabel='Contact rate (beta)', ylabel='Fraction infected') savefig('figs/chap13-fig03.pdf') Saving figure to file figs/chap13-fig03.pdf gamma = 0.58.0 0.6 Fraction infected 0.4 0.2 0.0 0.2 0.4 0.6 8.0 1.0 Contact rate (beta) From the above plot, it appears that 0.4 fraction infected occurs at a contact rate (beta) of ~0.6. We use np.interp() to find the exact value and solve for tc: In [48]: beta_d = np.interp(0.4, infected_sweep.values, beta_array) tc = 1 / beta d #derived from beta equation round(tc,2) Out[48]: 1.59 We see that the time between contacts (tc) appears to be ~1.59 days.