SIMIODE Challenge Using Differential Equations Modeling (SCUDEM). Training Session 2: Crash Course in Modeling

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   - Equations that mimic the dynamics of complex biological systems to provide evidences on its behavior.

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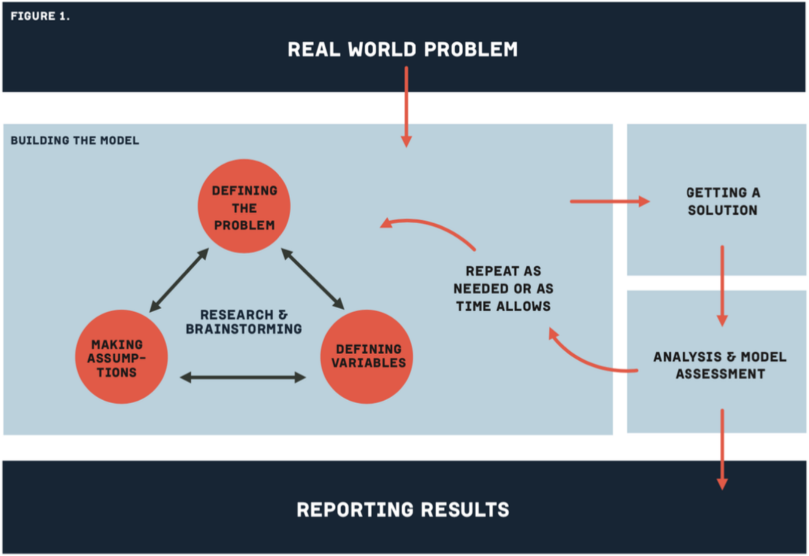
1. Mathematical descriptions of evolving biological phenomena
   - Equations that mimic the dynamics of complex biological systems to provide evidences on its behavior.
2. Theoretical representation of real-world situations
   - A conceptual framework that helps us understand and predict the behavior of a particular real - life system.
3. Variable-parameter-output linker
   - A structure that links input variables, controllable parameters, and output variables to explain or forecast their relationships.
4. Consider the relation

$$Y = aX + b \tag{1}$$

   - Is (1) a model? Write down your answer now and come back to it at the end of this training

Mathematical Models life cycle



Defining the Problem

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- Modeling problems are often open ended.
- Goal: Refine the conceptual idea into a concise problem statement which will indicate exactly what the output of your model will be.
- Defining the problem generally requires:
  - Literature review and brainstorming
  - Define the model variables (outputs & inputs) and control parameters
  - The (possible) form of relationship between those variables
  - At each step during the model formulation, it is critically important to record the assumptions
  - Refined problem starts with,“How”, “Why”, “Which”,

Defining the Problem Example:

- Suppose we want to investigate the interactions between fox and rabbit populations.

Conceptual illustration of the interaction Fox-Rabbit (Srinivasarao Thota, 2019)

Defining the Problem Example:

- Start with literature review: to help learn about fox and rabbit populations from a biological standpoint and how other researchers (if any) have modeled their relationships.

- This review revealed that this relationship can be modeled using Lotka-Volterra models
- Our research provides us with the background needed to form a specific goal for our model.
- We choose to focus on the number of rabbits ($:= R$) in an area, and the number of foxes ($:= F$) in the same area over time.
- A refined problem statement is:
  - What is the long term behavior of rabbit populations in a region where they are the primary prey for foxes?

Making Assumptions

- Assumptions help simplify the problem and sharpen the focus.
- Help deciding which factors are most important.

Making Assumptions

- Assumptions help simplify the problem and sharpen the focus.
- Help deciding which factors are most important.
- You should do some preliminary research and may find data to help you make assumptions. In the absence of relevant data, make a reasonable assumption and justify the assumption in your write-up.
- Different assumptions can lead to different, equally valid models at different mathematical levels.

Making Assumptions Example

What assumptions could we make about our model?

Making Assumptions Example

Some possible assumptions:

- The growth rate of the rabbit population is proportional to its size (exponential growth).
- The rabbits are the only food source for the foxes.
- In the absence of a food source, the death rate of the fox population is proportional to its size (exponential decay).

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- In the absence of a food source, the death rate of the fox population is proportional to its size (exponential decay).
- The interactions between the two species do not change with the seasons.
- There is no spatial component to the interactions.
- The two populations are homogeneous.

Defining Variables

- What are the primary factors influencing the phenomenon you are trying to understand?
- Can you list those factors as quantifiable variables with specified units?
- You may need to distinguish between independent variables, dependent variables, and model parameters.

Defining Variables Example of Foxes and Rabbits

Independent variables:

- R: number of rabbits
- F: number of foxes

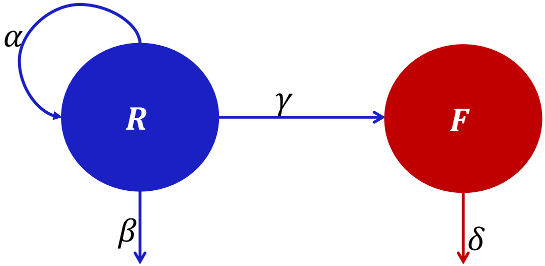
Dependent variable:

- time (in day, week, month, $\cdots$)

Parameters: **Be careful with units.**

- $0 < \alpha$: rabbit birth rate
- $0 < \beta$: rabbit death rate from predation
- $0 < \gamma$: fox birth date from predation
- $0 < \delta$: fox death rate

Model formulation



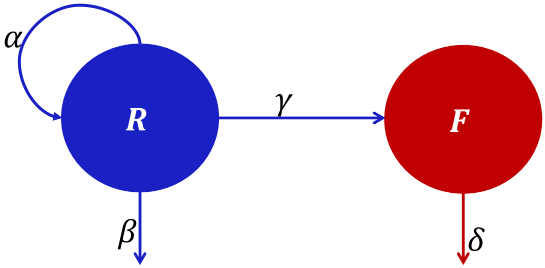
Flow diagram of the model of the relationship Fox-Rabbit populations. Ont his figure, α is rabbits birth rate, β is their death rate due to predation by foxes, γ is the fox growth rate due to the predation, and δ is fox death rate.

Model equations:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \textbf{GAIN} - \textbf{LOSE}, \tag{2}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \textbf{GAIN} - \textbf{LOSE}. \tag{3}$$

Model formulation



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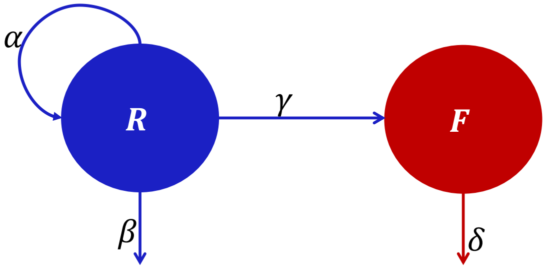

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Model equations:

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \textbf{GAIN} - \textbf{LOSE} = \underbrace{\alpha R}_{\textbf{GAIN}} - \underbrace{\beta RF}_{\textbf{LOSE}} \tag{4}$$

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \textbf{GAIN} - \textbf{LOSE} = \underbrace{\gamma RF}_{\textbf{GAIN}} - \underbrace{\delta F}_{\textbf{LOSE}} \tag{5}$$

Getting Solutions

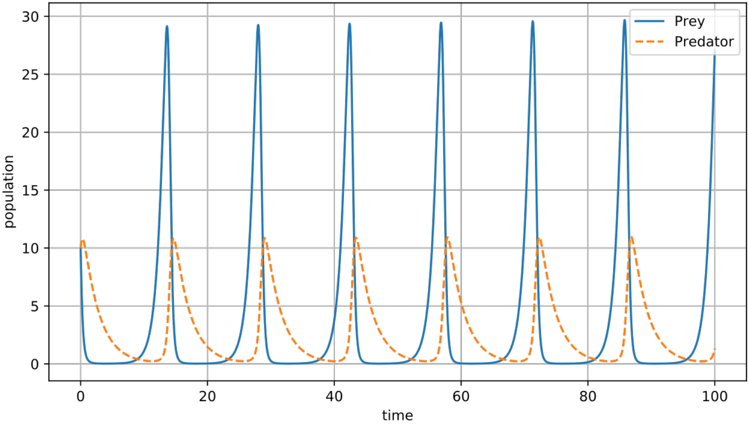
- There is often more than one way to tackle a problem, so just start and see what happens.
- If you don't immediately know how to solve the problem at hand, ask yourself:
  - Have I seen this type of problem before? If so, how did I solve it? If not, how is this problem different?
  - Do I have a single unknown, or is this a multivariable problem with many interdependent variables?
  - Is the model linear or nonlinear?
  - Am I solving a system of equations simultaneously, or can I solve sequentially?
  - What software or computational tools are available to me? Would a graph or other visual schematic help provide insight?

Getting Solutions

- How to find the value of each parameters?
  - Found some in the literature
  - Estimated some using their definition and literature review
  - Fit you model to available data (using LSQ for instance)
- What can you learn from your model?
- Does it answer the questions asked in the problem? Determining a solution may involve
  - Pencil and paper calculations
  - Evaluating a function
  - Running simulations
  - Solving an equation
- It might be helpful to use software or some other computational technology.

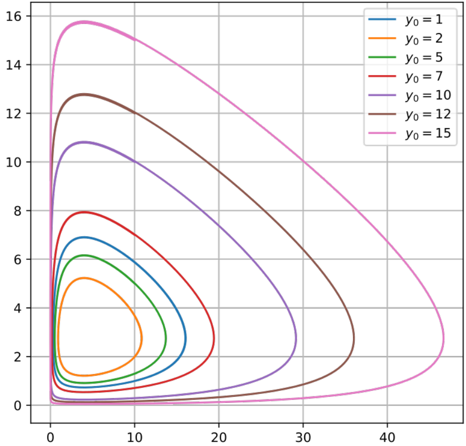
Getting Solutions Example [1]

- Solve by hand (Sometime, these are not useful)
- Solve numerically



Getting Solutions Example [1]

- Qualitative analysis
  - Equilibria, nullclines, and stability analysis
  - Bifurcation analysis
  - Phase planes, etc.



Getting Solutions Example

The time independent solution of the model is obtained by setting the LHS to zero. That is:

$$0 = \alpha R - \beta RF$$
$$0 = R(\alpha - \beta F)$$

This yield the Equilibria : $(R, F) = (0, 0)$ or $(R, F) = (\frac{\delta}{\gamma}, \frac{\alpha}{\beta})$

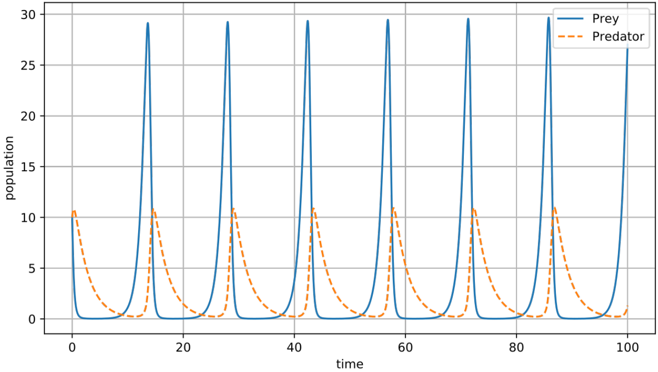
From here, we can linearize the system and find the eigenvalues of its Jacobian at each equilibrium point to determine their stability.

Analysis and Model Assessment

In the end, one must step back and analyze the results to assess the quality of the model.

- What are the strengths and weaknesses of the model?
- Always examine the output you get from your model and ask yourself if it makes sense. If your answer doesn't make sense, verify that you haven't made a mistake in implementing your model.
- Are there certain situations when the model doesn't work?
- How sensitive is the model if you alter the assumptions or change model parameters values?
- Is it possible to make (or at least point out) possible improvements?

Analysis and Model Assessment Example [1]



$$\frac{\mathrm{d}R}{\mathrm{d}t} = \alpha R - \beta R F$$
$$\frac{\mathrm{d}F}{\mathrm{d}t} = \gamma R F - \delta F$$

Do you have any ideas for how we could improve this model? Does anything seem unrealistic?

Analysis and Model Assessment Example

- One possible improvement involves the rabbit growth term.
- We could change our assumption from exponential growth to logistic growth.
- This would account for limited food and other resources, since populations generally cannot grow without bound.
- With this change, we introduce a carrying capacity κ that behaves like a horizontal asymptote.

$$\frac{\mathrm{d}R}{\mathrm{d}t} = \alpha R \left(1 - \frac{R}{\kappa}\right) - \beta RF$$
$$\frac{\mathrm{d}F}{\mathrm{d}t} = \gamma RF - \delta F$$

- After making this improvement, we will restart the modeling cycle until we are happy with our results.

Reporting the Results

Your model might be awesome, but no one will ever know unless you are able to explain how to use or implement it.

- Take notes throughout your entire modeling process so that you do not leave out anything important, especially assumptions made along the way.
- Give yourself enough time to focus on the writing process and to proofread the report.
- Keep in mind that this is a technical document, not a story about your modeling experience.
- Follow the guidelines for MCM/ICM for the summary report and paper.
- Pat yourself on the back for your accomplishments!

Wikipedia contributors.
Lotka–volterra equations — Wikipedia, the free encyclopedia.
https://en.wikipedia.org/w/index.php?title=Lotka%E2%80%93Volterra_equations&oldid=1174565138, 2023.

1. Overview of Mathematical Modeling
2. A Modeling Example

Unraveling the dynamics of the Omicron and Delta variants of the 2019 coronavirus in the presence of vaccination, mask usage, and antiviral treatment

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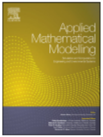
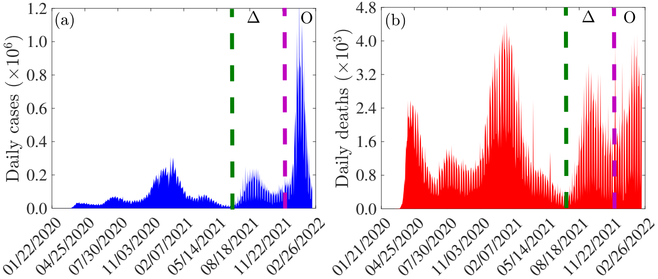


Unraveling the dynamics of the Omicron and Delta variants of the 2019 coronavirus in the presence of vaccination, mask usage, and antiviral treatment

Check for updates

Calistus N. Ngonghala[a,b,*], Hemaho B. Taboe[a,c], Salman Safdar[d], Abba B. Gumel[e,f,g]

What is the problem ?



Data for COVID-19 daily (a) cases and (b) mortality for the United States for the period of the COVID-19 pandemic from January 2020 to February 2022. The data is obtained from the Johns Hopkins University COVID-19 Dashboard. The burden of the Delta variant is in the regions between the green and purple dashed vertical lines (denoted by Δ), while that of the Omicron variant is in the region to the right of the dashed purple vertical line (denoted by O). (Calistus et. al, 2023)

The context/ problem and how our model will help to deal with ?

- FDA-approved vaccines in the United States were designed against the original SARS-Cov-2 strain, and only offer cross-protective efficacy against the variants

- How the emerging of the new variant will affect the dynamic of COVID19 in face of current policies (vaccination, isolation, mask usage,...) in place ?

- What will be the suitable responses to the new context ?

Model formulation: State variables

State var	Description
S	Unvaccinated susceptible individuals
V_f	Fully-vaccinated but not boosted
V_b	Fully-vaccinated individuals & booster dose
E_j	Exposed ($j = d :=$ Delta,$j = o :=$ Omicron,)
P_j	Pre-symptomatically infectious individuals
A_j	Asymptomatically-infectious individuals
Q_j	Detected (positive)
I_{j1}	Symptomatically-infectious within the 1st 5 days
I_{j2}	Symptomatically-infectious survived $>$ 5d symptoms
H_j	Population of hospitalized individuals
R_j	Recovered and successfully treated
N	Total population $N = S + V_f + V_b + E_d + P_d + A_d + Q_d + I_{d1} + I_{d2} + H_d + R_d + +E_o + P_o + A_o + Q_o + I_{o1} + I_{o2} + H_o + R_o)$

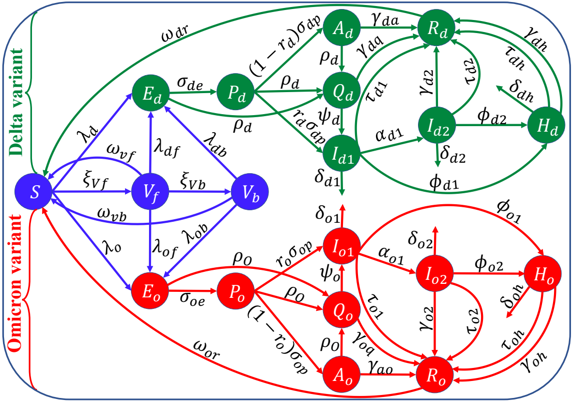
The goal and method

- To assess the qualitative dynamics of the two dominant SARS-CoV-2 variants co-circulating in the US (Delta and Omicron) and provide quantitative information as guidance for Politics

- How ?

- Develop a mathematical model :
  - that incorporate the two variants and the policies in place
  - Analyse it analytically and numerically along with the daily cases .

Model formulation (Conceptualization)



Flow diagram of the model. Although recruitment into the population and natural deaths occur (at the rate Λ and μ, respectively), these rates are not illustrated in the flow diagram to make it less crowded and easier to follow. The state variables and parameters are described in Tables S1 and S2 of the Supplementary Information (SI).(Calistus et. al, 2023)

- ASSUMPTIONS:

Description of the parameters (complete list)

Param	Description
Λ	Recruitment rate
β_{jk}	Effective contact rate for P_j, A_j , I_{jk}, and H_j
q_1	Modification parameter accounting for the proportion of individuals in Q_j who are infectious
ξ_{vf}	Rate at which susceptible individuals are fully-vaccinated
ξ_{vb}	Rate at which fully-Vaccinated receive the booster
ε_{jf}	Cross-protective efficacy of the vaccine
ε_{jb}	Cross-protective efficacy of the vaccine (booster)
ω_{jf}	Rate of waning of vaccine-derived immunity

(See the ref paper for the complete list of the parameters)

Assumptions made in the formulation of the model

(a) Only the Delta and Omicron variants were co-circulating (i.e., they were the most predominant of all the variants of concern at the time of this study).

(b) A well-mixed population, where every individual is equally likely to mix with every other individual in the community.

(c) Vaccines only offer cross-protective efficacy against the variants

(d) Natural immunity and vaccine-derived immunity for fully-vaccinated and boosted humans wane over time.

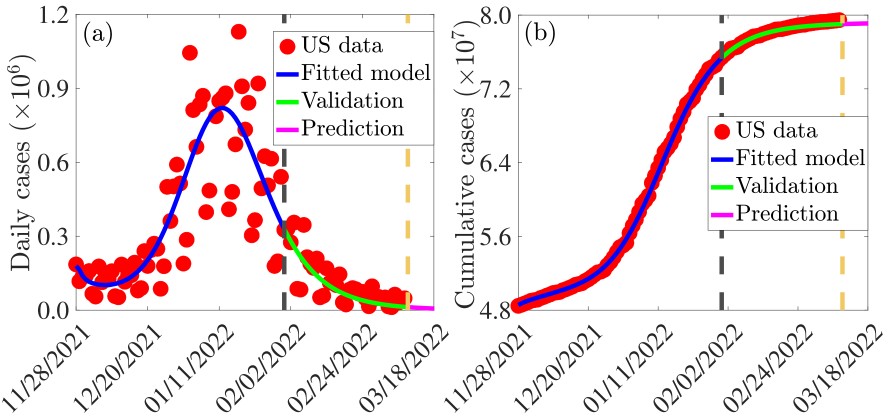
The mathematical form of the model (Equations)

$$
\begin{aligned}
\dot{S} &= \Lambda + \omega_{vf}V_f + \omega_{vb}V_b + \omega_{dr}R_d + \omega_{or}R_0 - (\lambda_d + \lambda_o + \xi_{vf} + \mu)S,\\
\dot{V}_f &= \xi_{vf}S - (\lambda_{df} + \lambda_{of} + \xi_{vb} + \omega_{vf} + \mu)V_f,\\
\dot{V}_b &= \xi_{vb}V_f - (\lambda_{db} + \lambda_{ob} + \omega_{vb} + \mu)V_b,\\
\dot{E}_j &= \lambda_j S + \lambda_{jf}V_f + \lambda_{jb}V_b - (\sigma_{je} + \rho_j + \mu)E_j,\\
\dot{P}_j &= \sigma_{je}E_j - (\sigma_{jp} + \rho_j + \mu)P_j,\\
\dot{A}_j &= (1 - r_j)\sigma_{jp}P_j - (\gamma_{ja} + \rho_j + \mu)A_j,\\
\dot{Q}_j &= \rho_j(E_j + P_j + A_j) - (\gamma_{jq} + \psi_j + \mu)Q_j,\\
\dot{I}_{j1} &= r_j\sigma_{jp}P_j + \psi_j Q_j - (\tau_{j1} + \alpha_{j1} + \phi_{j1} + \mu + \delta_{j1})I_{j1},\\
\dot{I}_{j2} &= \alpha_{j1}I_{j1} - (\tau_{j2} + \gamma_{j2} + \phi_{j2} + \mu + \delta_{j2})I_{j2},\\
\dot{H}_j &= \phi_{j1}I_{j1} + \phi_{j2}I_{j2} - (\tau_{jh} + \gamma_{jh} + \mu + \delta_{jh})H_j,\\
\dot{R}_j &= \gamma_{ja}A_j + \gamma_{jq}Q_j + \tau_{j1}I_{j1} + (\tau_{j2} + \gamma_{j2})I_{j2} + (\tau_{jh} + \gamma_{jh})H_j\\
&\quad -(\omega_{jr} + \mu)R_j, \text{ with } j \in \{d, o\}.
\end{aligned}
\tag{6}
$$

Model Fitting and Parameter Estimation (key points)

- Some of the parameters are fixed based on their availability and their importance
- The key unknown parameters and which were estimated are:
  - the effective community transmission rates
  - the rate at which individuals are fully-vaccinated , and
  - the rate at which fully-vaccinated individuals are boosted
- These parameters were estimated by fitting the model (6) to the confirmed daily COVID-19 case data for the US from 11/28/2021 to 01/31/2022 LSQ method implemented in *MATLAB2022b*.

Model Fitting and validation



(a) Time series illustration of the least squares fit of the model (6), showing the model's output for the daily cases (blue curve) compared to the observed daily confirmed cases for the United States (red dots) from November 28, 2021 to January 31, 2022 (segment to the left of the dashed vertical black line). (b) Simulation result of the model (6), showing cumulative COVID-19 cases for the United States as a function of time, using the fixed and estimated baseline parameter values given in Tables S3 and S4. The segment from February 1, 2022 to March 18, 2022 (i.e., solid green and magenta curves or the entire segment to the right of the dashed black vertical line) illustrates the performance of the model (6) in predicting the daily and cumulative cases in the United States.

Main results (output): (1) vaccination reproduction number

The *vaccination reproduction number* of the model, with respect to variant j (with $j \in \{d, o\}$), denoted by $\mathbb{R}_{jv}$, can be obtained using the *next generation operator method* [**?**, **?**]. It is given by the following expression:

$$\mathbb{R}_{jv} = \mathbb{R}_{jp} + \mathbb{R}_{ja} + \mathbb{R}_{jq} + \mathbb{R}_{j1} + \mathbb{R}_{j2} + \mathbb{R}_{jh}, \tag{7}$$

where,

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where,

$$\begin{aligned}
\mathbb{R}_{jp} &= \frac{\beta_{jp}\sigma_{je}G_{j1}G_{j2}G_{ja}G_{jq}G_{jh}}{G_{je}G_{jp}G_{ja}G_{jq}G_{j1}G_{j2}G_{jh}}H^*, \\
\mathbb{R}_{ja} &= \frac{\beta_{ja}\sigma_{je}\sigma_{jp}G_{jq}G_{j1}G_{j2}G_{jh}(1-r_j)}{G_{je}G_{jp}G_{ja}G_{jq}G_{j1}G_{j2}G_{jh}}H^*, \\
\mathbb{R}_{jq} &= \frac{\beta_{jq}G_{j1}G_{j2}G_{jh}\rho_j\{[G_{ja}+(1-r_j)\sigma_{jp}]\sigma_{je}+G_{ja}G_{jp}\}}{G_{je}G_{jp}G_{ja}G_{jq}G_{j1}G_{j2}G_{jh}}H^*,
\end{aligned} \tag{8}$$

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\mathbb{R}_{jq} &= \frac{\beta_{jq}G_{j1}G_{j2}G_{jh}\rho_j\{[G_{ja}+(1-r_j)\sigma_{jp}]\sigma_{je}+G_{ja}G_{jp}\}}{G_{je}G_{jp}G_{ja}G_{jq}G_{j1}G_{j2}G_{jh}}H^*,
\end{aligned} \tag{8}$$

Notice that here I did not display all the formula

Main results (output): (1) DFE of the model locally asymptotically stable

Theorem

The DFE of the model (6) *is locally-asymptotically stable if* $\mathbb{R}_c < 1$*, and unstable if* $\mathbb{R}_c > 1$.

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Theorem

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- The epidemiological implication of Theorem 1 is that a small influx of infected individuals will not generate a large outbreak of the SARS-CoV-2 virus in the community.

Main results (output): (1) DFE of the model locally asymptotically stable

Theorem

The DFE of the model (6) *is locally-asymptotically stable if* $\mathbb{R}_c < 1$*, and unstable if* $\mathbb{R}_c > 1$.

- The epidemiological implication of Theorem 1 is that a small influx of infected individuals will not generate a large outbreak of the SARS-CoV-2 virus in the community.

- Thus, the SARS-CoV-2 pandemic can be controlled effectively if the control reproduction number of the model ($\mathbb{R}_c$) can be brought to a value less than one (and maintained), provided the initial number of infected individuals is small enough

Main results (output): (2) Vaccine-derived Herd Immunity Threshold

$$f_v = \frac{1}{\varepsilon_{jv}}\left(1 - \frac{1}{\mathbb{R}_{0j}}\right) = f_v^c. \tag{9}$$

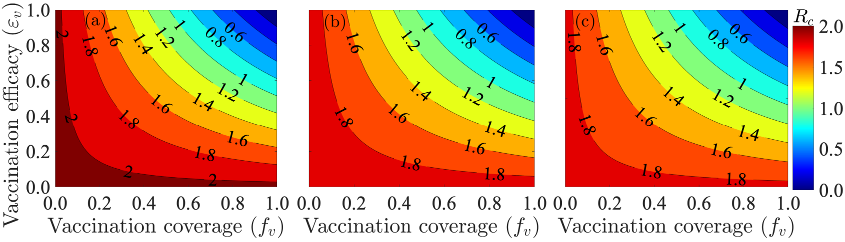
Main results (output): (2) Vaccine-derived Herd Immunity Threshold

$$f_v = \frac{1}{\varepsilon_{jv}}\left(1 - \frac{1}{\mathbb{R}_{0j}}\right) = f_v^c. \tag{9}$$

Theorem

The DFE of Model (6) is locally-asymptotically stable if $f_v > f_v^c (\mathbb{R}_c < 1)$, and unstable if $f_v < f_v^c (\mathbb{R}_c > 1)$.

Main results (output): (2) Vaccine-derived Herd Immunity Threshold



Contour plots of the control reproduction number of the model (6), $\mathbb{R}_c$, as a function vaccine coverage (i.e., proportion of fully-vaccinated individuals, f_v) and cross-protective vaccine efficacy against the variants ($\varepsilon_v = \min(\varepsilon_{vf}, \varepsilon_{vb})$) for the case when (a) mask coverage is maintained at its baseline value, (b) surgical mask is prioritized and the coverage in its usage is increased by 10% from its baseline value, (c) N95 mask is prioritized and the coverage in its usage is increased by 10% from its baseline value. The values of all other parameters used in the simulations are as given by the baseline values in Tables S3 and S4.

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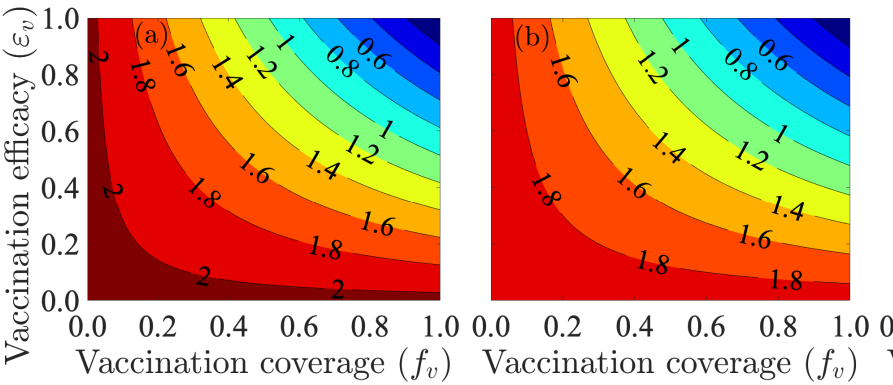

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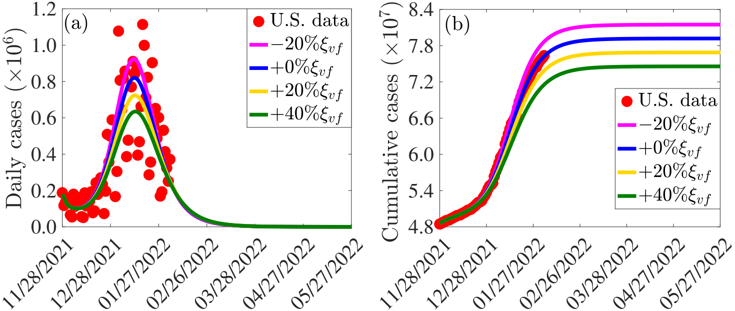
Main results (output): (3) Impact of vaccine-efficacy



Simulations of the model (6) showing the effect of increases or decreases in fully-vaccinated vaccination coverage rate (ξ_{vf}) on the COVID-19 pandemic in the United States. (a) Daily cases, as a function of time, for various values of the fully-vaccinated vaccination coverage rate. (b) Cumulative cases, as a function of time, for various values of the fully-vaccinated vaccination coverage rate. The values of all other parameters used in these simulations are given by the baseline values in Tables S3 and S4.

Conclusion

- The constituent reproduction number:
  - $R_{cd} = 0.28$
  - $R_{co} = 0.96$
- Vaccine-derived herd immunity: can be achieved if at least 68% of the population is fully-vaccinated with either the Pfizer or Moderna vaccine

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  - $R_{cd} = 0.28$
  - $R_{co} = 0.96$
- Vaccine-derived herd immunity: can be achieved if at least 68% of the population is fully-vaccinated with either the Pfizer or Moderna vaccine
- We showed that the proportion of individuals who need to be fully-vaccinated to achieve herd immunity decreases with increasing coverage of face masks in the community

References

This presentation was extracted from:

Ngonghala, C. N., Taboe, H. B., Safdar, S., & Gumel, A. B. (2023). Unraveling the dynamics of the Omicron and Delta variants of the 2019 coronavirus in the presence of vaccination, mask usage, and antiviral treatment. Applied mathematical modelling, 114, 447-465.