



Andrew Becker

PhD Candidate

Computational Mathematics

Introduction to The Spanish Lady Problem



Andrew Becker

AI Statement

9/3/20XX

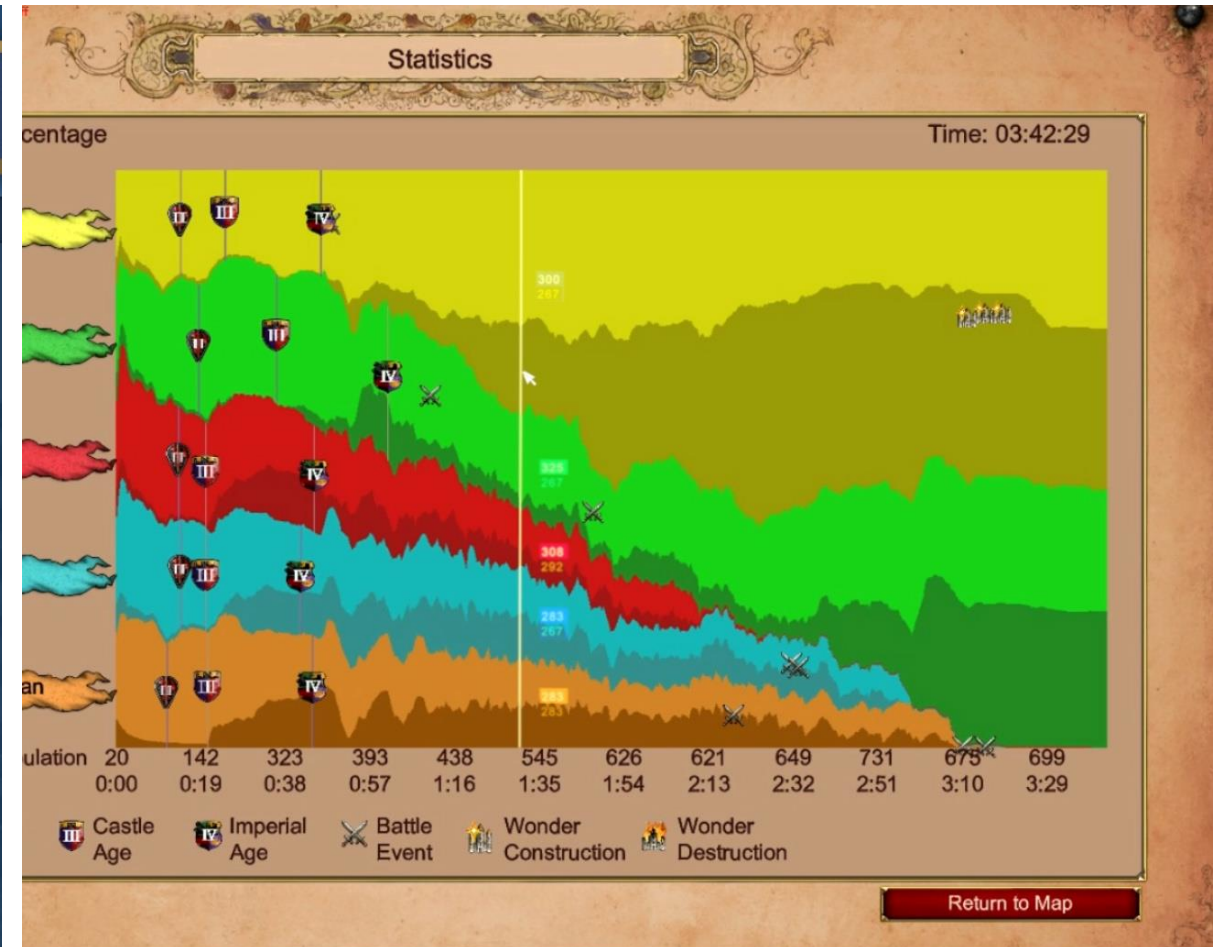
Presentation Title



Who am I?

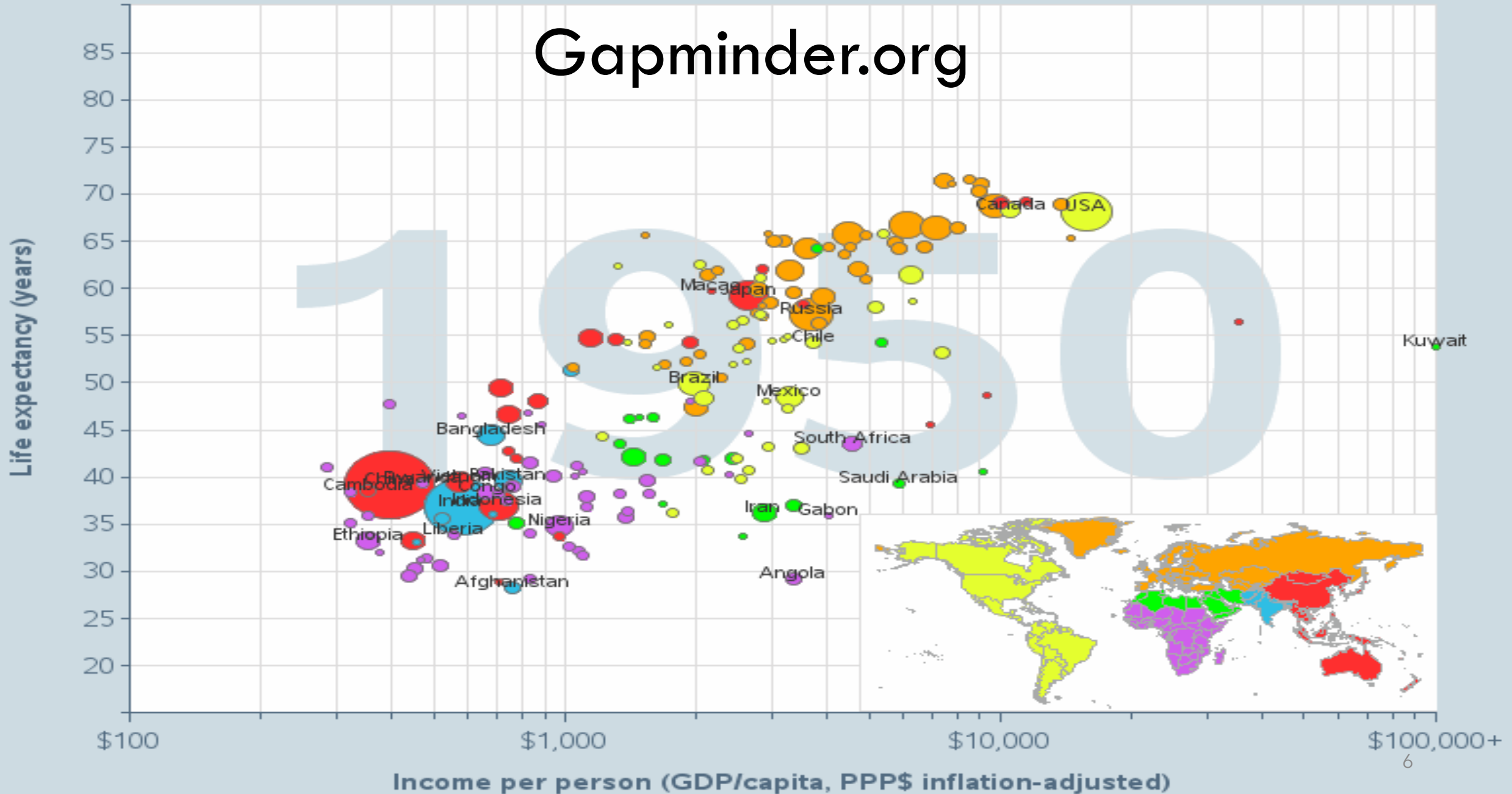


Civilization & Age of Empires Game Over Screen Graphs



Wealth & Health of Nations

Gapminder.org



Project Development

9/3/20XX

Presentation Title

Computational Science Project Schedule

Week of June 7

- Defining the project scope and goals.
 - Clarity and feasibility of the project scope and goals.
 - Completeness of the project proposal

For June 21

- Literature review and research on existing methods
 - Breadth and depth of the literature review
 - Relevance of the literature to the project
 - Evidence of understanding the existing methods

For June 30

- Developing the computational method/algorithm:
 - Quality and completeness of the implementation
 - Evidence of testing and debugging of the method/algorithm
 - Evidence of understanding and implementation of the method/algorithm

Future Goals and Objectives

July 14

- Testing and optimization of the method/algorithm:
 - Evidence of understanding and implementation of optimization techniques
 - Evidence of testing and debugging of the optimization techniques
 - Scalability and computational efficiency of the method.

July 28

- Verification and validation of the method/algorithm:
 - Evidence of understanding and implementation of verification and validation techniques
 - Evidence of testing and debugging of the optimization techniques
 - Quality and completeness of the results

August 11

- Final Report/Presentation Preparation
 - Clarity and organization of the final report/presentation
 - Quality and completeness of the visual aids
 - Effectiveness of the delivery



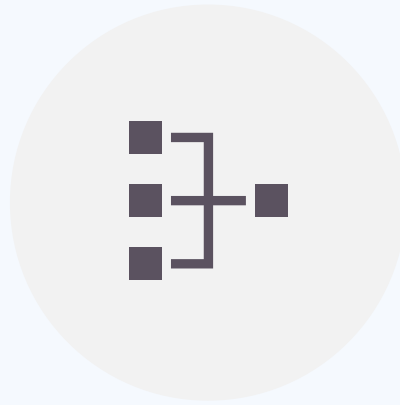
Echoes of the Spanish Lady: Navigating the Maze of Epidemic Models

A Look at the 1918 Flu Epidemic Models

Introduction



MATHEMATICAL MODELING
OF INFECTIOUS DISEASES

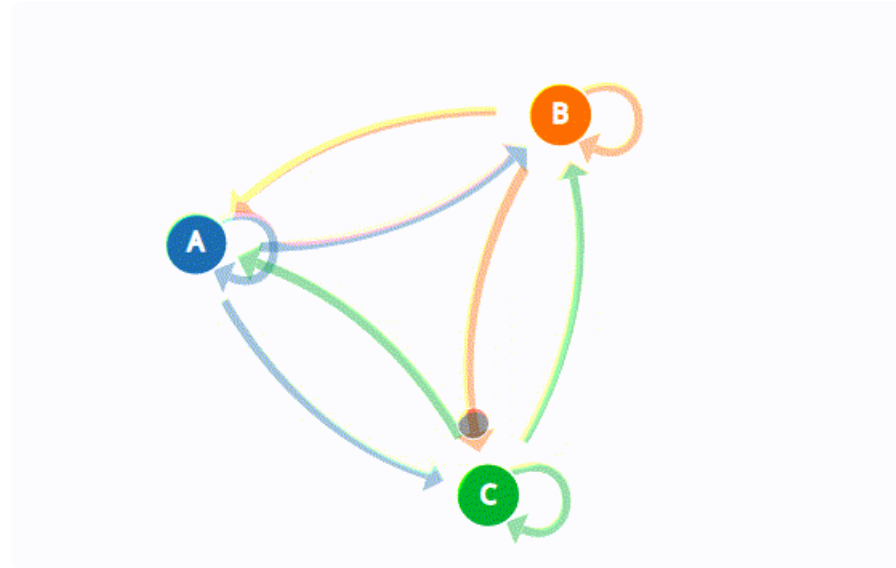


KERMACK-MCKENDRICK
MODEL



CELLULAR AUTOMATA AND
MARKOV CHAINS

Markov Chain Example & Walk





The Corrupted Blood Incident

09/13/2005, Azeroth: Zul'Gurub (World of Warcraft)

- Release of new gaming content: Blood God "Hakkar the Soulflayer" for high level Avatars
- During battle, Hakkar cast the spell "corrupted blood" (CB) on random Avatars
- CB hit with severe damage once plus additional damage over time; duration 10 seconds
- CB spread from Avatar to Avatar: INFECTIOUS
- CB was never meant to leave Zul'Gurub, but: - Infected Avatars could teleport to cities - Hunters could dismiss their infected pets in Zul'Gurub and later call them back - still infected- in cities



Markov Walks

I-A. Contextual Explanation Touch a little more on where Markov chains are practically used. For instance, weather models, stock price predictions, Google's PageRank algorithm, and natural language processing can be examples.

I-B. Graphical Illustrations Including animated visuals of the restaurant serving different dishes and the Markov chain evolving would make it even more engaging.

I-C. Clarify Terminology While you've done a good job explaining most terms, some might benefit from a brief aside or definition. For example, when you first mention 'states', it could help to clarify that it's just a term for the different situations or outcomes in our model (like "hamburger day").

I-D. Python Script Mention Mentioning the python script was a great way to demonstrate practical application. It would be helpful to either showcase snippets of the script or provide a link for viewers who might want to see it in action or try it themselves.

I-E. Linear Algebra Part This section is crucial, but it's also where some viewers might get lost, especially if they're not familiar with linear algebra concepts. Taking a bit more time here, maybe with an extended example or more visuals, can help cement understanding.

I-F. Concluding Thoughts It might be useful to wrap up with a quick recap, highlighting the main points again, and maybe pointing to advanced topics related to Markov chains for those interested in diving deeper

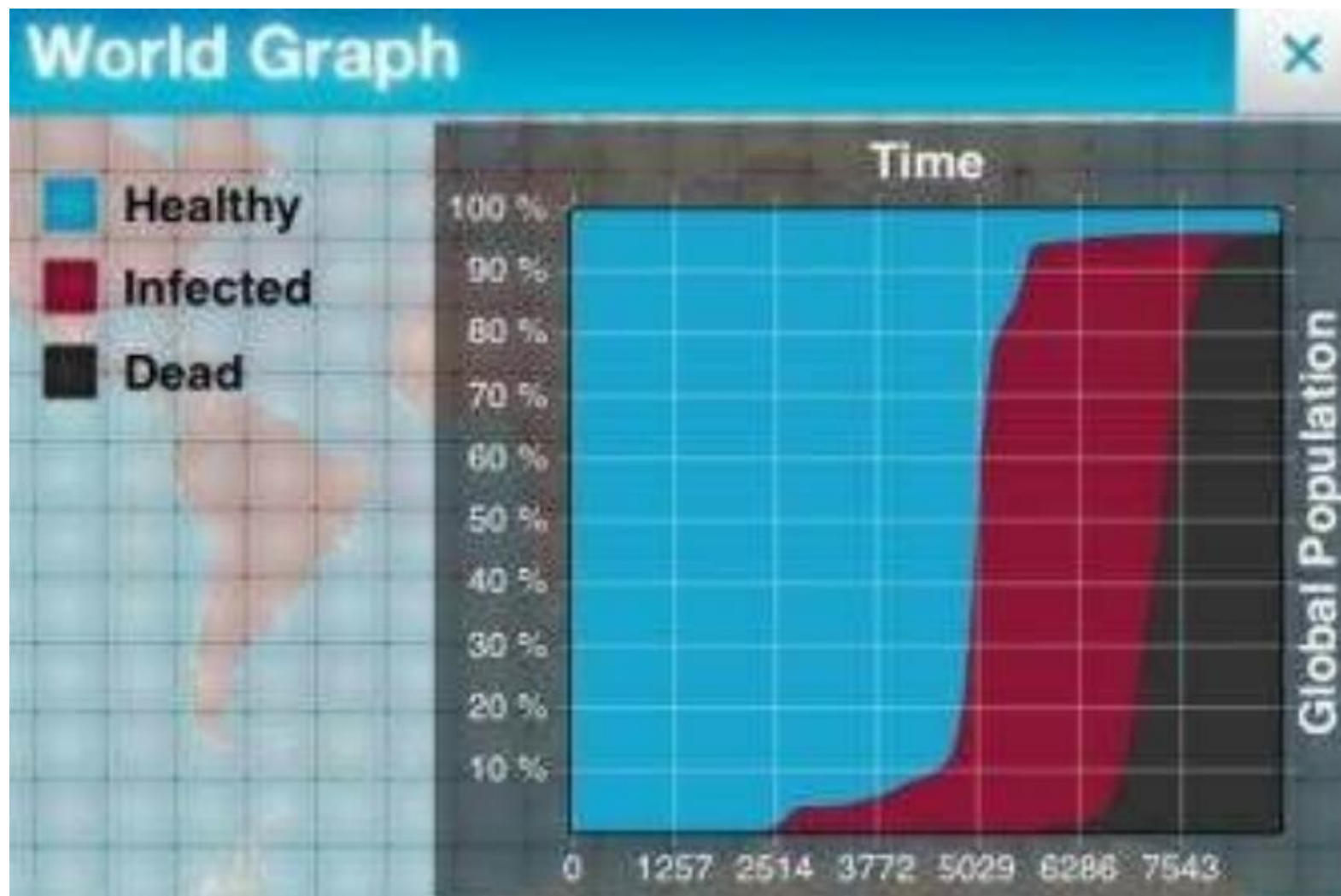


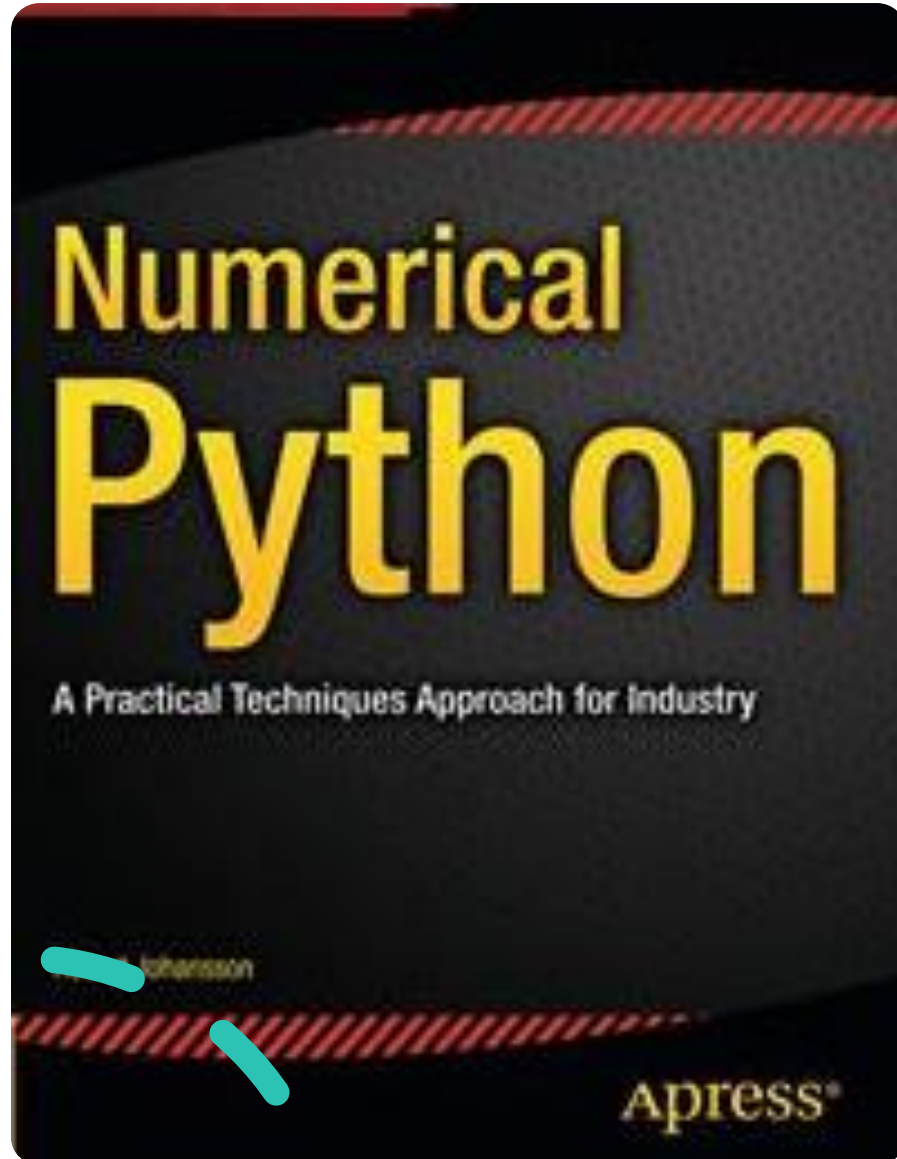
Background



Project Focus

Plague Inc., Video Game





Additional Resources

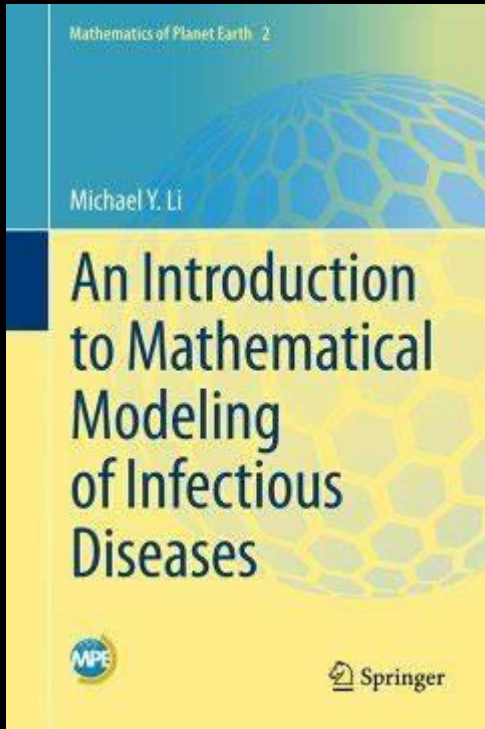
[Numerical Python](#) Robert Johansson

The Extrapolation of First Order
Methods for Parabolic Partial
Differential Equations

J.D. Lawson and J. Ll. Morris SIAM 1978

Recent Progress of the combinatorial
diameter of polytopes and simplicial
complexes

Francisco Santos Jul 2013



Mathematical Modeling of Infectious Diseases

Keywords: Infectious diseases, Mathematical modeling, Epidemiology, Public health

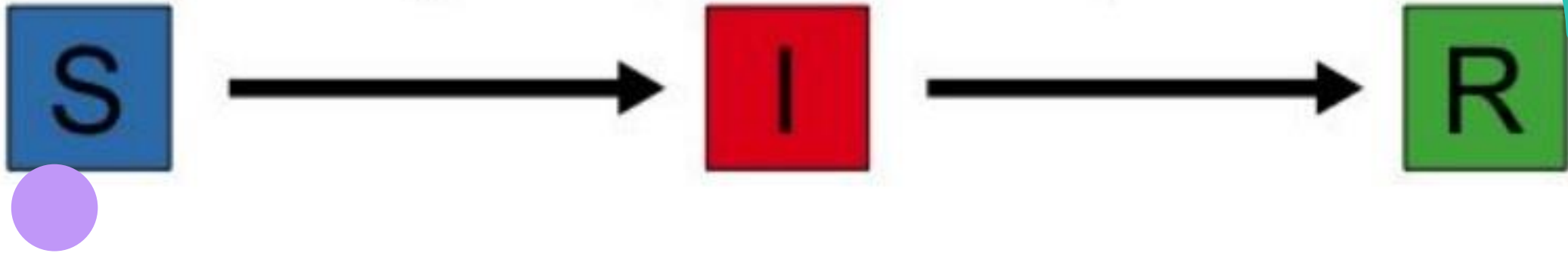


Susceptible- set of people in the model who have not had the disease.

Infected- set of people in the model who have had the disease currently

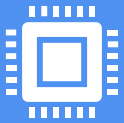
Recovered- set of people in the model who have recovered from the disease.

SIR (Susceptible, Infectious, Recovered)



Basic SIR Model

Project Focus



1. Leveraging cellular automata for simulating epidemic models, specifically the SIR (Susceptible, Infected, Recovered) and SEIR (Susceptible, Exposed, Infected, Recovered) models.



2. The goal is to compare the efficiency and accuracy of these models with traditional techniques like Markov Chains, to develop more efficient and practical tools for simulating disease spread.



3. Additionally, the project aims to explore the use of machine learning for model refinement and seeks potential applications of these models beyond public health, such as in game development.

Project Description & Scientific Problem



The scientific problem being addressed in this project is the efficient and accurate simulation of epidemic models, specifically the SIR and SEIR models, using parallel processing techniques and cellular automata.



Traditional techniques like Markov Chains can be computationally intensive and might not scale efficiently. The project aims to overcome the challenge of refining these models to better fit real-world observations without overfitting.



Ultimately, the project seeks to develop practical tools for simulating disease spread that can also be applied in diverse fields such as game development.

Scientific Conclusions



Through this project, we hope to achieve several scientific conclusions:



1. Demonstrate the effectiveness of parallel processing and cellular automata in simulating the SIR and SEIR epidemic models, potentially showcasing an alternative to traditional methods like Markov Chains that can be more efficient and scalable.



2. Determine the accuracy of these simulations compared to real-world data and understand the balance between model refinement and overfitting.



3. Explore the practicality and applicability of these simulation tools beyond academic research, such as their use in public health planning or game development.



4. Provide insights into the potential integration of machine learning techniques for automatic model refinement and adaptive simulation techniques.



5. Establish a groundwork for future research, such as the inclusion of more complex factors in epidemic models (like carrier states or vaccination rates) and the potential for a reverse-engineering approach to model selection.

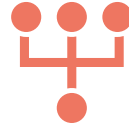
Simulation & Data Analysis



The simulation in this project will involve the use of cellular automata to model the spread of an infectious disease based on SIR and SEIR models. We'll represent the population as a two-dimensional grid, where each cell corresponds to an individual and their state: Susceptible, Exposed, Infected, or Recovered. The initial state of each cell will be randomly assigned to reflect a realistic distribution of population states at the start of a disease spread.



This simulation will run on a parallel computing environment, leveraging technologies like MPI and OpenMP. By assigning different portions of the grid to multiple processes, we aim to enhance computational efficiency.



Once the simulation is running, it will apply the rules defined by the SIR and SEIR models for each time step. Each individual's state will evolve based on these rules, and the aggregate state of the population will be captured and analyzed.



In terms of data analysis, we will introduce the concept of an 'error function' that assesses the difference between the simulated data and real-world observations. This approach will allow us to refine the parameters of our model iteratively to improve its predictive accuracy while preventing overfitting.



Ultimately, we aim to generate a rich dataset that provides insight into the temporal dynamics of disease spread and the comparative efficiency and accuracy of SIR and SEIR models when implemented in parallel computing environments.

Algorithms & Numerical Methods



Several algorithms and numerical methods are anticipated to be applied:



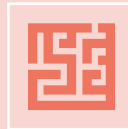
1. **Cellular Automata:** This will be the preliminary method for modeling the disease spread. Each cell in a grid represents an individual, and their state (Susceptible, Exposed, Infected, Recovered) evolves according to the SIR/SEIR model rules.



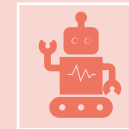
2. **Numerical Integration:** As the SIR and SEIR models involve ordinary differential equations, numerical integration methods might be used for their solution, especially if we wish to simulate continuous time models.



3. **Random Number Generation:** Some initial states of individuals (cells) in the grid will be assigned randomly, which will require a reliable method for generating random numbers.



4. **Error Function and Optimization Algorithms:** To refine the model parameters, we will define an error function that quantifies the difference between simulated data and real-world observations. Then, we can use optimization algorithms (e.g., gradient descent, stochastic gradient descent, etc.) to adjust parameters and minimize this error.



5. **Machine Learning Algorithms:** Depending on the direction of the research, we might employ machine learning techniques to automate model refinement, or even reverse-engineer the best-fitting model based on observed data.

Programing & Development

The project will be developed in Python and the programming work will likely involve the following:

1. Setting Up the Simulation Environment:

This would involve setting up the cellular automata grid, initializing individual states randomly according to the SIR/SEIR model rules, and defining the transition functions for changing states. Libraries such as NumPy can be used to efficiently handle arrays representing the population grid.

2. Implementing SIR/SEIR Models:

You would be writing functions or classes to represent the SIR and SEIR models, which will include the associated differential equations. These will be used to determine state transitions in the simulation. SciPy's integrate module can be utilized for numerically solving these equations.

3. Running the Simulation:

This would involve iterating over the defined time steps, updating the state of each cell according to the SIR/SEIR rules at each step, and storing or outputting the state of the entire system at each step for subsequent analysis.

4. Data Analysis and Model Refinement:

Here, we write code to analyze the results of the simulation, such as computing the error between the simulated data and real-world data. We also use this analysis to iteratively refine model parameters. Libraries like Pandas for data handling and Matplotlib for visualization can aid in this process.

5. Machine Learning Integration:

Depending on the project's scope, we could also implement machine learning models using libraries such as Scikit-Learn or TensorFlow. These models could help automate the process of model refinement or even potentially reverse-engineer the best fitting model based on real-world data.

Python's extensive standard library and the availability of scientific computing packages like NumPy, Scipy, Pandas, and Scikit-learn make it a great choice for such a project.

Relevant Papers

Deep-Data-Driven Neural Networks for COVID-19 Vaccine Efficacy by Thomas K. Torku, Abdul Q.M. Khaliq & Khaled M. Furati

This paper develops a vaccination model with an efficacy rate, using a hybrid neural network approach for reliable daily case predictions, demonstrating through data-driven simulations that higher vaccination rates with more effective vaccines decrease the infectiousness and basic reproduction number, using data from Tennessee as a case study.

"Modeling Infectious Diseases in Humans and Animals" by Keeling, M. J., & Rohani, P. (2008, Princeton University Press).

This is not a paper but a comprehensive book that provides a thorough introduction to the mathematical modeling of infectious diseases, including both the SIR and SEIR models.

"Parallel discrete event simulation of SEIR epidemic models"

by Perumalla, K. S., & Seal, S. K. (2013, in Winter Simulations Conference (WSC)).

This paper presents an approach for accelerating the simulation of SEIR epidemic models using parallel discrete event simulation. Although you mentioned that parallel processing is not important for this project, this paper can provide useful insights on how such models are typically parallelized.

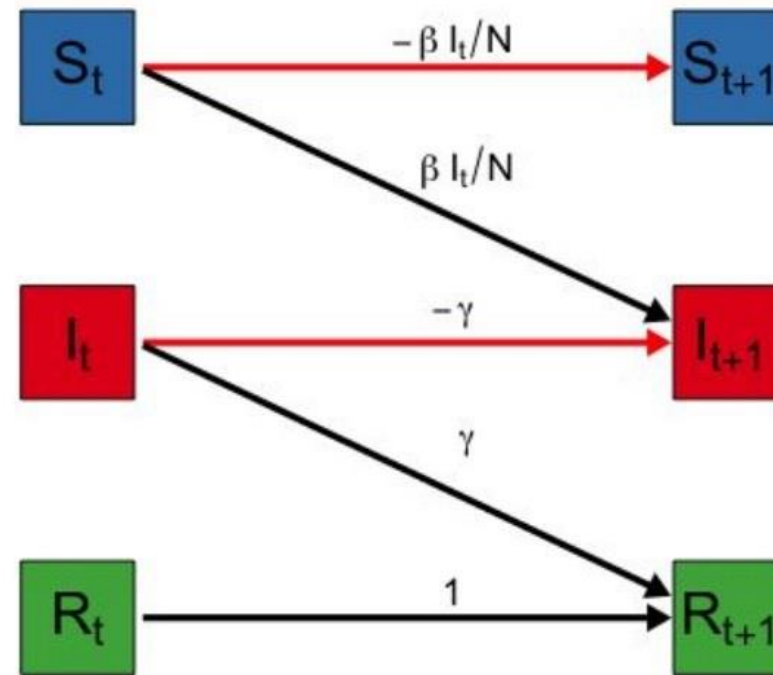
"An efficient solution to the inverse problem of epidemic models using sequential Monte Carlo"

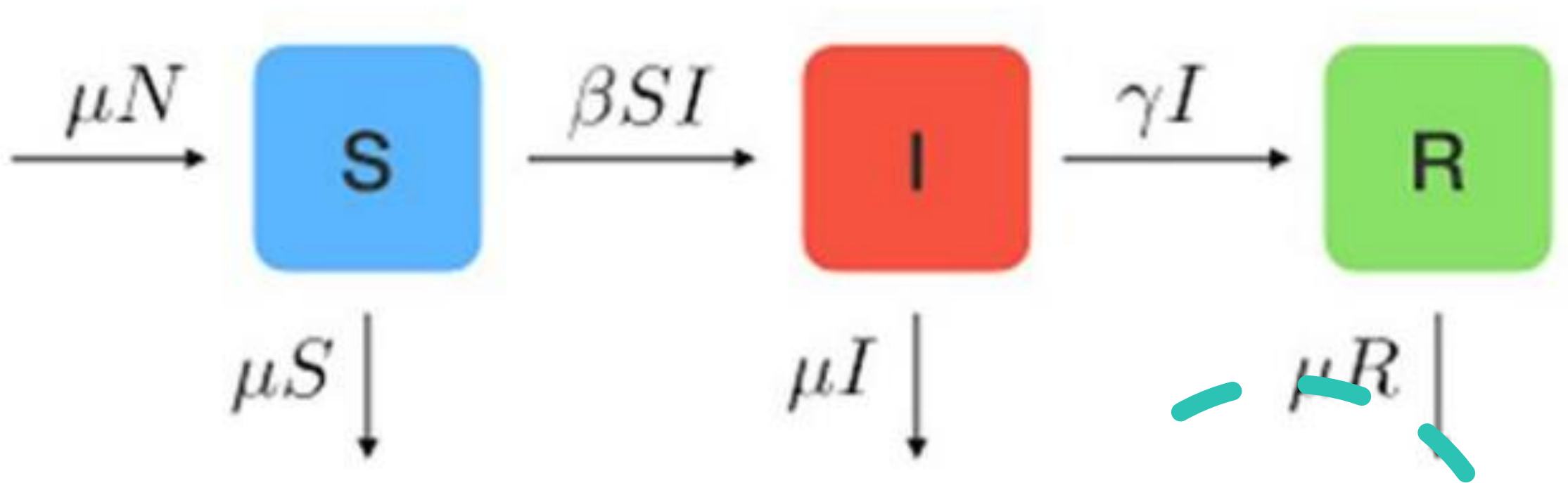
by Cantwell, C. J., Ruktanonchai, N., & Tildesley, M. J. (2019, PLoS One). This paper addresses the reverse problem in epidemic models, i.e., determining parameters given observed data, using a sequential Monte Carlo method. The methodology proposed could provide insights for your own reverse-engineering approach.



Basic SIR Model

Differential Equations Model of SIR Transformations





● Basic SIR Model

SEIR (Susceptible, Exposed, Infectious, Recovered)

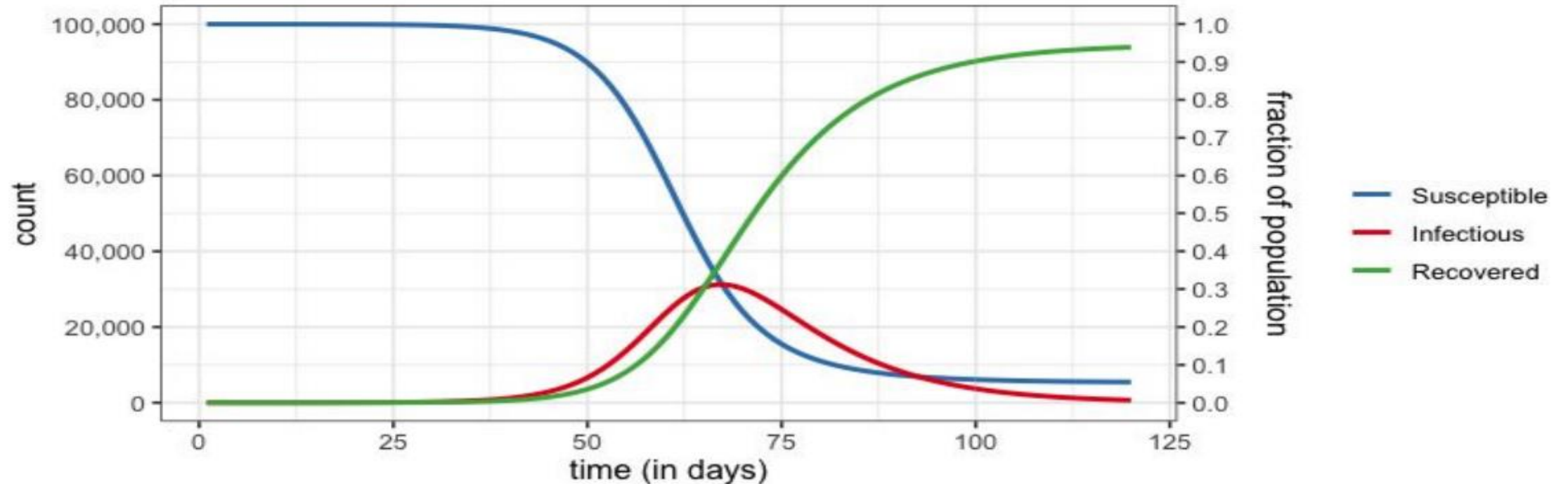


Basic SEIR Model

- E (Exposed) - Set of people in the model who have been exposed to the disease, and do not show symptoms.

SIR Example over Time

SIR : $\beta = 0.3$, $\gamma = 0.1$

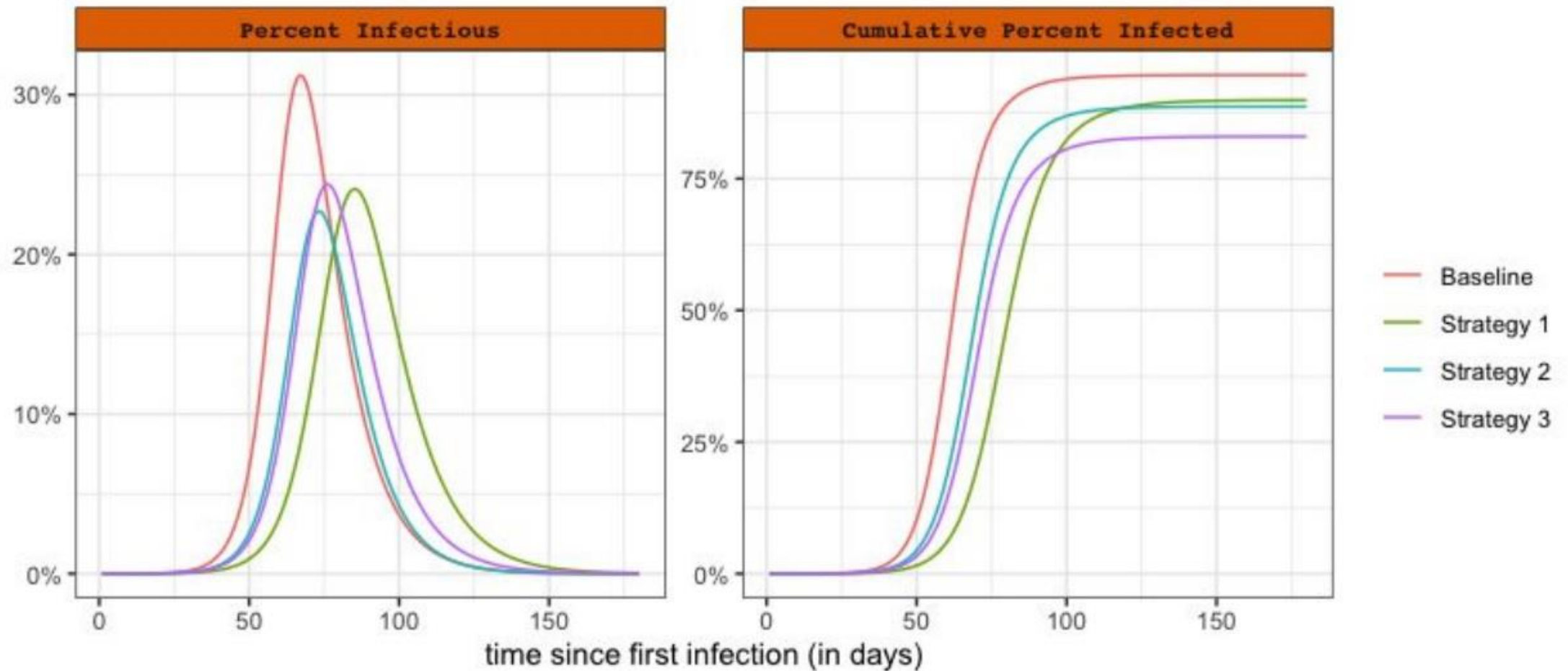



- Graphical representation on the SIR model (Susceptible, Infected and Recovered) on the right, and bellow their structure and dynamics in flow charts.



Oversimplified (simple
forced probability) Model

Models Derived through Different Strategies





The Extrapolation of First Order Methods for Parabolic Partial Differential Equations

J.D. Lawson and J. Ll. Morris
December 1978

Abstract: J.D. Lawson and J. Li. Morris Dec 1978

Splitting methods for parabolic partial differential equations based on (1,1) Padé approximations (Crank-Nicolson replacements) are well known to produce poor numerical results when a time discretization is imposed with time steps which are "too large" relative to the spatial discretization.

In particular such numerical solutions exhibit an oscillatory behavior which increases in amplitude with a reduction in the spatial discretization, keeping the time step constant.

In contrast, (1,0) Padé approximations (backwards difference, or fully implicit replacements) do not suffer from these drawbacks but are of lower order accuracy.

In the present paper, a combination of fully implicit methods is used to attain second order accuracy and to retain the favorable property of the fully implicit scheme.

The method is tested on a heat equation in two space dimensions which possesses a discontinuity between the initial and boundary conditions.



Recent progress on the combinatorial diameter of polytopes and simplicial complexes

Francisco Santos July 24, 2013

Abstract: Francisco Santos July 24, 2013

The Hirsch conjecture, posed in 1957, stated that the graph of d -dimensional polytope with n facets cannot have diameter greater than $n - d$.

The conjecture itself has been disproved, but what we know about the underlying question is quite scarce.

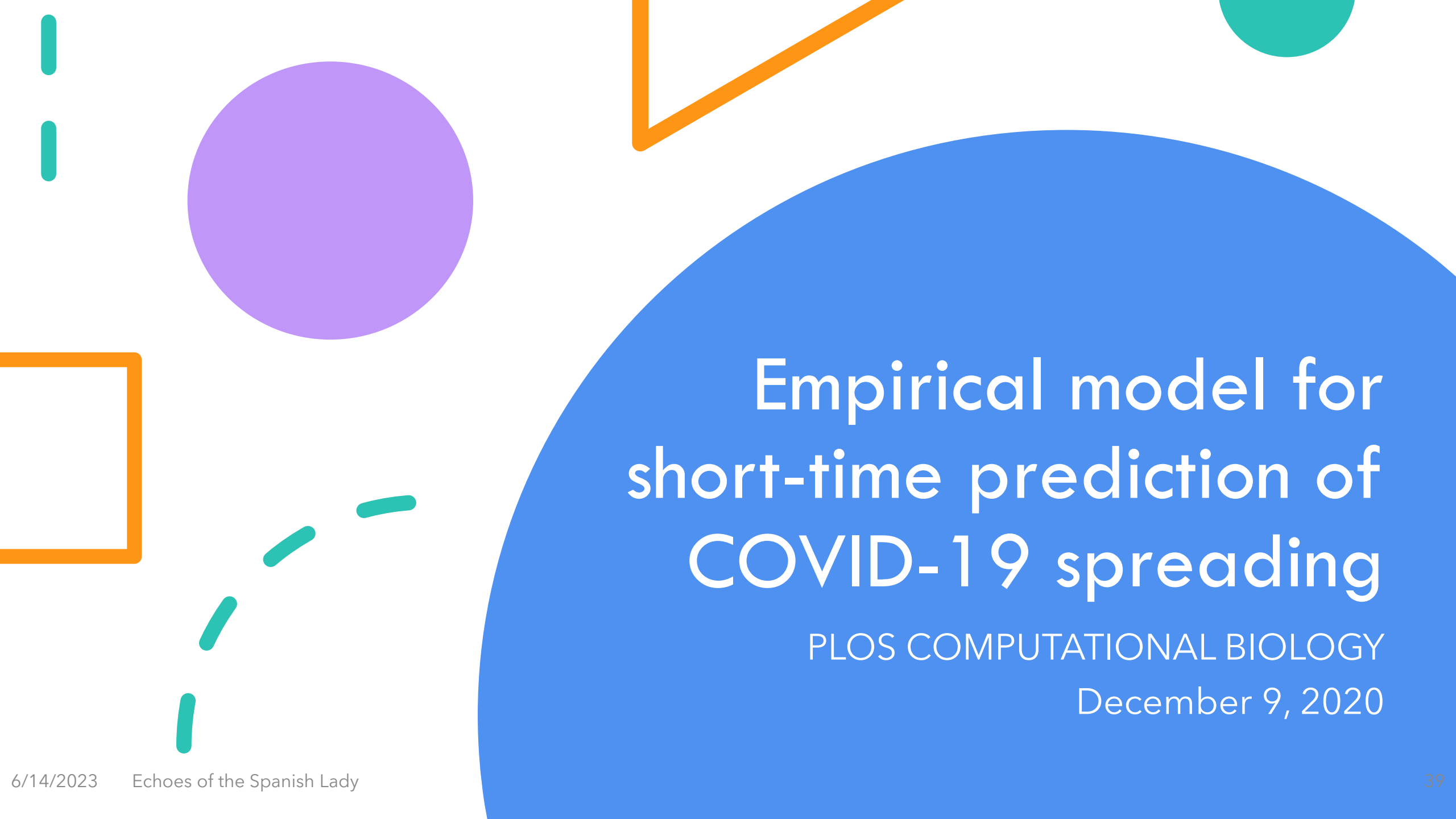
Most notably, no polynomial upper bound is known for the diameters that were conjectured to be linear. In contrast, no polyhedron violating the conjecture by more than 25% is known.

This paper reviews several recent attempts and progress on the question.

Some work in the world of polyhedral or (more often) bounded polytopes, but some try to shed light on the question by generalizing it to simplicial complexes.

In particular, we include here our recent and unpublished proof that the maximum diameter of arbitrary simplicial complexes is in $n^{\Theta(d)}$ and we summarize the main ideas in the **polymath 3** project, a web-based collective effort trying to prove an upper bound of type nd for the diameters of polyhedral and of more general objects (including, e.g., simplicial manifolds).

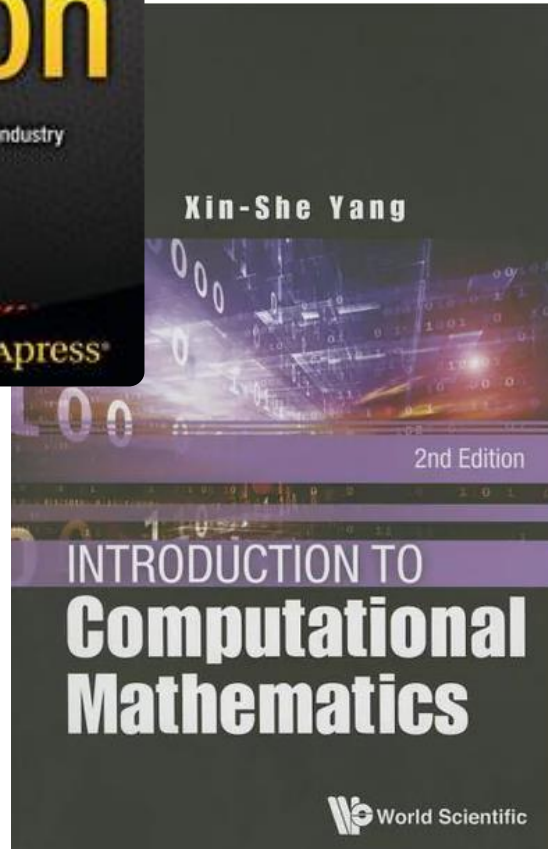
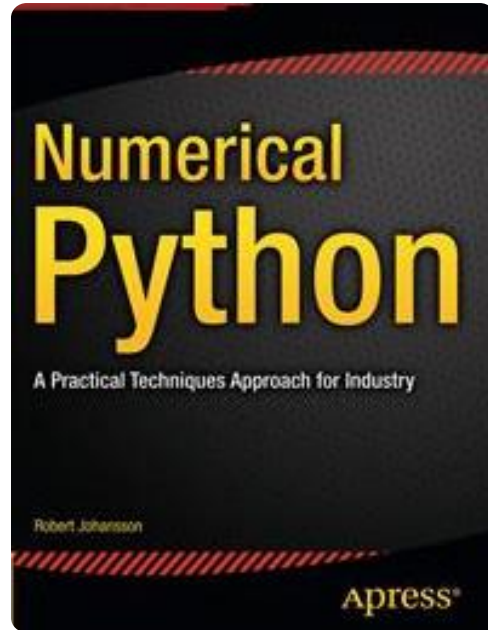
Keywords Polyhedra, diameter, Hirsch conjecture, simplex method, simplicial method.



Empirical model for short-time prediction of COVID-19 spreading

PLOS COMPUTATIONAL BIOLOGY

December 9, 2020



Continuing Focus

[Numerical Python](#) Robert Johansson

Harvard CS50's Introduction to
Programming with Python – Full University
Course https://youtu.be/nLRL_NcnK-4

[CS50's Introduction to Programming with Python
\(harvard.edu\)](https://www.harvard.edu/cs50/)

Introduction to Computational
Mathematics (2nd Edition) [Xin-She Yang](#)

Video Games as Models



World of Warcraft



- Massively multiplayer online role playing game (MMORPG) by Blizzard Entertainment



- Launched 11/2004, 7/2007: 9 Mio players



- Players create "Avatars" from a set of races and classes, can learn professions



- Interaction with other Avatars



- LOTS of out-of-game activity

A World of Adventure

- Avatars adventure the virtual world "Azeroth" and progress from Level 1 to Level 60 (70, 80)
- Each new level makes Avatars more powerful: more life, talents, spells, better armory etc.
- Powerful enemies ("Bosses") can only be defeated by several coordinated max. level Avatars ("raid")