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Modeling Infectious Disease Spread: Comparison of the Agent-Based Modeling and Differential-Equation Approaches

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Introduction

- In epidemiology, the **SIR model** is commonly used to describe the population dynamics of infectious diseases.
- It divides the population into three categories: **Susceptible (S)**, **Infected (I)**, and **Recovered (R)**.
- We consider two approaches to describe its population dynamics.

1. Ordinary Differential Equation (ODE)

Mathematical equations tracking population-level changes, ideal for predicting large-scale trends and getting quick insights into disease spread patterns.

ODE has two model parameters, **infection strength (b)** and **recovery rate (k)**.

$$\begin{aligned} \frac{ds}{dt} &= -b s(t) i(t), & s(0) &= 1 - \epsilon, & \epsilon &= 1 \times 10^{-8} \\ \frac{di}{dt} &= b s(t) i(t) - k i(t), & i(0) &= \epsilon \\ \frac{dr}{dt} &= k i(t), & r(0) &= 0 \end{aligned}$$

Figure 1. ODE of SIR model

2. Agent-Based Model (ABM)

A grid simulation where each cell represents an individual, allowing us to capture local interactions and spatial effects that ODEs can't model. This helps us understand how individual behavior influences disease spread. ABM has three model parameters, **recovery rate (α)**, **infection rate (β)**, and **diffusion rate (γ)**.

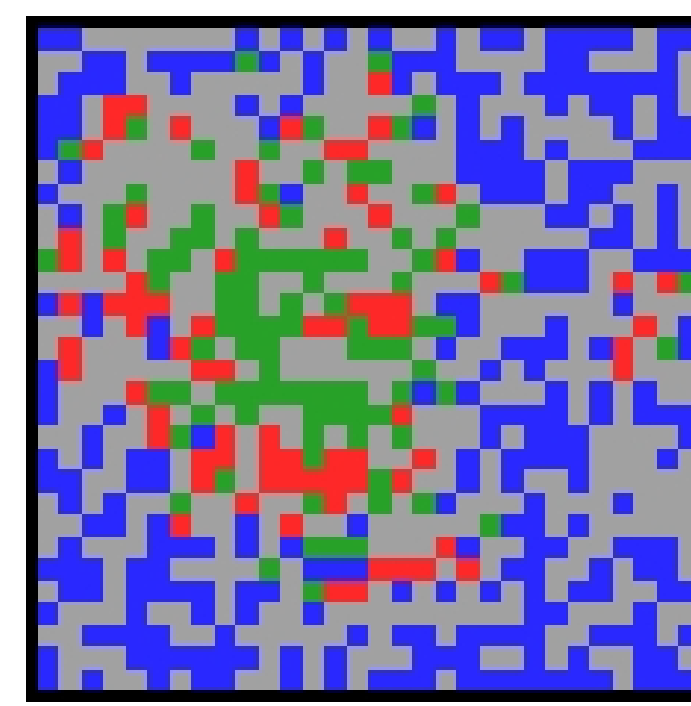


Figure 2. Example image of ABM

Each color represents: **Susceptible**, **infected**, **recovered**, empty site

Research Aims: To compare the two approaches by establishing relationships between the ODE and ABM parameters, bridging the gap between population-level predictions and individual-based simulations.

Methods and Materials

- ODE:** To numerically solve the ODE, we used the **Runge-Kutta method**.
- ABM:** We used **SPPARKS (Stochastic Parallel Particle Kinetic Simulator)**, a kinetic Monte Carlo simulator, to simulate the ABM.
- To compare the two parameters, we first run the simulation with fixed ABM parameters. We then find the optimal ODE parameters that would produce the most similar result (SIR graph) as the ABM.
- We use two methods when determining whether an ODE parameter is producing the most similar result as the ABM.

Method 1: Least Squares

Using the **differential evolution method**, we find optimal ODE parameters, **b** and **k** values that minimize the least squared difference between ODE and ABM results.

Method 2: Contact Number

Contact number is the number of close contacts per infected individual.

- Using SPPARKS, we find the proportion of the population that stayed susceptible during the epidemic (S_∞).
- We obtain contact number (**c**) using S_∞ , then find **b** value when **k** is known.

$$c = \frac{\ln S_\infty}{1 - S_\infty}, \quad c = \frac{b}{k}$$

Figure 3. Contact number

SIR Graph of epidemic that has an infectious period of 14 days and contact number of 2, generated using ABM parameters below.

$$b = \frac{1}{7}, \quad k = \frac{1}{14}, \quad \gamma = 30$$

Visualization of ABM at different times (T, days)

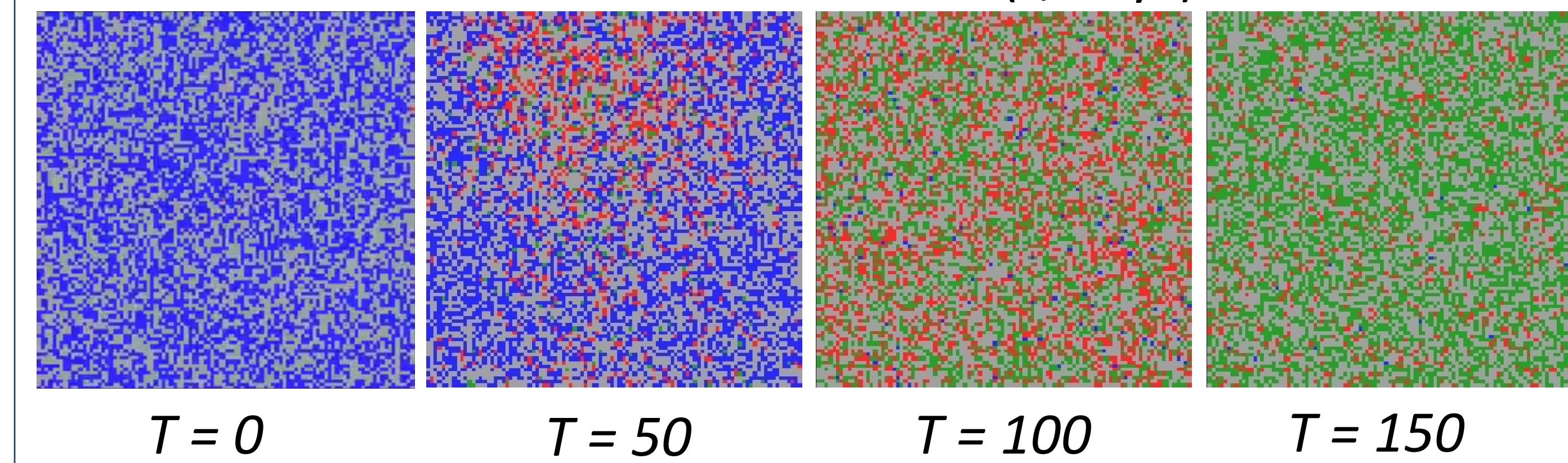


Figure 4. Image of ABM, at different time T.

Optimized parameter using

Method 1: **b** = 0.453768, **k** = 0.0719541

Method 2: **b** = 0.486128, assuming **k** as 0.714285

The two methods give very similar number for **b** and **k**.

Relationship between **α** and optimal **k** value

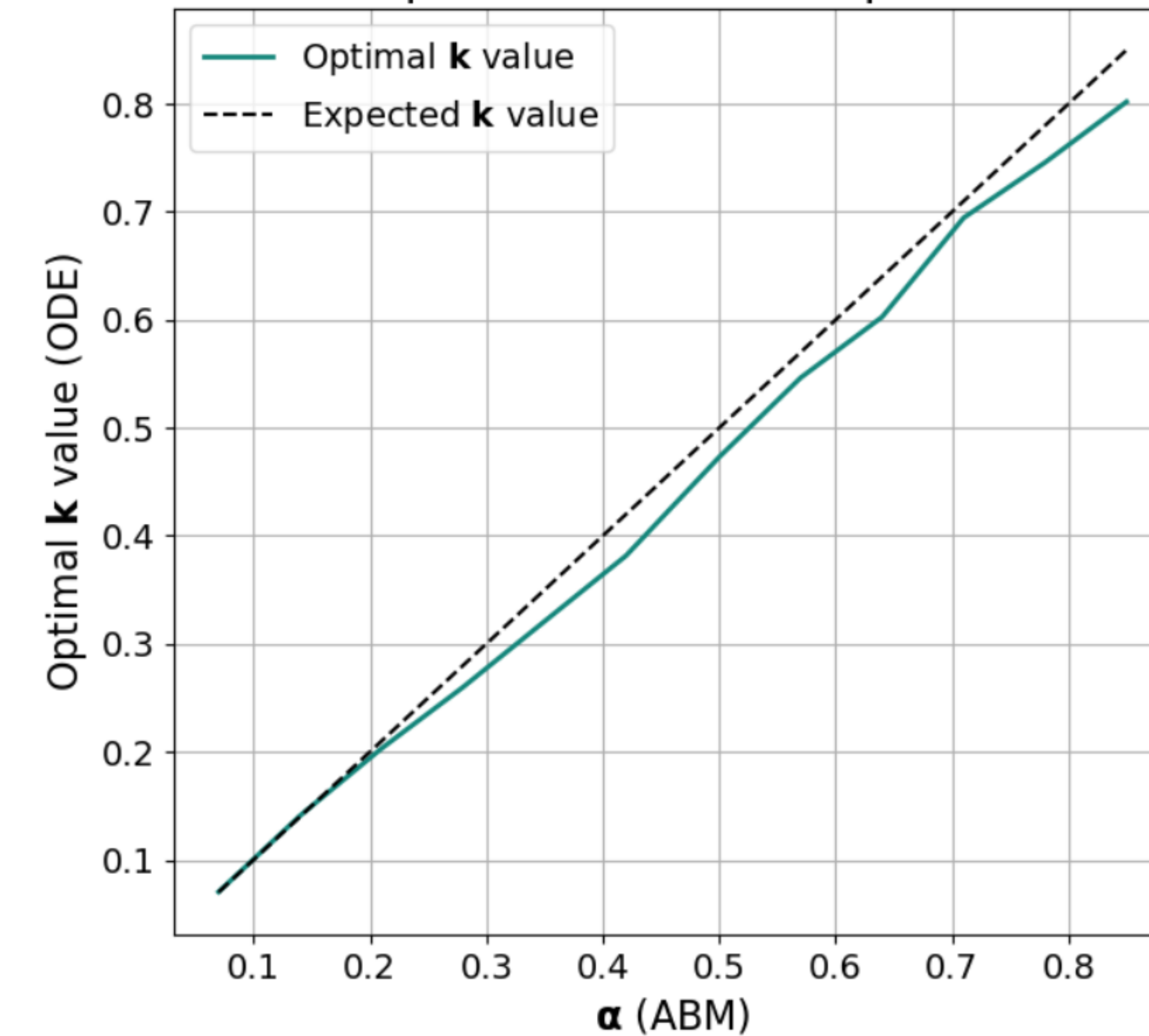


Figure 6. This plot was obtained using Method 1.

This graph shows that **α** and **k** has one-to-one correspondence.

We ran multiple sets of SPPARKS simulations using various values for **α**, and obtained corresponding **k** values. **b** and **γ** were set to 0.3 and 50, respectively.

Results

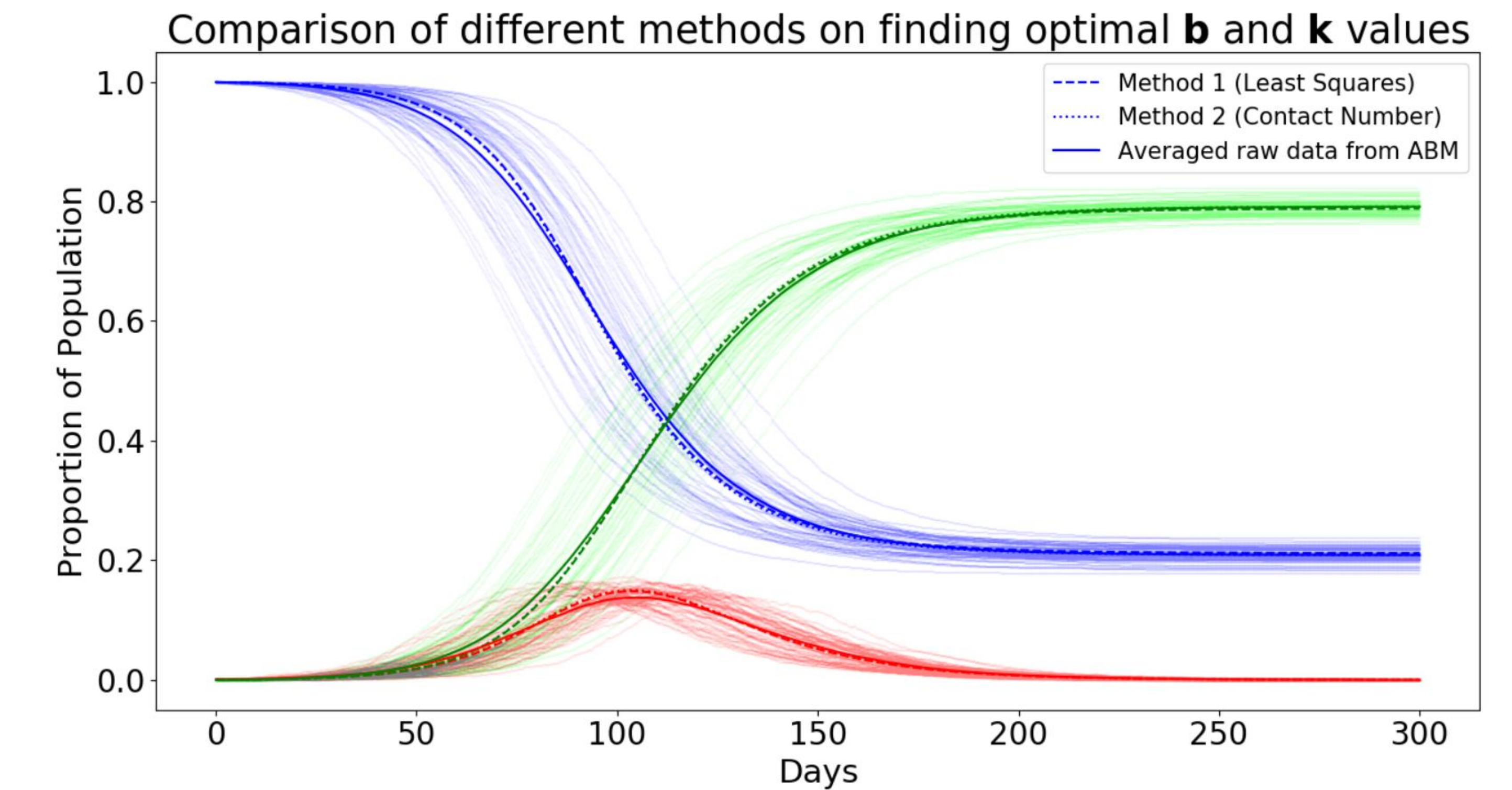


Figure 5. SIR graph with ABM results and optimal ODE using Methods 1 and 2. The soft lines represent the individual simulation that are used to generate the averaged raw data.

Relationship between **γ** and optimal **b** value using two methods, when **β** = 0.3

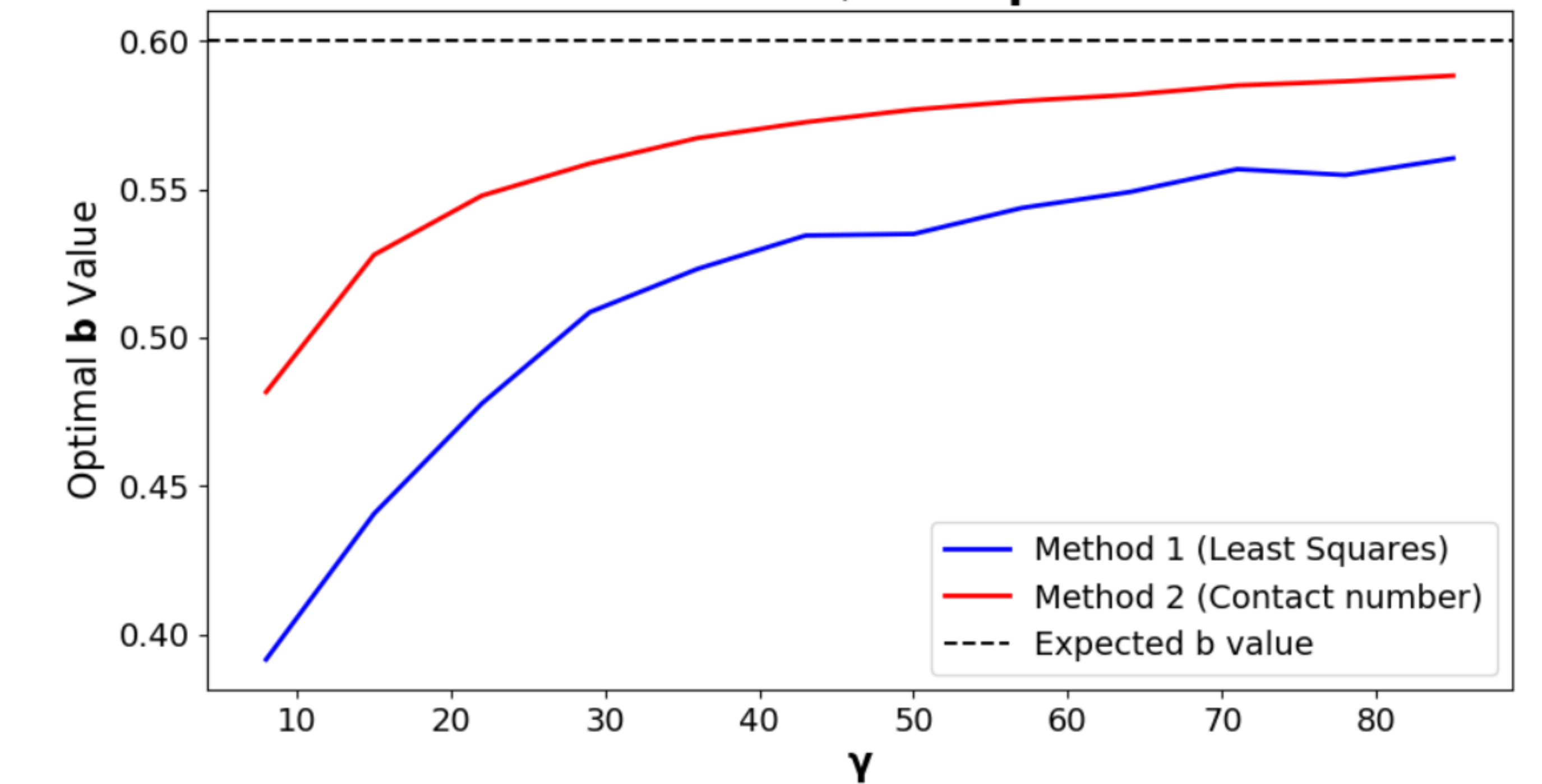


Figure 7. Plot of Relationship between **γ** and optimal **b** value using two methods.

As **γ** increases, we find that optimal **b** value from both methods getting closer to **β**, which is 0.6 in this case. **α** were set to 0.3.

Conclusion

Key Parameter Relationships:

- Discovered one-to-one relationship between recovery parameters, ($\alpha = k$)
- Established relationship between: ABM diffusion rate (γ), ABM infection rate (β), and ODE infection strength (**b**).
- As diffusion rate (γ) increases (greater mobility in the model):
 - ODE infection strength (**b**) approaches ABM infection rate (β)
 - This convergence reflects how increased mobility bridges the gap between spatial (ABM) and non-spatial (ODE) disease spread dynamics.
- Our findings reveal a fundamental connection between microscopic (ABM) and macroscopic (ODE) descriptions of epidemic dynamics, despite their distinct modeling approaches:
 - These relationships provide guidance for modelers choosing between or transitioning between ABM and ODE approaches, enabling more informed parameter selection based on the desired scale of analysis.

References & Acknowledgements

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