Simulation and Theory of Bacterial Transformation

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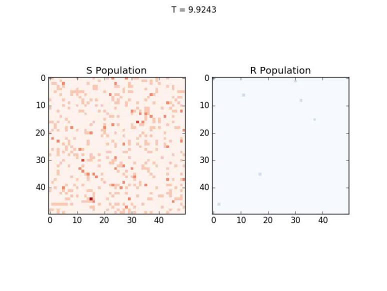


Outline

Motivation

- Ubiquitous threat of antibiotic resistance
- Main mechanisms of transmission

Goal

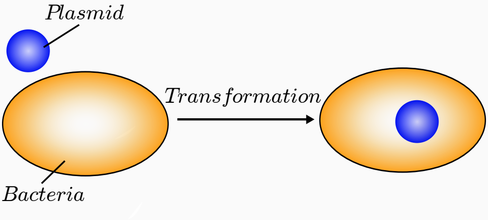
Identify what most significantly affects resistant cell dominance.

Plasmids

- Small, independently replicating genetic material
- Often include DNA segments encoding antibiotic resistance
- Imposes a fitness cost on host cell

Transformation and Conjugation

- **Transformation:** Cell incorporates plasmid from environment
- **Conjugation:** Plasmid transferred between cells



Outline

Simulation vs Modeling

- Stochastic vs Deterministic
- Information about average behavior vs specific system

Simulation vs Modeling

Reaction $$R \xrightarrow{\delta} \varnothing \quad (1)$$

Simulation vs Modeling

Reaction $$R \xrightarrow{\delta} \varnothing \tag{1}$$

Differential equation $$\frac{dR}{dt} = -\delta R \tag{2}$$

$$R(t) = R_0 e^{-\delta t} \tag{3}$$

Population Dynamics Model - Constant

$$\frac{dS}{dt} = b_S \left(1 - \frac{S+R}{K}\right) S - \alpha S$$

$$\frac{dR}{dt} = b_R \left(1 - \frac{S+R}{K}\right) R + \alpha S - \delta R$$

Population Dynamics Model - Linear

$$\frac{dS}{dt} = b_S \left(1 - \frac{S+R}{K}\right) S - \alpha \left(\frac{P}{P_0}\right) S$$

$$\frac{dR}{dt} = b_R \left(1 - \frac{S+R}{K}\right) R + \alpha \left(\frac{P}{P_0}\right) S - \delta R$$

$$\frac{dP}{dt} = -\alpha \left(\frac{P}{P_0}\right) S$$

Population Dynamics Model - Recycled

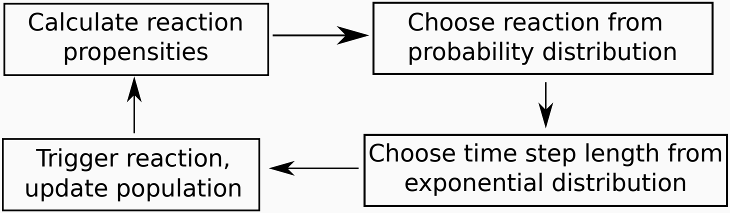
$$\frac{dS}{dt} = b_S \left(1 - \frac{S+R}{K}\right) S - \alpha \left(\frac{P}{P_0}\right) S$$

$$\frac{dR}{dt} = b_R \left(1 - \frac{S+R}{K}\right) R + \alpha \left(\frac{P}{P_0}\right) S - \delta R$$

$$\frac{dP}{dt} = -\alpha \left(\frac{P}{P_0}\right) S + \delta R$$

Kinetic Monte Carlo Method

- Initially used to simulation chemical reactions
- Captures information about dynamics of a growing system



Optimizations

- Sets vs. lists
- Occupancy lists
- `imshow` vs. `plcolor`

Outline

Parameter Space

Outline

Backup slides

References i