PatchSim Model Description

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Mechanistic approaches to disease simulation often fall under one of two categories:

- **ODE models** Approaches of this kind are based on ordinary differential equations with the central assumption being *homogeneous mixing* of individuals within the population of interest. While easy to setup and simulate, they often cannot reproduce spatial or social heterogeneity observed in the ground truth.
- **Network models** Approaches of this kind simulate the disease dynamics on a graph (e.g., social network) where disease propagates from infected to susceptible individuals through the edges of the graph, capturing social interactions. They can be implemented in an agent-based manner and allow for high fidelity of representation. However, such models are tough to setup and pose computational challenges in model simulation and calibration.

Metapopulation models take advantage of both these approaches, and are well suited to capture spatial heterogeneity in disease dynamics. The population of interest is divided into spatially distinct *patches*, and within each patch the disease dynamics are simulated with a homogeneous mixing assumption. The patches are also connected to each other through a weighted directed network capturing movement of individuals between the patches. The movement is often representative of *commuting* (as against *migration*), thus preserving the home population counts of each patch. While within a single patch the disease evolution resembles a homogeneous ODE model, the mobility network generates heterogeneity and longer hops between the spatial sub-populations. PatchSim is a deterministic implementation of this approach.

Let $\mathcal{N}$ represent the set of all patches (with $N = |\mathcal{N}|$). Associated with each patch i, we have population P_i, and state tuple $Z_i(t)$ denoting number of individuals in each of the disease states at time t. For a typical SEIR (Susceptible $\rightarrow$ Exposed $\rightarrow$ Infected $\rightarrow$ Recovered) model, the set of states is given by $\mathcal{Z} = \{S, E, I, R\}$. The state tuple is then $Z_i(t) = (S_i(t), E_i(t), I_i(t), R_i(t))$, with $\sum_{z\in\mathcal{Z}} z_i(t) = P_i$. Between a pair of patches i and j, we have the flow F_{ij}, denoting the fraction of individuals belonging to *home* patch i spending their day in *away* patch j. In order to conserve patch populations (i.e., commuting model), we assume $\sum_{j\in\mathcal{N}} F_{ij} = 1$. The mobility is assumed to be *homogeneous* and *memory-less*, i.e., the commuting individuals according to F_{ij} are assumed to be picked at random from the population P_i independent of their disease state, and independently for each day of the simulation. Due to the movement of individuals, the *effective* population of patches may differ from their home population P_i. This in turn also affects the state tuple Z_i. We denote the effective population as $P_i^{\mathtt{eff}}$ and the effective state tuple as $Z_i^{\mathtt{eff}}(t)$. Then, $P_i^{\mathtt{eff}} = \sum_{k\in\mathcal{N}} F_{ki}P_i$ and $z_i^{\mathtt{eff}} = \sum_{k\in\mathcal{N}} F_{ki}z_i$ for $z \in \mathcal{Z}$.

PatchSim steps through the disease simulation in daily epochs. In order to compute the change in state tuple $\Delta Z(t) = Z(t+1) - Z(t)$, it incorporates (i) movement of individuals from their respective home patches to away patches according to F_{ij}, (ii) exposures, infections, and recoveries happening in the away patches, and (iii) integration of state updates at the home patches. Let β represent the probability of exposure per day per $S - I$ contact, α the infection rate and γ recovery rate. α can be thought of as the reciprocal of mean incubation period, and γ the reciprocal of mean infectious period. Additionally, let $X_i(t)$ represent the spatio-temporal seeding profile. This captures the number of individuals of patch i

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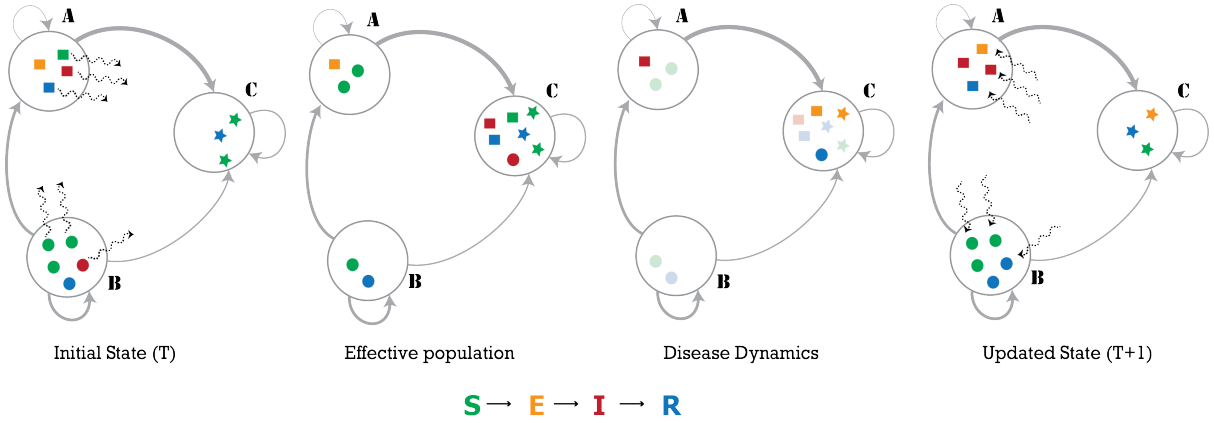

Figure 1: The large circles represent the patches in the simulation, and the grey edges represent the travel network, with varying thickness denoting heterogeneity in flow volumes. The sample population shows 4 individuals in patch A (squares), 5 in patch B (circles) and 3 in patch C (stars). The colors represent the disease state the individuals are in (susceptible, exposed, infected or recovered). The wavy dashed arrows show movement of individuals (randomly chosen according to outgoing edge probabilities). In the first step, individuals are moved from their home patch to another patch (first panel), creating the effective population (second panel). The disease dynamics may constitute an exposure event (transition from S to E), onset of infectiousness (E to I), or recovery event (I to R). The nodes undergoing these transitions are highlighted in third panel, where we see an onset of infectiousness in patch A, two exposures and a recovery in patch C. Finally, the individuals return to their home patch (fourth panel).

who are extraneously moved from S to E to indicate external exposure ('seed' cases). The state update equations can then be written down as below for each $z \in \mathcal{Z}$ (omitting time index t for clarity):

$$\Delta S_i = -X_i - \sum_{j \in \mathcal{N}} F_{ij} \beta \frac{I_j^{\mathtt{eff}}}{P_j^{\mathtt{eff}}} S_i \tag{1}$$

$$\Delta E_i = X_i + \sum_{j \in \mathcal{N}} F_{ij} \beta \frac{I_j^{\mathtt{eff}}}{P_j^{\mathtt{eff}}} S_i - \alpha E_i \tag{2}$$

$$\Delta I_i = \alpha E_i - \gamma I_i \tag{3}$$

$$\Delta R_i = \gamma I_i \tag{4}$$

The summation in Equation 1 captures new exposures for individuals with home patch i, summed across potential away patches j. F_{ij} denotes the movement to away patch j, $\frac{I_j^{\mathtt{eff}}}{P_j^{\mathtt{eff}}}$ is the proportion of infectious individuals in the effective population at patch j, and β the probability of exposure given contact. Note that, unlike exposure, becoming infectious ($E \to I$) and recovery ($I \to R$) are independent of the away patch j visited by an individual, hence need not be explicitly summed across $j \in \mathcal{N}$.

Thus, given the disease parameters (β, α, γ) and a seeding profile X, PatchSim uses the population vector P and flow matrix F to produce the spatio-temporal evolution of disease states Z.