FUNMANAbstraction

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1 Introduction

We describe methods to stratify and abstract (de-stratify) Petrinets for compartmental models. The motivation for abstracting a Petrinet is to reduce its size, which becomes exponential in the number of stratified variables. Reducing the size of the model can have a significant impact on runtime, and it is possible to answer useful queries with the abstract model. The following sections include a background (defining the models), a description of abstraction, an approach needed to bound the abstracted models, and then a comparison of simulation results for several variations of a baseline model that applies stratification, bounding, and abstraction.

2 Background

Definition 1 *A Petrinet Ω is a directed graph (V, E) with vertices $V = (V_x, V_z)$ partitioned into sets V_x of state vertices and V_z of transition vertices, and edges $E = (E_{in}, E_{out})$ partitioned into collections E_{out} of flow-out and E_{in} flow-in edges (relative to state vertices).*

Definition 2 *A flow-out edge $e \in E_{out}$ comprises a pair of vertices (v_x, v_z), where $v_x \in V_x$ is a state vertex, $v_z \in V_z$ is a transition vertex, and the flow is directed from v_x to v_z.*

Definition 3 *A flow-in edge $e \in E_{in}$ comprises a pair of vertices (v_z, v_x), similar to a flow-out edge, except that the flow is directed from v_z to v_x.*

Example 1 *The SIR model that stratifies the S state variable into S_1 and S_2 for two susceptible populations and defines Ω by:*

$$\begin{aligned}
V_x &= \{v_{S_1}, v_{S_2}, v_I, v_R\}\\
V_z &= \{v_{inf_1}, v_{inf_2}, v_{rec}\}\\
E_{in} &= ((v_{inf_1}, v_{S_1}), (v_{inf_1}, v_I), (v_{inf_1}, v_I), (v_{inf_2}, v_{S_2}), (v_{inf_2}, v_I), (v_{inf_2}, v_I), (v_{rec}, v_R))\\
E_{out} &= ((v_{S_1}, v_{inf_1}), (v_{S_2}, v_{inf_2}), (v_I, v_{inf_1}), (v_I, v_{rec}))
\end{aligned}$$

Definition 4 *The ODE semantics Θ of the Petrinet Ω defines a tuple $(P, X, Z, \mathcal{I}, \mathcal{P}, \mathcal{X}, \mathcal{Z}, \mathcal{R})$ where*

- *P is a set of parameters;*
- *X is a set of state variables;*
- *Z is a set of transitions;*
- *$\mathcal{I} : S \rightarrow \mathbb{R}$ assigns the initial value of state variables to a real number;*
- *$\mathcal{P} : P \rightarrow \mathbb{R} \cup \mathbb{R} \times \mathbb{R}$ assigns parameters to a real number, or a pair of real numbers defining an interval;*

- *$\mathcal{X}: X \rightarrow V_x$ assigns state variables to state vertices;*
- *$\mathcal{Z}: Z \rightarrow V_z$ assigns transtions to transition vertices; and*
- *$\mathcal{R}: \mathbf{P} \times \mathbf{X} \times Z \rightarrow \mathbb{R}$ defines the rate of each transition $z \in Z$ in terms of the set of parameter vectors $\mathbf{P}$ and state variable vectors $\mathbf{X}$.*

The elements of the Petrinet Ω and semantics Θ define the partial derivative $\frac{d\mathbf{x}}{dt}$, so that for each state variable $x \in X$:

$$\frac{dx}{dt} = \sum_{v_z \in V_z^{in(x)}} \mathcal{R}(\mathbf{p}, \mathbf{x}, z) - \sum_{v_z \in V_z^{out(x)}} \mathcal{R}(\mathbf{p}, \mathbf{x}, z) \tag{1}$$

where $V_z^{in(x)} = \{v_z \in V_z | (v_z, v_x) \in E_{in}\}$ and $V_z^{out(x)} = \{v_z \in V_z | (v_x, v_z) \in E_{out}\}$ are the transition vertices that flow in and out of the vertex v_x, respectively. We denote by $\nabla_{\Omega,\Theta}(\mathbf{p}, \mathbf{x}, t) = (\frac{dx_1}{dt}, \frac{dx_2}{dt}, \ldots)^T$, the gradient comprised of components in Equation (1).

Example 2 *The stratified SIR model defines Θ by:*

$$\begin{aligned}
P &= \{\beta_1, \beta_2, \gamma\} \\
X &= \{S_1, S_2, I, R\} \\
Z &= \{inf_1, inf_2, rec\} \\
\mathcal{I} &= \begin{cases} 0.45 & : S_1 \\ 0.45 & : S_2 \\ 0.1 & : I \\ 0.0 & : R \end{cases} \\
\mathcal{P} &= \begin{cases} 1e{-}7 & : \beta_1 \\ 2e{-}7 & : \beta_2 \\ 1e{-}5 & : \gamma \end{cases} \\
\mathcal{X} &= \{ \; v_x \quad : x \in X \\
\mathcal{Z} &= \{ \; v_z \quad : z \in Z \\
\mathcal{R} &= \begin{cases} \beta_1 S_1 I & : z_{inf_1} \\ \beta_2 S_2 I & : z_{inf_2} \\ \gamma I & : z_{rec} \end{cases}
\end{aligned}$$

Using the partial derivatives defined by the Petrinet graph and semantics, we can define the state vector at given time $t + dt$ with the forward Euler method as:

$$\begin{aligned}
\frac{d\mathbf{x}}{dt} &= \nabla_{\Omega,\Theta}(\mathbf{p}, \mathbf{x}, t) \\
\frac{\mathbf{x}(t + dt) - \mathbf{x}(t)}{dt} &= \nabla_{\Omega,\Theta}(\mathbf{p}, \mathbf{x}, t) \\
\mathbf{x}(t + dt) &= \nabla_{\Omega,\Theta}(\mathbf{p}, \mathbf{x}, t)dt + \mathbf{x}(t)
\end{aligned}$$

3 Abstraction

Definition 5 *An abstraction (Θ', Ω') of a Petrinet and the associated semantics (Θ, Ω) that is produced by the abstraction operator A has the following properties:*

- *State: For each* $x \in X$, $A(x) = x'$, *where* $x' \in X'$. *For each vertex* $v_x \in V_x$, $A(v_x) = v'_x$ *where* $v'_x \in V'_x$. *For each* $x \in X$ *where* $\mathcal{X}(x) = V_x$, $A(x) = x'$, *and* $A(v_x) = v'_x$, *then* $\mathcal{X}'(x') = v'_{x'}$. *For each* $x' \in X'$, $\mathcal{I}'(x') = \sum_{x \in X : A(x) = x'} \mathcal{I}(x)$.
- *Parameters: For each* $p \in P$, $A(p) = p'$, *where* $p' \in P'$. *For each* $p' \in P'$, $\mathcal{P}'(p') = \sum_{p \in P : A(p) = p'} \mathcal{P}(p)$.
- *Transitions: For each* $z \in Z$, $A(z) = z'$, *where* $z' \in Z'$. *For each vertex* $v_z \in V_z$, $A(v_z) = v'_z$, *where* $v'_z \in V'_z$. *For each* $z \in Z$, *if* $\mathcal{Z}(z) = v_z$, $A(z) = z'$, *and* $A(v_z) = v'_z$, *then* $\mathcal{Z}'(z') = v'_{z'}$.
- *In Edges: For each edge* $(v_z, v_x) \in E_{in}$, $A((v_z, v_x)) = (v'_z, v'_x)$, $A(v_x) = v'_x$, *and* $A(v_z) = v'_z$, *where* $(v'_z, v'_x) \in E'_{in}$;
- *Out Edges: For each edge* $(v_x, v_z) \in E_{out}$, $A((v_x, v_z)) = (v'_x, v'_z)$; $A(v_x) = v'_x$, *and* $A(v_z) = v'_z$, *where* $(v'_x, v'_z) \in E'_{out}$;
- *Transition Rates: For each* $z' \in Z'$,

$$\mathcal{R}'(\mathbf{p}', \mathbf{x}', z') = \sum_{z \in Z : A(z) = z'} \mathcal{R}(\mathbf{p}, \mathbf{x}, z) \tag{2}$$

Example 3 *The abstraction* (Θ', Ω') *of the stratified SIR model defines (with the changed elements highlighted by "*"):*

$$A = \begin{cases} S & : S_1 & * \\ S & : S_2 & * \\ I & : I & \\ R & : R & \\ \beta & : \beta_1 & * \\ \beta & : \beta_2 & * \\ \gamma & : \gamma & \\ inf & : inf_1 & * \\ inf & : inf_2 & * \\ rec & : rec & \\ v_S & : v_{S_1} & * \\ v_S & : v_{S_2} & * \\ v_I & : v_I & \\ v_R & : v_R & \\ (v_S, v_{inf}) & : (v_{S_1}, v_{inf_1}) & * \\ (v_S, v_{inf}) & : (v_{S_2}, v_{inf_2}) & * \\ (v_I, v_{inf}) & : (v_I, v_{inf_1}) & * \\ (v_I, v_{inf}) & : (v_I, v_{inf_2}) & * \\ (v_I, v_{rec}) & : (v_I, v_{rec}) & \\ (v_{inf}, v_I) & : (v_{inf_1}, v_I) & * \\ (v_{inf}, v_I) & : (v_{inf_2}, v_I) & * \\ (v_{rec}, v_R) & : (v_{rec}, v_R) & \end{cases}$$

$$\mathcal{R} = \begin{cases} \beta_1 S_1 I + \beta_2 S_2 I & : z_{inf} & * \\ \gamma I & : z_{rec} & \end{cases}$$

In Example 3, the abstraction (Θ', Ω') maps the S_1 and S_2 state variables to the S state variable (effectively de-stratifying the base Petrinet). In combining the state variables, the abstract Petrinet consolidates the transitions inf_1 and inf_2 and associated rates from susceptible to infected.

Like the base model, the abstraction (Θ', Ω') defines a gradient $\nabla_{\Omega',\Theta'}(\mathbf{p}', \mathbf{x}', t) = (\frac{dx'_1}{dt}, \frac{dx'_2}{dt}, \ldots)^T$, in terms of Equation 1. Via Equation 2, the abstraction thus expresses the gradient by aggregating terms from the base Petrinet and semantics. It preserves the flow on consolidated transitions, but expresses the transition rates in terms of the base states. As such, the abstraction compresses the Petrinet graph structure, but at the cost of expanding the expressions for transition rates. Moreover, the transition rates refer to state variables and parameters (e.g., β_1, β_2, S_1, and S_2) that are not expressed directly by the abstract Petrinet and semantics (e.g., as β and S), and by extension, the gradient.

4 Bounded Abstraction

We modify the abstraction in what we call a *bounded abstraction*, so that it refers to the abstract, and not the base, Petrinet and semantics. This bounded abstraction replaces base elements with corresponding bounded elements. For example, if $A(S_1) = S$ and $A(S_2) = S$ (S_1 and S_2 are base variables represented by S in the abstraction), the transition rate associated with the inf transition is $\mathcal{R}'(\mathbf{p}', \mathbf{x}', z_{inf}) = \beta_1 S_1 I + \beta_2 S_2 I$. By construction, we know that $S_1 + S_2 = S$. However, in general $\beta_1 \neq \beta_2$, and we cannot say that $\beta_1 S_1 I + \beta_2 S_2 I = \beta S I$ for some definition of β. Yet, if we replace β_1 and β_2 by $\beta^{ub} = \max(\beta_1, \beta_2)$, then $\beta^{ub} S_1 I + \beta^{ub} S_2 I \geq \beta S I$. Simplifying, we get $\beta^{ub} S_1 I + \beta^{ub} S_2 I = \beta^{ub}(S_1 + S_2) I = \beta^{ub} S I \geq \beta S I$. A similar argument can be made for the lower bound where $\beta^{lb} = \min(\beta_1, \beta_2)$ and we find that $\beta^{lb} S I \leq \beta S I$.

By introducing the bounded parameters, we no longer rely upon the base state variables or parameters. However, in tracking the effect of the bounded parameters, the bounded abstraction must also track bounded rates and bounded state variables. The resulting bounded abstraction thus over-approximates the abstraction and base model, wherein we can derive bounds on the state variables at each time, which may correspond to a larger (hence over-approximation) set of state trajectories.

Definition 6 *A bounded abstraction (Θ^B, Ω^B) of an abstraction (Θ', Ω') of (Θ, Ω) replaces each element of (Θ', Ω') by a pair of elements denoting the lower and upper bound of that element (and referred to with the "lb" and "ub" superscripts). The bounded abstraction defines:*

- *State: For each $x' \in X'$, $x^{lb}, x^{ub} \in X^B$. For each $v'_{x'} \in V'_x$, $\mathcal{X}^B(x^{lb}) = v^B_{x^{lb}}$ and $\mathcal{X}^B(x^{ub}) = v^B_{x^{ub}}$. For each $x^{lb}, x^{ub} \in X^B$, $\mathcal{I}^B(x^{lb}) = \mathcal{I}^B(x^{ub}) = \mathcal{I}'(x')$.*
- *Parameters: For each $p' \in P'$, let $\mathcal{P}^B(p^{lb}) = \min\limits_{p \in P : A(p) = p'} \mathcal{P}(p)$ and $\mathcal{P}^B(p^{ub}) = \max\limits_{p \in P : A(p) = p'} \mathcal{P}(p)$.*
- *Transitions: For each transition $z' \in Z'$ and state variable $x' \in \{x' \in X' | (v_{z'}, v_{x'}) \in E_{in}\} \cup \{x' \in X' | (v_{x'}, v_{z'}) \in E_{out}\}$, $z^{lb}_{x'}, z^{ub}_{x'} \in Z^B$. For each vertex $v_z \in V_z$, if $A(v_z) = v'_z$ then $v^B_{z^{lb}}, v^B_{z^{ub}} \in V^B_z$.*
- *In Edges: For each edge $(v^B_{z'}, v^B_{x'}) \in E'_{in}$, $(v^B_{z^{lb}}, v^B_{x^{lb}}), (v^B_{z^{ub}}, v^B_{x^{ub}}) \in E^B_{in}$.*
- *Out Edges: For each edge $(v^B_{x'}, v^B_{z'}) \in E'_{out}$, $(v^B_{x^{ub}}, v^B_{z^{lb}}), (v^B_{x^{lb}}, v^B_{z^{ub}}) \in E^B_{out}$.*
- *Transition Rates: For each transition $z^{lb} \in Z^B$ and , $\mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z^{lb}) = \min\limits_{z \in Z : A(z) = z'} \mathcal{R}(\mathbf{p}, \mathbf{x}, z)$ (replacing $\mathbf{p}$ and $\mathbf{x}$ of the minimal rate by the elements in $\mathbf{p}^B$ and $\mathbf{x}^B$ respectively, which minimize the rate), and $\mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z^{ub}) = \max\limits_{z \in Z : A(z) = z'} \mathcal{R}(\mathbf{p}, \mathbf{x}, z)$ (similarly replacing $\mathbf{p}$ and $\mathbf{x}$ of the maximal rate by the elements in $\mathbf{p}^B$ and $\mathbf{x}^B$ respectively, which maximize the rate).*

Example 4 *The bounded abstraction* (Θ^B, Ω^B) *of the stratified SIR model defines:*

$$\begin{aligned}
V_x^B &= \{v_S^{lb}, v_S^{ub}, v_I^{lb}, v_I^{ub}, v_R^{lb}, v_R^{ub}, \} \\
V_z^B &= \{v_{inf}^{lb}, v_{inf}^{ub}, v_{rec}^{lb}, v_{rec}^{ub}\} \\
E_{in}^B &= ((v_{inf}^{lb}, v_S^{lb}), (v_{inf}^{lb}, v_I^{lb}), (v_{inf}^{lb}, v_I^{lb}), (v_{rec}^{lb}, v_R^{lb}), (v_{inf}^{ub}, v_S^{ub}), (v_{inf}^{ub}, v_I^{ub}), (v_{inf}^{ub}, v_I^{ub}), (v_{rec}^{ub}, v_R^{ub}) \\
E_{out}^B &= ((v_S^{lb}, v_{inf}^{ub}), (v_I^{lb}, v_{inf}^{ub}), (v_I^{lb}, v_{rec}^{ub}), (v_S^{ub}, v_{inf}^{lb}), (v_I^{ub}, v_{inf}^{lb}), (v_I^{ub}, v_{rec}^{lb})) \\
P^B &= \{\beta^{lb}, \beta^{ub}, \gamma^{lb}, \gamma^{ub}\} \\
X^B &= \{S^{lb}, S^{ub}, I^{lb}, I^{ub}, R^{lb}, R^{ub}\} \\
Z^B &= \{inf^{lb}, inf^{ub}, rec^{lb}, rec^{ub}\} \\
\mathcal{I}^B &= \begin{cases} 0.9 & : S^{lb} \\ 0.9 & : S^{ub} \\ 0.1 & : I^{lb} \\ 0.1 & : I^{ub} \\ 0.0 & : R^{lb} \\ 0.0 & : R^{ub} \end{cases} \\
\mathcal{P}^B &= \begin{cases} 1e{-}7 & : \beta^{lb} \\ 2e{-}7 & : \beta^{ub} \\ 1e{-}5 & : \gamma^{lb} \\ 1e{-}5 & : \gamma^{ub} \end{cases} \\
\mathcal{X}^B &= \begin{cases} v_x^{lb} & : x^{lb} \in X^B \\ v_x^{ub} & : x^{ub} \in X^B \end{cases} \\
\mathcal{Z}^B &= \begin{cases} v_z^{lb} & : z^{lb} \in Z^B \\ v_z^{ub} & : z^{ub} \in Z^B \end{cases} \\
\mathcal{R}^B &= \begin{cases} \beta^{lb} S^{lb} I^{lb} & : z_{inf}^{lb} \\ \beta^{ub} S^{ub} I^{ub} & : z_{inf}^{ub} \\ \gamma^{lb} I^{lb} & : z_{rec}^{lb} \\ \gamma^{ub} I^{ub} & : z_{rec}^{ub} \end{cases}
\end{aligned}$$

The gradient for the bounded abstraction defines:

$$\nabla_{\Theta^B,\Omega^B} = \begin{bmatrix} \frac{dS^{lb}}{dt} \\ \frac{dS^{ub}}{dt} \\ \frac{dI^{lb}}{dt} \\ \frac{dI^{ub}}{dt} \\ \frac{dR^{lb}}{dt} \\ \frac{dR^{ub}}{dt} \end{bmatrix} = \begin{bmatrix} -\mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{inf}^{ub}) \\ -\mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{inf}^{lb}) \\ \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{inf}^{lb}) - \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{rec}^{ub}) \\ \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{inf}^{ub}) - \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{rec}^{lb}) \\ \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{rec}^{lb}) \\ \mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z_{rec}^{ub}) \end{bmatrix} = \begin{bmatrix} -\beta^{ub} S^{ub} I^{ub} \\ -\beta^{lb} S^{lb} I^{lb} \\ \beta^{lb} S^{lb} I^{lb} - \gamma^{ub} I^{ub} \\ \beta^{ub} S^{ub} I^{ub} - \gamma^{lb} I^{lb} \\ \gamma^{lb} I^{lb} \\ \gamma^{ub} I^{ub} \end{bmatrix} \tag{3}$$

5 SIR Example Results

Figures 1 to 5 illustrate several variations of the SIR model and an example simulation of the model. The variations correspond to the model at different points in the process of stratifying, abstracting, and bounding the model. The simulation results were computed by FUNMAN for each model, and the output variables differ by model.

Figure 1 is the original SIR model. The model includes the S, I, and R variables, and the two transitions inf and rec. The model simulation uses parameters $\beta = 0.00035$ and $\gamma = 0.1$. The total population size is 1001, and the simulation uses 100 timepoints. The initial state assigns $S = 1000$, $I = 1$ and $R = 0$. The peak infections occur at approximately day 40.

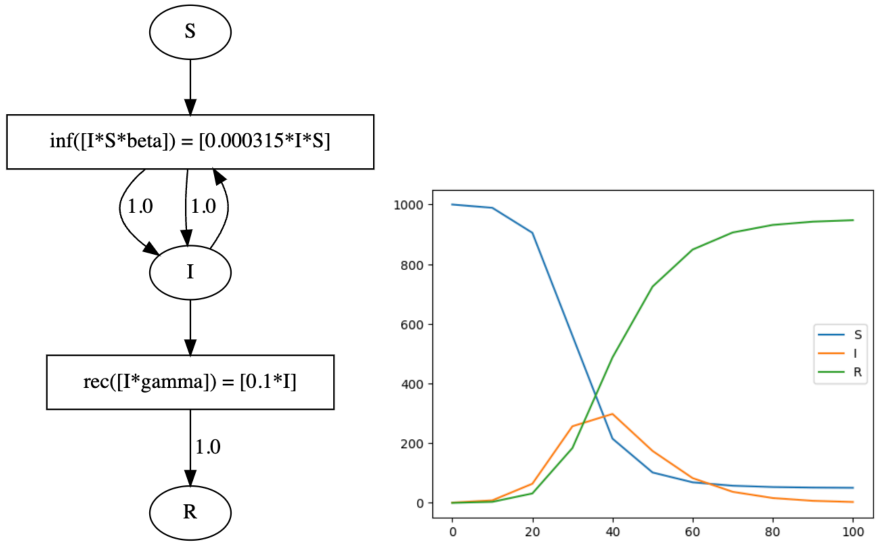

Figure 1: Stratified SIR Model (left) and Simulation (right)

Figure 2 illustrates the baseline SIR after transforming it to bound S, I, and R. The corresponding lower and upper bounds for each state variable are denoted by a $\_lb$ or $\_ub$ suffix. The model is different from the baseline in the following ways: there are six state variables and eight transitions, and the transitions use custom rates. Each baseline transition is replaced by four transitions. The four transitions differ in whether they define a lower or upper bound, and whether they define the flow into or out from a transition. For example, the first transition 'inf_in_lb' defines the lower bound on the flow from S_lb into the 'inf' transition. The least flow expression is illustrated in the box for the transition. Simulating this model with the same initial state and parameters (where the lower and upper bounds are initially equal) results in a simulation where the lower and upper bounds are equal for all variables. While bounding this model in this fashion is not useful in itself, it illustrates a simple application of the bounding transformation. The bounded abstraction, described below, is similar except that it uses alternative bounds on the parameters.

Figure 3 illustrates the stratified SIR model (wrt. S). It uses state variables that distinguish two S populations and two inf transitions that distinguish different rates due to two β parameters. We modified the β parameters to be slightly less and greater than β from the previous models. The simulation illustrates a difference between the S variables.

Figure 4 illustrates a bounded stratified model, for the sake of illustration. It resembles the bounded baseline model aside from incorporating the stratified S variable. The simulation shows how it is possible to bound the stratified variables and achieve similar results to prior models. The primary distinction with this model is how it bounds the stratified variables individually instead of collectively. The collective bounding can be achieved by first abstracting and then bounding the stratified variables.

Figure 5 illustrates the bounded abstracted model. It resembles the bounded baseline model, except that it incorporates upper and lower bounds on the β parameter due to the stratified populations. By propagating lower and upper bounds that are not equal, this variation of the model captures lower and upper bounds on the abstracted state variables. The bounds are tight enough to answer several queries about the model. For example, it can assess whether a upper threshold (that does not fall between the bounds) on peak infected I is satisfied. The threshold $I \leq 400$ is satisfied because $I\_ub \leq 400$. However, the threshold $I \leq 300$ may or may not be satisfied because $I\_lb \leq 300 \leq I\_ub$.

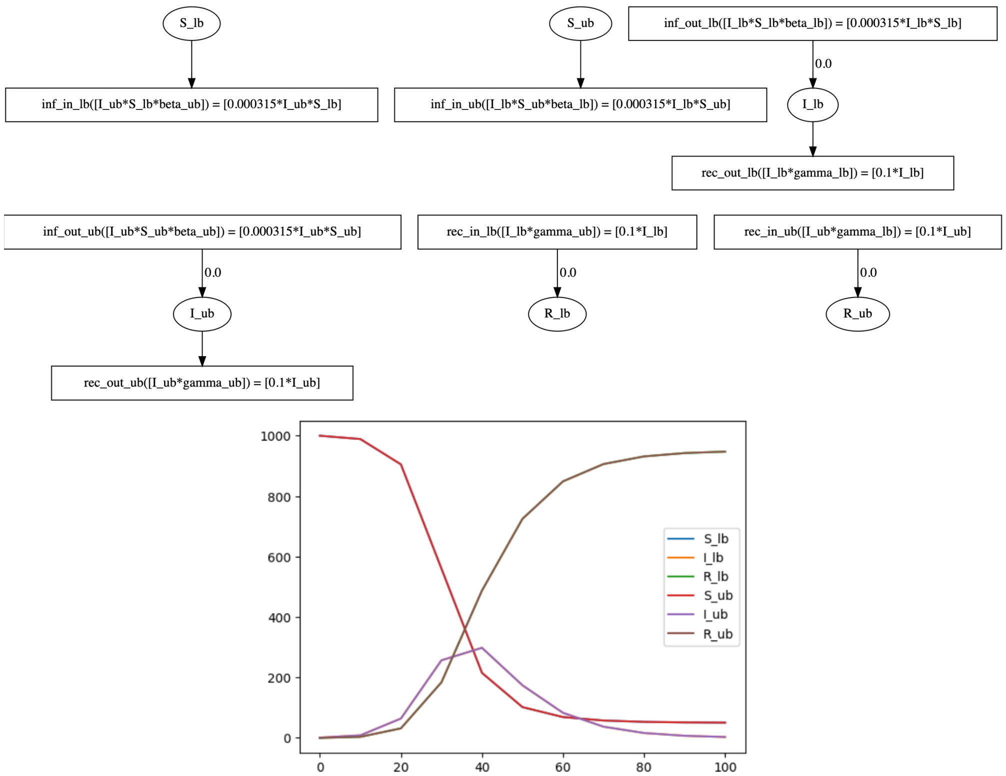

Figure 2: Bounded SIR Model (top) and Simulation (bottom)

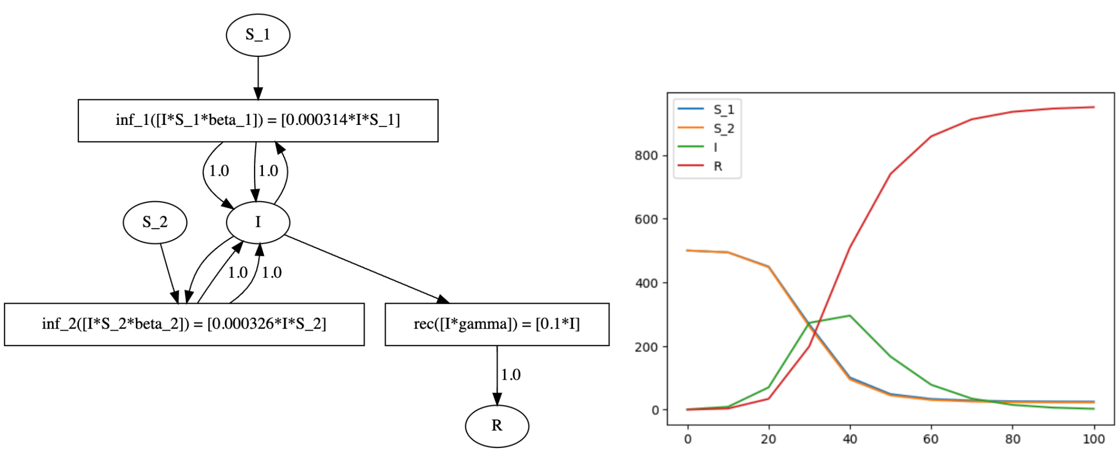

Figure 3: Stratified SIR Model (top) and Simulation (bottom)

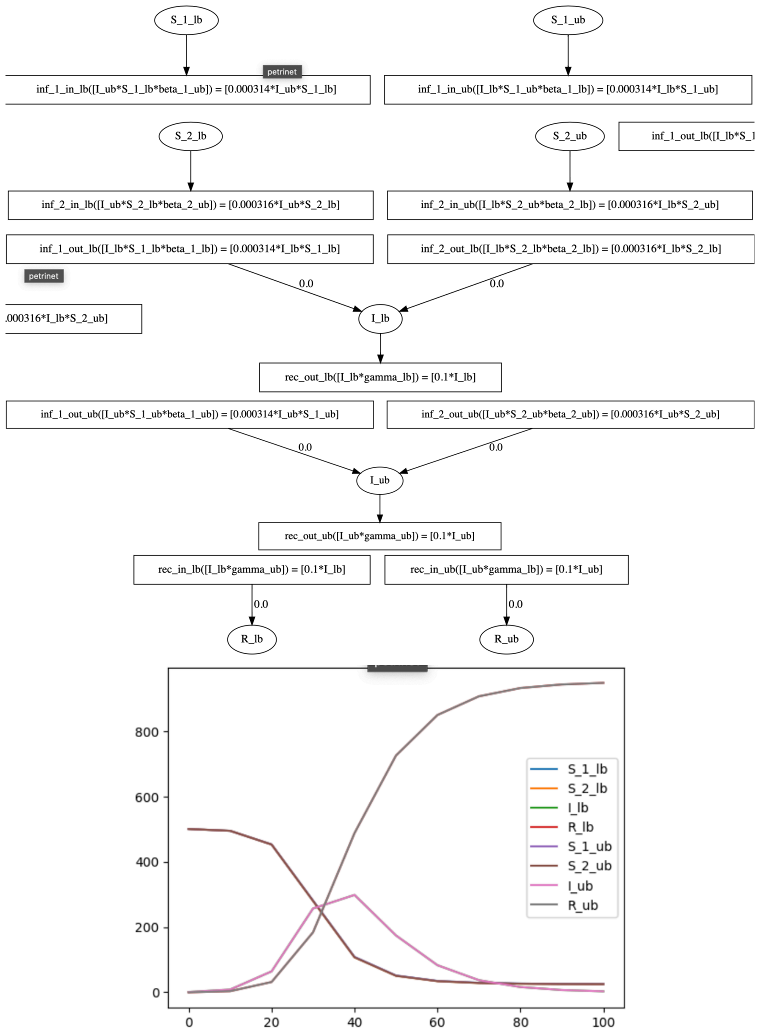

Figure 4: Bounded Stratified SIR Model (top) and Simulation (bottom)

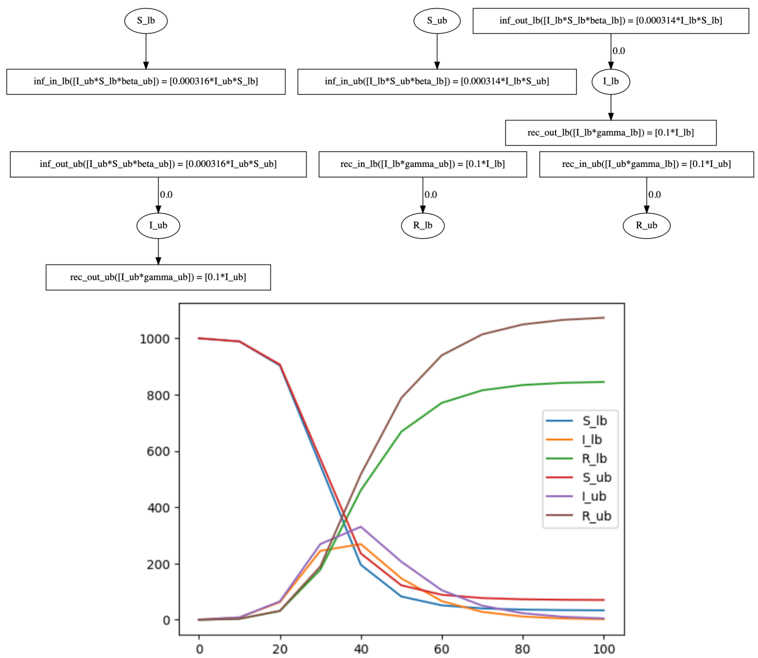

Figure 5: Bounded Stratified SIR Model (top) and Simulation (bottom)