FUNMANAbstraction

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1 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 $\frac{\mathbf{dx}}{\mathbf{dt}}$, 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:*

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

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:

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

2 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 "*"):*

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

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

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.

3 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 $z' \in Z'$, $z^{lb}, z^{ub} \in Z^B$. 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 $z^{lb} \in Z^B$, $\mathcal{R}^B(\mathbf{p}^B, \mathbf{x}^B, z^{lb}) = \min\limits_{z \in Z: A(z) = z'} \mathcal{R}(\mathbf{p}, \mathbf{x}, z)$ (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:*

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

The gradient for the bounded abstraction defines:

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

The bounded abstraction defines lower and upper bounds on the abstract state variables, for example:

$$
\begin{array}{rcl}
\frac{dS^{lb}}{dt} & \leq \frac{dS}{dt} & \leq \frac{dS^{ub}}{dt} \\
-\beta^{ub} S^{ub} I^{ub} & \leq \frac{dS}{dt} & \leq -\beta^{lb} S^{lb} I^{lb} \\
-\max(\beta_1, \beta_2) S^{ub} I^{ub} & \leq \frac{d(S_1+S_2)}{dt} & \leq -\min(\beta_1, \beta_2) S^{lb} I^{lb} \\
-\max(\beta_1, \beta_2) S^{ub} I^{ub} \leq -\max(\beta_1, \beta_2)(S_1 + S_2) I^{ub} & \leq \frac{dS_1}{dt} + \frac{dS_2}{dt} & \leq -\min(\beta_1, \beta_2)(S_1 + S_2) I^{lb} \leq -\min(\beta_1, \beta_2) S^{lb} I^{lb} \\
-\max(\beta_1, \beta_2) S^{ub} I^{ub} \leq -\max(\beta_1, \beta_2)(S_1 + S_2) I^{ub} & \leq \frac{dS_1}{dt} + \frac{dS_2}{dt} & \leq -\min(\beta_1, \beta_2)(S_1 + S_2) I \leq -\min(\beta_1, \beta_2)(S_1 + S_2) I^{lb} \leq
\end{array}
$$