Simplified Unimodal Influence Networks

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1. Simplified Unimodal Influence Networks

This note provides supplementary material to the LICS'16 submission titled "Comparing Chemical Reaction Networks: A Categorical and Algorithmic Perspective". It presents a technique that can be used to speed up the calculation of Algorithm 2 in the case of unimodal influence networks.

Definition 1. *Let (S, R) be a unimodal influence network and $v(0) \in \mathbb{R}^S$ the underlying initial condition. Define for each set of ODEs*

$$\dot{x}_0 = -\alpha_{01} \cdot x_0 \cdot y_i + \alpha_{10} \cdot x_1 \cdot z_j$$
$$\dot{x}_1 = -\alpha_{10} \cdot x_1 \cdot z_j - \alpha_{12} \cdot x_1 \cdot y_i + \alpha_{01} \cdot x_0 \cdot y_i + \alpha_{21} \cdot x_2 \cdot z_j$$
$$\dot{x}_2 = -\alpha_{21} \cdot x_2 \cdot z_j + \alpha_{12} \cdot x_1 \cdot y_i$$

underlying a triplet (x_0, x_1, x_2) of (S, R) the set of simplified ODEs

$$\dot{\underline{x}}_0 = -\alpha_{01} \cdot \underline{x}_0 \cdot \underline{y}_i + \alpha_{10} \cdot \Big(\sum_{j=1}^{3} v_{x_j}(0) - \underline{x}_0 - \underline{x}_2 \Big) \cdot \underline{z}_j$$

$$\dot{\underline{x}}_2 = -\alpha_{21} \cdot \underline{x}_2 \cdot \underline{z}_j + \alpha_{12} \cdot \Big(\sum_{j=1}^{3} v_{x_j}(0) - \underline{x}_0 - \underline{x}_2 \Big) \cdot \underline{y}_i$$

Let $\underline{f} : \mathbb{R}^{\underline{S}} \to \mathbb{R}^{\underline{S}}$ denote the so constructed simplified drift, where $\underline{S} = \{\underline{x}_0 \mid x_0 \in S\} \cup \{\underline{x}_2 \mid x_2 \in S\}$.

The simplified drift is closely related to the drift $f : \mathbb{R}^S \to \mathbb{R}^S$ of (S, R). In particular, if $\dot{v} = f(v)$ and $\dot{w} = \underline{f}(w)$ with $v_{x_0}(0) = w_{\underline{x}_0}(0)$ and $v_{x_2}(0) = w_{\underline{x}_2}(0)$ for all triplets (x_0, x_1, x_2) of (S, R), it holds that $v_{x_0} \equiv w_{\underline{x}_0}$ and $v_{x_2} \equiv w_{\underline{x}_2}$ for all triplets (x_0, x_1, x_2) of (S, R). This property can be used to show the following result.

Proposition 1. *Fix a $\delta > 0$, a unimodal influence network (S, R) and let $\underline{f} : \mathbb{R}^{\underline{S}} \to \mathbb{R}^{\underline{S}}$ denote the simplified drift in the case where $\sum_{j=1}^{3} v_{x_j}(0) = \delta$ for all triplets (x_0, x_1, x_2) of (S, R). Similarly, let $(\hat{S}, \hat{R})$ denote a unimodal influence network and let $\underline{\hat{f}} : \mathbb{R}^{\underline{\hat{S}}} \to \mathbb{R}^{\underline{\hat{S}}}$ denote the simplified drift in the case where $\sum_{j=1}^{3} \hat{v}_{\hat{x}_j}(0) = \delta$ for all triplets $(\hat{x}_0, \hat{x}_1, \hat{x}_2)$ of $(\hat{S}, \hat{R})$. Assume that $\mu : S \to \hat{S}$ is a triplet preserving emulation. Then, $\underline{\mu} : \underline{S} \to \underline{\hat{S}}, \underline{x} \mapsto \underline{\mu(x)}$ is an emulation.*

Proof. Assume that $\mu : S \to \hat{S}$ is a triplet preserving emulation and let $\mathcal{H}$ denote the underlying union BDE partition. Then, for any $H \in \mathcal{H}$, it holds that H contains either only middle species with index one, or has no middle species at all. Moreover, by choosing the initial conditions $v \in \mathbb{R}^S$ and $\hat{v} \in \mathbb{R}^{\hat{S}}$ as in the construction of $\underline{f}$ and $\underline{\hat{f}}$, the trajectories of the simplified drifts coincide with those underlying the original drifts f and $\hat{f}$. This yields the claim. □

Note that if $\mu : S \to \hat{S}$ is a triplet preserving emulation and $\mu(x_0) \in \{y_0, y_2\}$, then $\mu(x_1) = y_1$. Thus, any triplet preserving emulation can be reconstructed from $\underline{\mu}$, meaning that the above result shows that one can find all triplet preserving emulations by studying the emulations between the simplified drifts.

The motivation to work on simplified drifts $\underline{f}$ is rooted in the fact that $\underline{f}$ arises from f by removing redundancy. This usually implies that the largest dimension of all generalized eigenspaces underlying the Jacobian of $\underline{f}$ at point $\mathbb{1}$ is substantially smaller than the largest dimension of all generalized eigenspaces underlying the Jacobian of f at point $\mathbb{1}$. This, in turn, greatly improves the performance of Algorithm 2.

We applied this simplification to some models studied in Section 5 to speed up the calculation. The underlying `crn` files contain `simp` in their name.