Asymptotic state lumping in network problems

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Figure: The theory refers to the question how to deal with complex and interrelated models such as description of a metapopulation consisting of several interacting with each other subpopulations.

From macro to micro models

Let us assume that we have a macromodel of a metapopulation. In order to build resonable relations in a micro scale we can:

1. Enhance the macromodel introducing dynamics into vertices.
2. Identify time scales that refer to the behaviour of, first, individuals and then the whole society.
3. Check the consistency of the micromodel by comparing dynamics of both models at the macroscale.

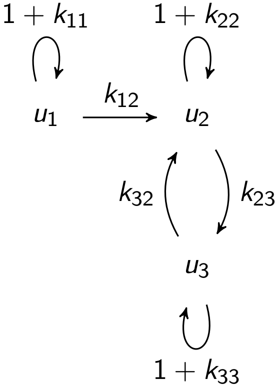
Consider the population described by $\mathbf{u} = (u_1, u_2, u_3)$, where u_j is the number of cells whose genotype belongs to the class j.

Evolution can be described by the system

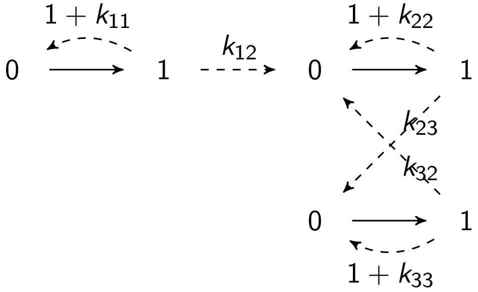
$$\mathbf{u}' = \mathbb{K}\mathbf{u},$$

where matrix $\mathbb{K}$ describing connections between the nodes is given in the form

$$\mathbb{K} = \begin{pmatrix} 1+k_{11} & 0 & 0 \\ k_{12} & 1+k_{22} & 0 \\ 0 & k_{23} & 1+k_{33} \end{pmatrix}$$



In order to introduce dynamics we identify each node with one-dimensional domain. Position at the interval $[0,1]$ related to the vertex u_j informs about the age of individual whose genotype belongs to the class j. The process of aging is described by transport along the edges.



Let us consider an oriented metric graph with weights $G = (V, E, \mu)$, where $V = \{v_1, v_2, \ldots, v_n\}$ is a set of n vertices, $E = \{e = v_i v_j \times [0, 1] : \quad v_i, v_j \in V\}$ is a set of m edges and the function $\mu : E \to \mathbb{R}$ defines weights of edges such that

$$\forall_{i,j=1,2,...,n} \quad \mu(v_i v_j \times [0, 1]) = w_{ik} \quad \text{where } v_i \overset{e_k}{\to} v_j.$$

We suppose that G is connected but not necessarily strongly connected.

On each edge of a graph we define the function $\mathbf{u} = (u_1, u_2, ..., u_m)$ that depends on the position on the edge $x \in [0, 1]$ and the time $t \in \mathbb{R}_+$.

Let us define matrix $\mathbb{B} = (b_{ij})_{i,j=1,2,...,n}$ by

$$b_{ij} = \begin{cases} w_{ki} & \text{if } \exists_k \overset{e_j}{\to} v_k \overset{e_i}{\to} \\ 0 & \text{otherwise;} \end{cases}$$

which describes the relation between edges of the graph. We denote the matrix of speeds of transport at each edge by $\mathbb{C} = diag\,\{c_1, c_2, ..., c_m\} > 0$. Now, the transport problem on network can be formulated as follows

$$\begin{aligned} \partial_t \mathbf{u}(x,t) &= -\mathbb{C}\partial_x \mathbf{u}(x,t), \quad x \in (0,1) \times \mathbb{R}_+, \\ \mathbf{u}(0,t) &= \mathbb{C}^{-1}\mathbb{B}\mathbb{C}\mathbf{u}(1,t), \quad t > 0, \\ \mathbf{u}(x,0) &= \mathring{\mathbf{u}}(x), \quad x \in (0,1). \end{aligned} \tag{1}$$

Theorem

For an arbitrary matrix $\mathbb{B}$, the transport model on generalized network has a unique solution which can be represented by a semigroup $(T(t))_{t\geq 0}$,

$$\mathbf{u}(x,t) = T(t)\mathring{\mathbf{u}}(x)$$

generated by the operator $A := -\mathbb{C}\partial_x$ considered on the domain

$$D(A) = \left\{\mathbf{u} \in W_1^1([0,1])^m : \quad \mathbf{u}(0) = \mathbb{C}^{-1}\mathbb{B}\mathbb{C}\mathbf{u}(1)\right\}.$$

Additionally, the solution to system (1) is positive for each positive initial condition if and only if the matrix $\mathbb{B}$ is positive.

Processes in microscale occur much faster than those at the macroscale. To separate different scales we modify a the problem by introducing a small parameter:

$$\begin{cases} \partial_t \mathbf{u}(x,t) &= A_\epsilon \mathbf{u}(x,t); \quad x \in (0,1), \quad t \in \mathbb{R}_+ \\ \mathbf{u}(x,0) &= \mathring{\mathbf{u}}(x); \quad x \in (0,1), \end{cases} \tag{2}$$

where $(A_\epsilon)_{\epsilon \geq 0}$ is a family of operators $A_\epsilon = -\frac{1}{\epsilon}\partial_x$ with a domain of a form

$$D(A) = \left\{ \mathbf{u} \in (W_1^1([0,1]))^m : \quad \mathbf{u}(0) = (\mathbb{I} + \epsilon \mathbb{B})\, \mathbf{u}(1) \right\}.$$

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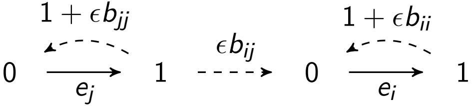


Theorem

For any $T \in (0, \infty)$ *there exists* $C(T, \mathbb{B})$ *such that for any (sufficiently small)* $\epsilon > 0$ *and* $\mathring{\mathbf{u}} \in \mathbf{W}_1^1([0,1])$ *the solution* $\mathbf{u}_\epsilon(x,t) = \left[e^{t\mathbf{A}_\epsilon}\mathring{\mathbf{u}}\right](x)$ *of (2) satisfies*

$$\|\mathcal{P}\mathbf{u}_\epsilon(\cdot, t) - \bar{\mathbf{v}}(t)\|_{\mathbb{R}^m} \leq \epsilon C(T, \mathbb{B})\|\mathring{\mathbf{u}}\|_{\mathbf{W}_1^1(I)}, \tag{3}$$

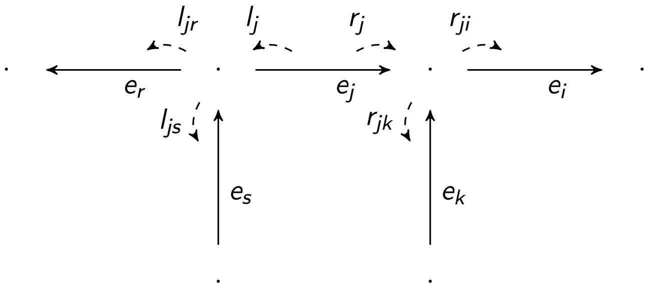
uniformly on $[0, T]$, *where* $\mathcal{P}\mathbf{u} = \int_0^1 \mathbf{u}(x)dx$ *and* $\bar{\mathbf{v}}$ *solves system of ordinary differential equations:*

$$\left\{\begin{array}{rcl} \partial_t \bar{\mathbf{v}}(t) & = & \mathbb{B}\bar{\mathbf{v}}(t), \\ \bar{\mathbf{v}}(0) & = & \mathcal{P}\mathring{\mathbf{u}}. \end{array}\right. \tag{4}$$

For a given (undirected) metric graph $G = (V, E)$, one can consider dynamical systems given on each edge, somehow coupled through interactions at the vertices. Here we assume that on each edge e_j there is a substance with density $u_j, j = 1, 2, ..., m$ which diffuses along this edge and can also enter adjacent edges through semipermeable membrane. The flux from edge j is proportional to the difference of weighted density at the endpoint of e_j and the densities at edges incident to this endpoint of e_j which results in a system of interlinked Robin boundary conditions.

To write down the analytical formulation of the problem, we find it useful to introduce an orientation on G noting that, since diffusion is invariant under the change of the direction, it does not matter which end point of e_j we identify with 0 and which one with 1. However, once such identification is made, we shall refer to the vertex incident to the edge at 0 as the left endpoint (tail) and the vertex incident at 1 as the right endpoint (head).

Let l_j and r_j be the probabilities of diffusing from e_j to the edges incident at the left and right, respectively and let l_{jk} and r_{jk} be the probabilities that, after diffusing from edge e_j to the left, a particle ends up in e_k and, respectively, after diffusing from e_j to the right, the particle ends up in e_k.



Then, the Fick's law at the head v of e_i (identified with 1 on e_i), takes the form

$$-u_i'(1) = r_i u_i(1) - \sum_{j \neq i} r_{ij} u_j(v), \tag{5}$$

where we have written $u_j(v)$ as v may be either the tail or the ahead of an incident edge e_j.

At the left endpoint w of e_i (identified with 0 on e_i) we have

$$u_i'(0) = l_i u_i(0) - \sum_{j \neq i} l_{ij} u_j(w), \qquad (6)$$

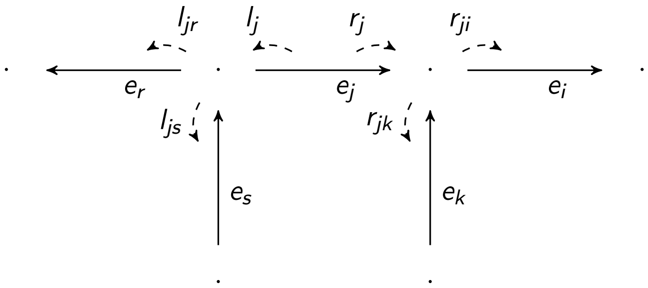
where w is the tail e_i. We adopted convention that if e_j is not incident with the the head of e_i, then $r_{ij} = 0$ and, similarly, if e_j is not incident with the tail of e_i, then $l_{ij} = 0$.

In order to present boundary conditions we introduce matrices K^{00}, K^{01}, K^{10}, K^{11}. For any $i, j = 1, 2, ..., m$ we have

$$k_{ij}^{00} = -l_{ij} \quad \text{if} \ \overset{e_j}{\leftarrow} \cdot \overset{e_i}{\rightarrow}, \qquad k_{ij}^{01} = -l_{ij} \quad \text{if} \ \overset{e_j}{\rightarrow} \cdot \overset{e_i}{\rightarrow},$$

$$k_{ij}^{10} = r_{ij} \ \text{if} \ \overset{e_i}{\rightarrow} \cdot \overset{e_j}{\rightarrow}, \qquad k_{ij}^{11} = r_{ij} \ \text{if} \ \overset{e_i}{\rightarrow} \cdot \overset{e_j}{\leftarrow}$$

$$k_{ii}^{00} = l_i \qquad k_{ii}^{11} = -r_i.$$



Then the model can be written as

$$\begin{aligned}
\partial_t \mathbf{u}(x,t) &= \mathbb{D}\partial_{xx}\mathbf{u}(x,t), \quad (x,t)\in(0,1)\times\mathbb{R}_+,\\
\partial_x \mathbf{u}(0,t) &= \mathbb{K}^{00}\mathbf{u}(0,t)+\mathbb{K}^{01}\mathbf{u}(1,t), \quad t>0,\\
\partial_x \mathbf{u}(1,t) &= \mathbb{K}^{10}\mathbf{u}(0,t)+\mathbb{K}^{11}\mathbf{u}(1,t), \quad t>0,\\
\mathbf{u}(x,0) &= \mathring{\mathbf{u}}(x), \quad x\in(0,1)\,,
\end{aligned} \tag{7}$$

where $\mathbf{u}=(u_1,\ldots,u_m)$, $\mathbb{D}=\mathrm{diag}\{\sigma_i\}_{1\le i\le m}$.

Note that there is no need to restrict ourselves to matrices $\mathbb{K}^{ij}$ arising from the diffusion on graphs. We can consider a family of diffusion processes depending on an abstract attribute $j=1,2,...,m$ which may switch between each other according to the rule given by $\mathbb{K}^{ij}$.

Theorem

For arbitrary matrices $\mathbb{K}^{00}$, $\mathbb{K}^{01}$ $\mathbb{K}^{10}$, $\mathbb{K}^{11}$, *the diffusion model on a generalized network has a unique solution which can be represented by a semigroup* $(T(t))_{t\geq 0}$,

$$\mathbf{u}(x,t) = T(t)\mathring{\mathbf{u}}(x)$$

generated by the operator $A := \mathbb{D}\partial_{xx}$ *considered on the domain*

$$D(A) = \left\{ \mathbf{u} \in \mathbf{Y} : \quad \begin{array}{c} \partial_x \mathbf{u}(0,t) = \mathbb{K}^{00}\mathbf{u}(0,t) + \mathbb{K}^{01}\mathbf{u}(1,t) \\ \partial_x \mathbf{u}(1,t) = \mathbb{K}^{10}\mathbf{u}(0,t) + \mathbb{K}^{11}\mathbf{u}(1,t) \end{array} \right\}$$

where $\mathbf{Y} = \mathbf{W}_1^2([0,1])$.

In analogy to the transport problem on a generalized network we can a introduce small parameter to identify different time scales. We obtain a family of problems for $\epsilon > 0$ of a form

$$\begin{aligned}
\partial_t \mathbf{u}(x,t) &= \frac{1}{\epsilon}\partial_{xx}\mathbf{u}(x,t), \quad (x,t) \in (0,1)\times\mathbb{R}_+, \\
\partial_x \mathbf{u}(0,t) &= \epsilon\mathbb{K}^{00}\mathbf{u}(0,t) + \epsilon\mathbb{K}^{01}\mathbf{u}(1,t), \quad t>0, \\
\partial_x \mathbf{u}(1,t) &= \epsilon\mathbb{K}^{10}\mathbf{u}(0,t) + \epsilon\mathbb{K}^{11}\mathbf{u}(1,t), \quad t>0, \\
\mathbf{u}(x,0) &= \mathring{\mathbf{u}}(x), \quad x \in (0,1)\,,
\end{aligned} \tag{8}$$

Theorem

Let $\mathbf{u}_\epsilon(t) = e^{t\mathbf{A}_\epsilon}\mathring{\mathbf{u}}$ *with* $\mathring{\mathbf{u}} \in \mathbf{W}_1^2([0,1])$ *be the solution of (8) in* $\mathbf{L}_1([0,1])$ *and* $\bar{\mathbf{v}}$ *and* $\widetilde{\mathbf{w}}_0$ *be the solutions, respectively, to*

$$\partial_t\bar{\mathbf{v}} = \left(\mathbb{K}^{10} - \mathbb{K}^{00} + \mathbb{K}^{11} - \mathbb{K}^{01}\right)\bar{\mathbf{v}}, \qquad \bar{\mathbf{v}}(0) = \mathcal{P}\mathring{\mathbf{u}} \tag{9}$$

$$\partial_\tau\tilde{\mathbf{w}}_0(x,\tau) = \partial_{xx}\tilde{\mathbf{w}}_0(x,\tau), \qquad \partial_x\tilde{\mathbf{w}}_0(1,\tau) = \partial_x\tilde{\mathbf{w}}_0(0,\tau) = 0,$$

$$\widetilde{\mathbf{w}}_0(x,0) = \mathring{\mathbf{u}}(x) - \mathcal{P}\mathring{\mathbf{u}}.$$

Then, for any $0 < T < \infty$*, there is* $C = C(T, \mathbb{K}^{00}, \mathbb{K}^{01}, \mathbb{K}^{10}, \mathbb{K}^{11})$ *such that, uniformly on* $[0,T]$*, the following condition is satisfied*

$$\|\mathbf{u}_\epsilon(t) - \bar{\mathbf{v}}(t) - \widetilde{\mathbf{w}}_0(t/\epsilon)\|_{\mathbf{L}_1([0,1])} \leq \epsilon C \|\mathring{\mathbf{u}}\|_{\mathbf{W}_1^2([0,1])}. \tag{10}$$

The result in the diffusion case is of a different type than in the transport equation. In the former, the initial layer term $\widetilde{\mathbf{w}}_0$ decays exponentially to 0 as $\epsilon \to 0$ for any $t > 0$. Hence, outside an $O(\epsilon)$ transition zone, the whole solution to the PDE problem on a network (8) can be approximated by the solution of an ODE system (9).

In contrast to the diffusion problem, in transport the solution outside the hydrodynamic space does not decay exponentially. Hence, we only can approximate the macroscopic characteristics of the flow; that is, the mass on each edge, given by $\mathcal{P}\mathbf{u}$, by the solution to ODE.

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IIASA

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