Rigorous Continuum Limit for the Discrete Network Formation Problem

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Transportation networks in biology

Continuum Limit for Network Formation
Discrete network models

- Static and dynamic discrete graph-based models, deterministic and random graphs.

- Solutions obtained by global energy minimization; combinatorial approach with NP-completeness issues.
Discrete modeling framework

- Flow of a material through the network-graph \((V, E)\)
  
  Pressures \(P_j\) on vertices \(j \in V\)
  Conductivities \(C_{ij}\) on edges \((i, j) \in E\)

- Assume low Reynolds number (Poiseuille flow), then
  
  Poiseuille fluxes \(Q_{ij} = C_{ij} \frac{P_i - P_j}{L_{ij}}\)

- Conservation of mass - Kirchhoff law with sources \(S_j\),
  
  \[- \sum_i Q_{ij} = - \sum_i C_{ij} \frac{P_i - P_j}{L_{ij}} = S_j \quad \text{for each } j \in V\]

- Topology, geometry and sources given as input.
Discrete modeling framework

Energy cost functional

\[ E[C] := \frac{1}{2} \sum_{(i,j) \in \mathcal{E}} \left( \frac{Q_{ij}^2}{C_{ij}} + \nu C_{ij}^\gamma \right) L_{ij} \]

consisting of

- **pumping power** (Joule’s law: power = potential diff. \( \times \) current)

\[ (P_i - P_j) Q_{ij} = \frac{Q_{ij}^2}{C_{ij}} L_{ij} \]

- **metabolic cost** \( \sim C_{ij}^\gamma L_{ij} \)
  - \( \gamma = 1/2 \) for blood flow (Murray’s theory)
  - \( 1/2 \leq \gamma \leq 1 \) for leaf venation

Gradient flow of \( E \), constrained by the Kirchhoff law \( \Rightarrow \) ODE system:

\[ \frac{dC_{ij}}{dt} = \left( \frac{Q_{ij}^2}{C_{ij}^2} - \nu \gamma C_{ij}^{\gamma-1} \right) L_{ij} \]
Simulation results [Hu-Cai’13]
Rigorous continuum limit
Transition to continuum description

- Kirchhoff law

\[ \sum_i C_{ij} \frac{P_i - P_j}{L_{ij}} = S_j \quad \text{for each } j \in \mathcal{V} \]

\[ \rightarrow \text{ Poisson equation } (C_{ij} \leftrightarrow c, P_i \leftrightarrow p) \]

\[ -\nabla \cdot (c \nabla p) = S \quad \text{for all } x \in \Omega \]

- The discrete energy functional

\[ E[C] = \sum_{(i,j) \in \mathcal{E}} \left( C_{ij} \left( \frac{P_i - P_j}{L_{ij}} \right)^2 + \frac{\nu}{\gamma} C_{ij} \right) L_{ij} \]

\[ \rightarrow \text{ continuum energy functional} \]

\[ \mathcal{E}[c] := \int_{\Omega} \nabla p[c] \cdot c \nabla p[c] + \frac{\nu}{\gamma} |c|^{\gamma} \, dx \]
Transition to continuum description

- To avoid issues with degeneracy: regularize
  replace $C_{ij}$ with $r + C_{ij}$

- Fix the network topology and geometry: rectangular networks

- The program:
  1. Establish a connection between the discrete solutions of the
     Kirchhoff law and weak solutions of the Poisson equation

     $$-\nabla \cdot ((r\mathbb{I} + c)\nabla p) = S$$

  2. Reformulate the discrete energy functional as an integral functional
     defined on the set of bounded tensor fields $c = c(x)$,

     $$\bar{E}[c] = \int_{\Omega} \nabla p[c] \cdot (rl + c)\nabla p[c] + \frac{\nu}{\gamma}|r + c|^{\gamma} \, dx$$

  3. Show $\Gamma$-convergence of the sequence of integral functionals.
1D equidistant case
Define the sequence of operators $Q_0^N : \mathbb{R}^N \rightarrow L^\infty(0, 1)$ by

$Q_0^N : (C_i)_{i=1}^N \mapsto c$, \hspace{1cm} $c(x) \equiv C_i$ for $x \in (x_{i-1}, x_i), \ i = 1, \ldots, N$.

**Step 1.** Kirchhoff with $C = (C_i)_{i=1}^N \longleftrightarrow$ Poisson with $Q_0^N[C],$

$$-\partial_x \left( (r + Q_0^N[C]) \partial_x p \right) = S,$$ no-flux BC

Using the "standard" hat function $\varphi_i^N$ as a test function, we obtain

$$(r + C_i) \frac{p(x_i) - p(x_{i-1})}{h} + (r + C_{i+1}) \frac{p(x_i) - p(x_{i+1})}{h} = S_i^N h,$$

for $i = 1, \ldots, N$, with

$$S_i^N := \frac{1}{h} \int_0^1 S(x) \varphi_i^N(x) \, dx$$

$\Rightarrow$ identification $P_i := p(x_i)$.
Step 2. Define the functionals $\bar{E}^N : L^\infty_+(0, 1) \mapsto \mathbb{R}$,

$$\bar{E}^N[c] := \int_0^1 (r + c) \left( Q_0^N[\Delta^h P] \right)^2 + \frac{\nu}{\gamma} (r + c)^\gamma \, dx,$$

with

$$(\Delta^h P)_i := \frac{P_i - P_{i-1}}{h}, \quad i = 1, \ldots, N,$$

and $P = (P_i)_{i=0}^N$ a solution of the Kirchhoff law with the conductivities

$$C_i := \frac{1}{h} \int_{x_{i-1}}^{x_i} c(x) \, dx, \quad i = 1, \ldots, N.$$

Then, the discrete energy functional can be written in the integral form as

$$E^N[C] = \bar{E}^N[Q_0^N[C]].$$
Step 3. Show the $\Gamma$-convergence of the sequence of functionals

$$\bar{\mathcal{E}}^N[c] := \int_0^1 (r + c) \left( \mathcal{Q}_0^N[\Delta_h P] \right)^2 + \frac{\nu}{\gamma} (r + c)^\gamma \, dx,$$

Towards

$$\bar{\mathcal{E}}[c] := \int_0^1 (r + c) (\partial_x p[c])^2 + \frac{\nu}{\gamma} (r + c)^\gamma \, dx,$$

with $p = p[c]$ a solution of the Poisson equation with conductivity $c = c(x)$,

$$-\partial_x ((r + c) \partial_x p) = S.$$
Prove $\Gamma$-convergence of $\bar{E}^N$ towards $\bar{E}$ as $h = 1/N \to 0$, with respect to the norm $L^2$-topology.

The obvious difficulty: Passage to the limit in the nonlinear term

$$(r + c^N) \left( Q_0^N [\Delta^h P] \right)^2$$

Weak-strong lemma:
Let $(c^N)_{N \in \mathbb{N}} \subset L^\infty(\Omega)$ be a sequence of nonnegative functions such that $c^N \to c \in L^2(\Omega)$ in the norm topology of $L^2(\Omega)$. Let $(p^N)_{N \in \mathbb{N}} \subset H^1(\Omega)$ be a sequence of zero-average weak solutions of the Poisson equation

$$-\nabla \cdot ((r + c^N) \nabla p^N) = S$$

subject to homogeneous Neumann boundary conditions on $\partial \Omega$. Then $\nabla p^N$ converges to $\nabla p$ strongly in $L^2(\Omega)$, where $p$ solves

$$-\nabla \cdot ((r + c) \nabla p) = S$$
2D rectangular case
The operator $Q^N_0$ maps $C$ onto piecewise constant $2 \times 2$ diagonal tensors,

$$Q^N_0 : (C_i)_{i \in EN} \mapsto \begin{pmatrix} c_1 & 0 \\ 0 & c_2 \end{pmatrix},$$

where $c_1$ is the conductivity of the horizontal edge and $c_2$ is the conductivity of the vertical edge.

**FEM**-discretization of the Poisson equation, establish connection to Kirchhoff by taking vertex values of the piecewise linear FE-functions.

Show $\Gamma$-convergence using

- FEM techniques (**Céa’s Lemma** in the energy norm)
- weak-strong convergence result for the Poisson equation
Grid (network) consisting of parallelograms with sides in linearly independent directions $\theta_1, \theta_2 \in S^1$. The coordinate transform

$$(1, 0) \mapsto \theta_1, \quad (0, 1) \mapsto \theta_2$$

leads to the transformed continuum energy functional

$$\mathcal{E}[c] = \int_{\Omega} \nabla p[c] \cdot \mathbb{P}[c] \nabla p[c] + \frac{\nu}{\gamma} (|r + c_1|^{\gamma} + |r + c_2|^{\gamma}) \, dx$$

coupled to the Poisson equation

$$-\nabla \cdot (\mathbb{P}[c] \nabla p) = S$$

with the permeability tensor

$$\mathbb{P}[c] = rl + c_1 \theta_1 \otimes \theta_1 + c_2 \theta_2 \otimes \theta_2$$
Formal $L^2$-gradient flow
The conductivity $c^k$ in the $k$-th spatial direction,

$$\partial_t c^k = (\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-2} c^k, \quad k = 1, \ldots, d,$$

coupled to the Poisson equation

$$-\nabla \cdot ((rI + c)\nabla p) = S, \quad c = \begin{pmatrix} c^1 \\ \vdots \\ c^d \end{pmatrix}$$

equipped with no-flux boundary condition.

**Regularization:** Random fluctuations of conductivity in the medium

$$\partial_t c^k = D^2 \Delta c^k + (\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-2} c^k, \quad k = 1, \ldots, d,$$

subject to homogeneous Dirichlet BC.
Formal $L^2$-gradient flow

Poisson equation for the pressure $p$

$$-\nabla \cdot ((rI + c)\nabla p) = S, \quad c = \begin{pmatrix} c^1 \\ \vdots \\ c^d \end{pmatrix}$$

coupled to the reaction-diffusion system for the conductivities $c^k$

$$\partial_t c^k = D^2 \Delta c^k + (\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-2} c^k$$

- $D^2 \geq 0$ - diffusivity, $\nu > 0$ - metabolic constant
- $\gamma \geq 1$ - relaxation exponent
- No-flux BC for the Poisson equation
- Homogeneous Dirichlet BC for conductivity
The system

\[-\nabla \cdot ((r\mathbb{I} + c)\nabla p) = S\]
\[\partial_t c^k = D^2 \Delta c^k + (\partial_{x_k} p)^2 - \nu |c^k|^{\gamma-2} c^k\]

is a formal $L^2$-gradient flow of the energy functional

\[\mathcal{E}[c] = \int_{\Omega} \frac{D^2}{2} |\nabla c|^2 + \nabla p \cdot (r\mathbb{I} + c)\nabla p + \frac{\nu}{\gamma} |c|^{\gamma} \, dx,\]

with $|\nabla c|^2 := \sum_{k=1}^d |\nabla c^k|^2$ and $|c|^{\gamma} := \sum_{k=1}^d |c^k|^{\gamma}$.

**Theorem:**
Let $S \in L^2(\Omega)$, $\gamma > 1$ and $c_0 \in L^\gamma(\Omega)^{d \times d}$.
Then the system admits a **global weak solution** in the energy space.
Introduce the regularized Poisson equation

\[-\nabla \cdot (P^\epsilon[c] \nabla p) = S\]

with the permeability tensor

\[P^\epsilon[c] := r I + c \ast \eta^\epsilon\]

with \(\eta^\epsilon\) a nonnegative, radially symmetric mollifier,

\[c^k \ast \eta^\epsilon(x) := \int_{\mathbb{R}^d} c^k(y) \eta^\epsilon(x - y) \, dy.\]

Introduce a compatible regularization of the conductivity eq.

\[\frac{\partial c^k}{\partial t} = D^2 \Delta c^k + (\partial_{x_k} p)^2 \ast \eta^\epsilon - \nu |c^k|^\gamma - 2 c^k\]

so that the system is the formal \(L^2\)-gradient flow of the energy

\[E^\epsilon[c] := \int_{\Omega} \frac{D^2}{2} |\nabla c|^2 + \nabla p \cdot P^\epsilon[c] \nabla p + \frac{\nu}{\gamma} |c|^\gamma \, dx\]
Proof of global existence

- **Leray-Schauder theorem** for the regularized system
- Compactness follows from the **weak-strong Lemma for the Poisson equation** and compact Sobolev embedding
- **Nonnegativity** of \( c^k_\varepsilon \) follows from the fact that solutions of the semilinear PDE
  \[
  \partial_t u = D^2 \Delta u - \nu |u|^{\gamma-2} u
  \]
  are subsolutions.
- Uniform a-priori estimates from the **energy dissipation inequality** facilitate the limit passage \( \varepsilon \to 0 \).
Conclusions

- The continuum limit depends on the **topology and geometry** of the network.

- **Goal:** random networks (graphs) - various models:
  - **Gilbert** $G(n, p)$ - every possible edge occurs independently with probability $0 < p < 1$
  - **Erdös-Rényi** $G(n, M)$ - assigns equal probability to all graphs with exactly $M$ edges

- Try to use convergence results from FEM (Nedelec elements?)


Thank you!
Thank you!
An excursion into graph limits
Motivation:

- **Classical optimization problem:** Find the minimum of \( x^3 - 6x \) over all numbers \( x \geq 0 \).
  
  **Answer:** \( x = \sqrt{2} \in \mathbb{R} \), but \( \not\in \mathbb{Q} \).

- **Graph optimization problem:** Find the minimum of \( t(C_4, G) \) over all graphs \( G \) with \( t(K_2, G) \geq 1/2 \).
  
  **Answer:** \( t(C_4, G) \geq t(K_2, G)^4 = (1/2)^4 \), but no finite \( G \) is a minimizer [Erdös].

- See [Lovász, Szegedy, Borgs, Chayes, Sós, Vesztergombi, Benjamini, Schramm, Hladký, ...] for more info.
Fix $F$ a graph of order $k$, $G$ is "large" of order $n > k$, and define the subgraph density

$$t(F, G) := \frac{\# \text{ of copies of } F \text{ in } G}{\binom{n}{k}} = \mathbb{P}(\text{random } k\text{-set of } G \simeq F)$$

**Def.:** A sequence of graphs $G_1, G_2, \ldots$ converges if for each $F$ the sequence $t(F, G_1), t(F, G_2), \ldots$ converges.

We get a limit object $\Psi$, with $t(F, \Psi) := \lim_{n \to \infty} t(F, G_n)$. 
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Observe: Works for dense graphs only, i.e., $|e(G_n)| \simeq n^2$, since otherwise the limit is trivial, $\lim_{n \to \infty} t(F, G_n) = 0$ for all $F$.

So, unfortunately, the theory is void for trees, planar graphs, ...
Example: Bipartite graphs

Represent these graphs by their adjacency matrices:

\[
\begin{array}{cc|ccc}
0 & 0 & 1 & 1 & \cdots & \cdots \\
1 & 0 & 1 & 1 & \cdots & \cdots \\
\end{array}
\]

... works if you do things the "right way". But:

\[
\begin{array}{cc|ccc}
0 & 0 & 1 & 1 & \cdots & \cdots \\
1 & 0 & 1 & 1 & \cdots & \cdots \\
\end{array}
\]

Szemerédi’s Regularity Lemma to determine the "right way" of ordering the vertices \( \sim \) graphon, symmetric Lebesgue measurable function \( W : [0, 1]^2 \to [0, 1] \).
Large dense graphs essentially behave like (connected sets of) random graphs.

Their limits are graphons and there is an established theory.

However: In our model, for $1/2 \leq \gamma < 1$, the minimizer is a tree, which is sparse (even very sparse - bounded degree).

The sparse theory is tricky (graphings $\simeq$ Borel measures; but no single "true" limit object).

[L. Lovász: Large networks and graph limits.]