Discrete-To-Continuum Limits of Dynamical Optimal Transport Problems

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Dynamics and Discretization: PDEs, Sampling, and Optimization

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Summary

(1) A general class of **dynamical transport problems** on $\mathbb{R}^d$.

(2) The **discrete optimal transport** problem on graphs.

(3) **Discrete-to-continuum** limits of transport problems on $\mathbb{Z}^d$-periodic graphs.

(4) Some examples: in particular, $\mathbb{Z}^d$-periodic **finite volume partitions**.

(1/4) Dynamical Transport Problems

The dynamical formulation of OT: Benamou–Brenier formula

$$\mathbb{W}_2(\mu,\nu)^2 := \min_{\pi} \left\{ \int_{\mathbb{R}^d \times \mathbb{R}^d} |x-y|^2 \, \mathrm{d}\pi(x,y) \ : \ \pi \in \Gamma(\mu,\nu) \right\} \qquad \text{(quadratic cost)}$$

Theorem [Benamou and Brenier, 2000] [Ambrosio, Gigli, and Savaré, 2008]: for any $\mu_0, \mu_1 \in \mathscr{P}_2(\mathbb{R}^d)$, we have the equality:

$$\mathbb{W}_2(\mu_0,\mu_1)^2 = \inf_{(\mu_t, v_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} |v_t|^2 \, \mathrm{d}\mu_t \, \mathrm{d}t \ : \ \underbrace{\partial_t \mu_t + \nabla \cdot (\mu_t v_t) = 0}_{\text{continuity equation}}, \ \mu_{t=i} = \mu_i \right\}$$

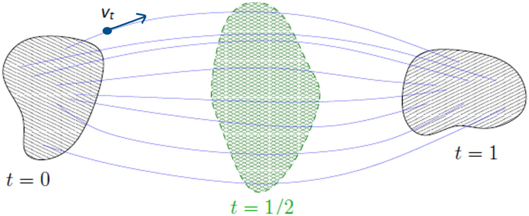


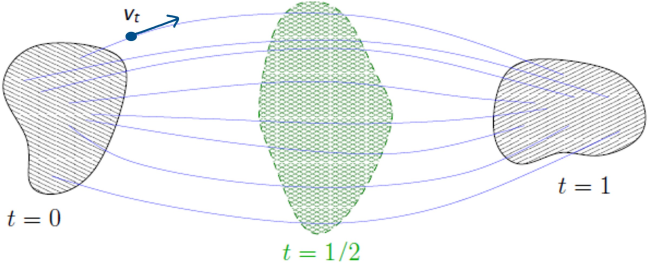
Figure: An evolution $(\mu_t)_t \subset \mathscr{P}_2(\mathbb{R}^d)$ from μ_0 to μ_1 (edited from [Villani, 2009]).

Dynamical transport problems in $\mathcal{M}_+(\mathbb{R}^d)$.

For a given convex, lsc function $f : \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$, we are interested in

$$C_f(\mu_0, \mu_1) := \inf_{(\mu_t, \xi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} f(\mu_t, \xi_t) \, dx \, dt \ : \ \underbrace{\partial_t \mu_t + \nabla \cdot \xi_t = 0}_{\text{continuity equation}}, \ \mu_{t=i} = \mu_i \right\}$$

where μ_0, $\mu_1 \in \mathcal{M}_+(\mathbb{R}^d)$ are given initial and final measures, $\xi_t := \mu_t v_t$ is the **flux**.



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Examples of transport problems (1).

$$C_f(\mu_0,\mu_1) := \inf_{(\mu_t,\xi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} f(\mu_t,\xi_t)\,\mathrm{d}x\,\mathrm{d}t \ : \ \underbrace{\partial_t \mu_t + \nabla \cdot \xi_t = 0,\ \mu_{t=i} = \mu_i}_{(\mu_t,\xi_t)_t \in \mathsf{CE}(\mu_0,\mu_1)} \right\}$$

- $f(\mu,\xi) = |\xi|^2/\mu$ corresponds to the **(2)-Wasserstein distance** $\mathbb{W}_2$:

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whose dynamical interpretation is due to [Benamou and Brenier, 2000].

- More general: $f(\mu,\xi) = |\xi|^p/m(\mu)^{p-1}$ for $m : \mathbb{R}^+ \to \mathbb{R}^+$ concave mobility:

$$\mathbb{W}_{p,m}(\mu_0,\mu_1)^p := \inf_{(\mu_t,\xi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} \frac{|\xi_t|^p}{m(\mu_t)^{p-1}}\,\mathrm{d}x\,\mathrm{d}t \ : \ (\mu_t,\xi_t)_t \in \mathsf{CE}(\mu_0,\mu_1) \right\}$$

are **generalised (p)-Wasserstein distances** [Dolbeault, Nazaret, and Savaré, 2012] .

Examples of transport problems (2).

$$C_f(\mu_0, \mu_1) := \inf_{(\mu_t,\xi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} f(\mu_t, \xi_t) \, \mathrm{d}x \, \mathrm{d}t \; : \; \underbrace{\partial_t \mu_t + \nabla \cdot \xi_t = 0, \;\; \mu_{t=i} = \mu_i}_{(\mu_t,\xi_t)_t \in \mathsf{CE}(\mu_0,\mu_1)} \right\}$$

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$$\int_0^1 \int_{\mathbb{R}^d} F(\xi_t)\,\mathrm{d}x\,\mathrm{d}t \overset{\text{Jensen}}{\geq} \int_{\mathbb{R}^d} F\Bigg(\underbrace{\int_0^1 \xi_t\,\mathrm{d}t}_{=:\bar\xi}\Bigg)\,\mathrm{d}x = \int_{\mathbb{R}^d} F(\bar\xi)\,\mathrm{d}x,$$

In this case, one has the equivalent **static** formulation:

$$C_f(\mu_0,\mu_1) = \inf_{\bar\xi} \left\{ \int_{\mathbb{R}^d} F(\bar\xi)\,\mathrm{d}x \;:\; \nabla\cdot\bar\xi = \mu_0 - \mu_1 \right\}.$$

This includes $\mathbb{W}_1$ ($F(\bar\xi) = |\bar\xi|$) and negative Sobolev distance H^{-1} ($F(\bar\xi) = |\bar\xi|^2$).

Motivations.

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(2) Application to PDEs: theory of metric **gradient flows**.

$$\partial_t \mu_t - \nabla \cdot (\mu_t \nabla (\mathsf{D}\mathsf{E}(\mu_t))) = 0, \quad \mathsf{E} : \mathcal{M}_+(\mathbb{R}^d) \to [0, +\infty].$$

[Jordan, Kinderlehrer, and Otto, 1998]: heat flow as gradient flow of the entropy

$$\partial_t \mu_t = \Delta \mu_t, \quad \mathsf{E}(\mu) = \int_{\mathbb{R}^d} \log\left(\frac{\mathrm{d}\mu}{\mathrm{d}x}\right) \mathrm{d}\mu.$$

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(3) Surprising connections with the **Riemannian geometry** (Lott–Villani–Sturm theory):

$$\mathrm{Ric}_{(M,g)} \geq 0 \quad \Longleftrightarrow \quad \mathsf{E}(\mu) = \int_M \log\left(\frac{\mathrm{d}\mu}{\mathrm{d}x}\right) \mathrm{d}\mu \quad \text{convex along } \mathbb{W}_2\text{-geodesics.}$$

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[Maas, 2011, Mielke, 2011] : generalisation of these ideas to the **discrete setting**.

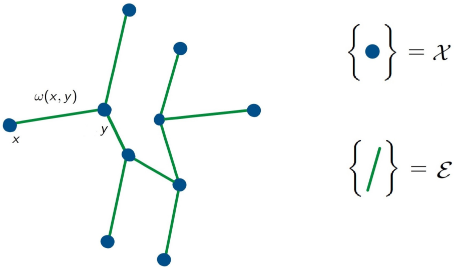
(2/4) **Discrete Optimal Transport**

Optimal transport on discrete spaces.

The dynamical formulation of **(2)-Wasserstein distance** $\mathbb{W}_2$ on $\mathscr{P}_2(\mathbb{R}^d)$:

$$\mathbb{W}_2(\mu_0,\mu_1)^2 = \inf_{(\mu_t,\xi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^d} \frac{|\xi_t|^2}{\mu_t} \,\mathrm{d}x\,\mathrm{d}t \;:\; \underbrace{\partial_t \mu_t + \nabla \cdot \xi_t = 0}_{\text{continuity equation}},\ \mu_{t=i} = \mu_i. \right\}$$

Discrete setting: $(\mathcal{X}, \mathcal{E}, \omega)$ a weighted graph, that is $\mathcal{X}$ finite set of *nodes*, $\mathcal{E}$ set of *edges*, and ω a weight function on $\mathcal{E}$. We fix a reference measure $\pi \in \mathscr{P}(X)$.



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Definition [Maas, 2011] [Mielke, 2011] : for $m_0, m_1 \in \mathscr{P}(\mathcal{X})$:

$$\mathcal{W}^\theta(m_0,m_1)^2 := \inf_{(m_t,j_t)} \left\{ \int_0^1 \frac{1}{2} \sum_{(x,y)\in\mathcal{E}} \frac{1}{\omega(x,y)} \frac{|j_t(x,y)|^2}{\theta\left(\frac{m_t(x)}{\pi(x)},\frac{m_t(y)}{\pi(y)}\right)} \,\mathrm{d}t \right\}.$$

where (m_t, j_t) is solution to the **discrete continuity equation** for $x\in\mathcal{X}$:

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Why the logarithmic average? Maas (2011), Mielke (2011)

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$$\boxed{\theta_{\log}(r,s) = \frac{r-s}{\log r - \log s}}, \quad r_t(x) := \frac{m_t(x)}{\pi(x)} \text{ (density)}.$$

Consider the discrete entropy functional $\mathcal{E} : (\mathscr{P}(\mathcal{X}), \mathcal{W}) \to \mathbb{R}^+$

$$\mathcal{E}(m) := \sum_{x\in\mathcal{X}} m(x) \log\left(\frac{m(x)}{\pi(x)}\right) = \sum_{x\in\mathcal{X}} r(x) \log r(x)\, \pi(x).$$

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The **gradient flow of** $\mathcal{E}$ in $(\mathscr{P}(\mathcal{X}), \mathcal{W})$ is the graph heat flow

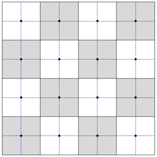
$$\dot{r}_t = \Delta_{\mathcal{X}} r_t, \quad \text{where} \quad \Delta_{\mathcal{X}} r = \sum_{y\sim x} \frac{\omega(x,y)}{\pi(x)}\big(r(y) - r(x)\big) \quad \text{(discrete Laplacian)}.$$

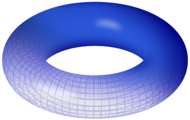
(3/4) Discrete-to-Continuum Limits of Transport Problems

- Gladbach, Kopfer, Maas, and Portinale. Homogenisation of one-dimensional discrete optimal transport. *J. Math. Pures Appl. (9)*, 139:204–234, 2020.
- Gladbach, Kopfer, Maas, and Portinale. Discrete-to-continuum limits of dynamical transport problems on periodic graphs. *http://arxiv.org/abs/2110.15321 (appeared today!)*.

Discrete-to-continuum limits of transport problems.

(1) **First convergence result** [Gigli and Maas, 2013]: transport metrics associated to the cubic mesh on the torus $\mathbb{T}^d$ converge to $\mathbb{W}_2$ in the limit of vanishing mesh size.





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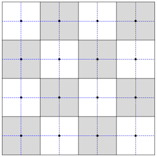

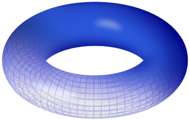

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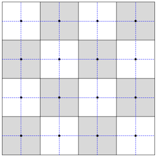

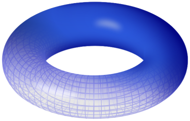

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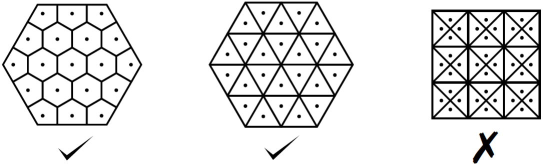
(3) **Finite volume partitions** $\mathcal{T}$ in $\mathbb{R}^d$ [Gladbach, Kopfer, and Maas, 2020]: convergence of $\mathcal{W}_\mathcal{T}$ to $\mathbb{W}_2$ as size$(\mathcal{T}) \to 0$ is essentially equivalent to an isotropy condition.



Discrete-to-continuum: transport on periodic graphs.

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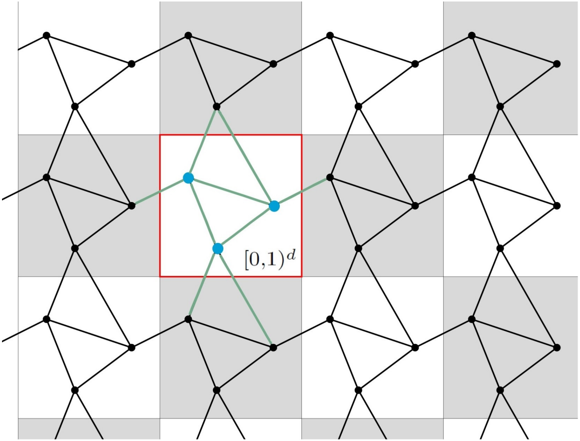
Setting: $\mathbb{Z}^d$-periodic, symmetric, connected, and locally finite graph $(\mathcal{X}, \mathcal{E})$ in $\mathbb{R}^d$.



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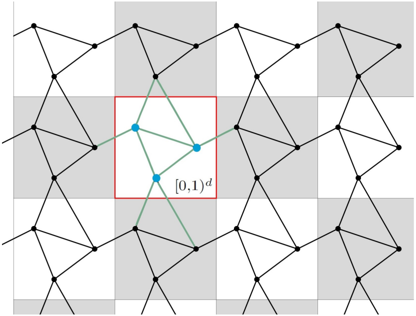
Given a convex, **local** function $f : \mathcal{M}_+(\mathcal{X}) \times \mathbb{R}^{\mathcal{E}} \to \mathbb{R} \cup \{+\infty\}$, we consider

$$\mathcal{C}_f(m_0, m_1) := \inf \left\{ \int_0^1 f(m_t, j_t)\,\mathrm{d}t \;:\; \partial_t m_t(x) + \frac{1}{2} \sum_{y \sim x} \big(j_t(x,y) - j_t(y,x)\big) = 0 \right\}$$

among $j_t \in \mathbb{R}^{\mathcal{E}}_{\mathrm{per}}$ and $m_t \in \mathcal{M}_+^{\mathrm{per}}(\mathcal{X})$, satisfying b.c. $m_{t=0} = m_0$, $m_{t=1} = m_1$.



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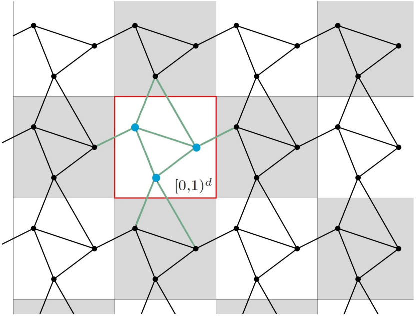

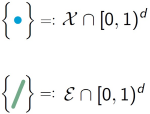

Transport on periodic graphs: some examples.

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- The **edge-based** case corresponds to the choice

$$f(m, j) = \frac{1}{2} \sum_{x \in \mathcal{X} \cap [0,1)^d} \sum_{y \sim x} f_{xy}(m(x), m(y), j(x, y)).$$

The $\mathfrak{m}$-Wasserstein-like distances are obtained using quadratic functions

$$f_{xy}(m, n, j) = \frac{1}{\omega(x, y)} \frac{|j|^2}{\mathfrak{m} \circ \theta\left(\frac{m}{\pi(x)}, \frac{n}{\pi(y)}\right)}, \quad m, n \in \mathbb{R}^+,\ j \in \mathbb{R}.$$

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- The **flow-based** case corresponds to the choice $f(m, j) = F(j)$ and

$$\mathcal{C}_f(m_0, m_1) = \inf\left\{ F(j) \;:\; \frac{1}{2} \sum_{y \sim x} \big(j(x, y) - j(y, x)\big) = m_0 - m_1 \right\}.$$

Transport on periodic graphs: the convergence result.

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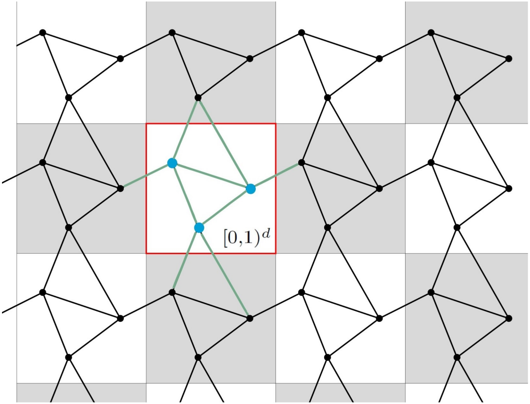

$\{\bullet\} =: \mathcal{X} \cap [0,1)^d$

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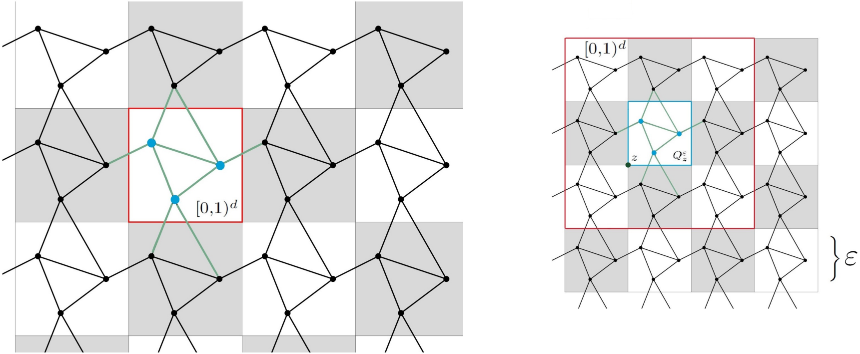

Figure: One the right, the rescaled graph $\mathcal{X}_\varepsilon = \varepsilon\mathcal{X}$, $\mathcal{E}_\varepsilon = \varepsilon\mathcal{E}$, for $\frac{1}{\varepsilon} \in \mathbb{N}$.

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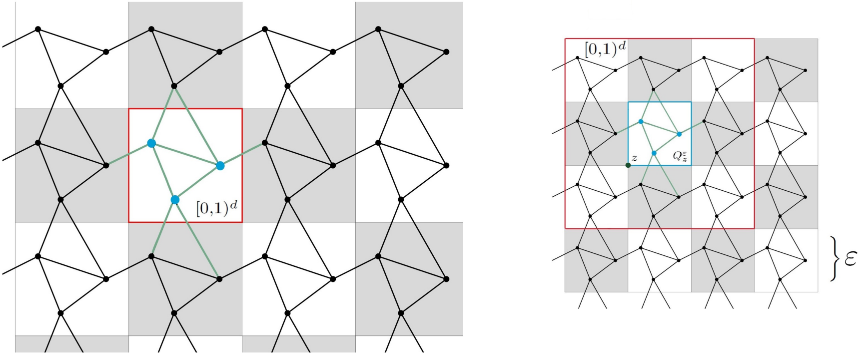

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Assume f is convex, lower semicontinuous, with superlinear growth$^{(*)}$ in j. Then $\mathcal{C}_f^\varepsilon$ Γ-converges in the weak*-topology as $\varepsilon \to 0$ to a continuous problem

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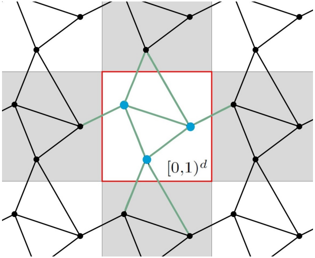
- In $d \geq 1$, it is achieved by (space-time) Γ-convergence and coercivity of the actions

$$\boldsymbol{m} := (m_t)_t \mapsto \mathcal{A}_\varepsilon(\boldsymbol{m}) := \inf_{\boldsymbol{j}} \left\{ \int_0^1 \sum_{z \in \mathbb{T}_\varepsilon^d} \varepsilon^d f\left(\frac{m_t(\cdot - z)}{\varepsilon^d}, \frac{j_t(\cdot - z)}{\varepsilon^{d-1}} \right) \mathrm{d}t \ : \ (m_t, j_t)_t \in \mathsf{CE}_{\mathcal{X}_\varepsilon} \right\}$$

The cell problem: a formula for the limit f_{hom}.



For $m \in \mathcal{M}_+^{\mathrm{per}}(\mathcal{X})$ and $\mathbb{Z}^d$-periodic $j \in \mathbb{R}_a^{\mathcal{E}}$, define:

$$\|m\| := \sum_{x \in \mathcal{X} \cap [0,1)^d} m(x) \in \mathbb{R}^+,$$

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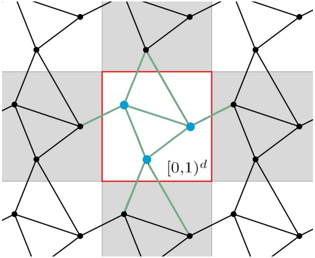

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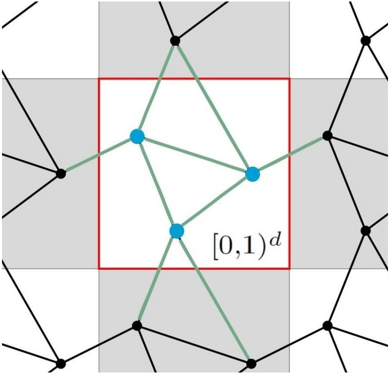
Cell problem: for any $\rho \in \mathbb{R}^+$, $\xi \in \mathbb{R}^d$, the limit cost is given by

$$\boxed{f_{\text{hom}}(\rho, \xi) := \inf_{m,j} \left\{ f(m,j) \;:\; \|m\| = \rho,\ \mathrm{Eff}(j) = \xi,\ \mathrm{div}\, j = 0 \right\}}$$

where the inf is taken over $m \in \mathcal{M}_+^{\text{per}}(\mathcal{X})$ and $\mathbb{Z}^d$-periodic, skew-sym. $j \in \mathbb{R}^{\mathcal{E}}$.

An example of a competitor for the cell problem

Example: $\rho = 5$, and $\xi = (2,3) \in \mathbb{R}^2$. We can obtain a representative of ρ, ξ as follows:



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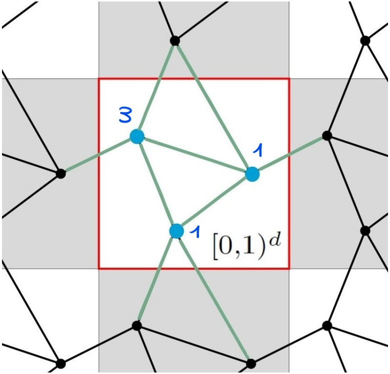

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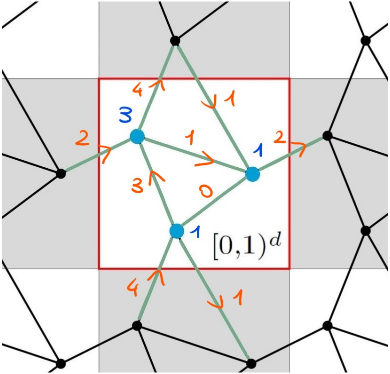

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(4/4) Application: periodic finite-volume partitions.

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where we choose: $\quad \omega_{\mathfrak{g}}(x,y) := \dfrac{\mathscr{H}^{d-1}(\partial K_x \cap \partial K_y)}{|y-x|}, \quad \pi(x) := \mathscr{L}^d(K_x)\,.$

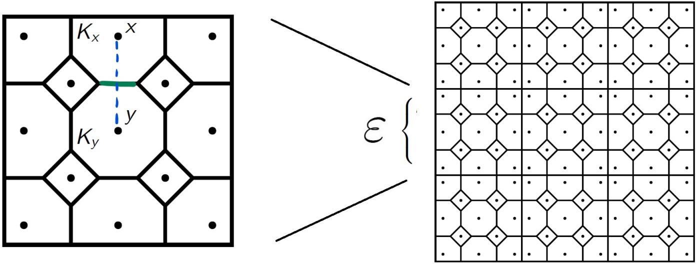

Figure: Periodic finite-volume partition of $\mathbb{T}^d$.

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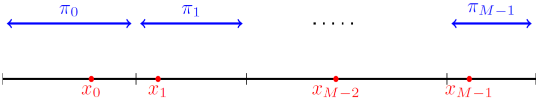

One-dimensional: $\mathcal{W}_\theta$ converges as $\varepsilon \to 0$ to $\mathbb{W}_{\mathrm{hom}} = f_{\mathrm{hom}}(1,1)\mathbb{W}_2$, where

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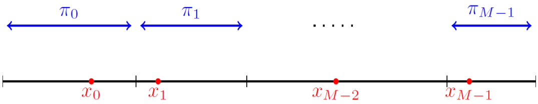

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Multidimensional: $\mathcal{W}_\theta$ converges as $\varepsilon\to 0$ to $\mathbb{W}_{\mathsf{hom}}$, where

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and $f_{\mathsf{hom}}(\mu,\xi) = \frac{\|\xi\|^2_{\mathsf{hom}}}{\mu}\le\frac{|\xi|^2}{\mu}$ with $\mathbb{W}_{\mathsf{hom}} = \mathbb{W}_2$ if and only if the mesh is isotropic.

The role of isotropy in the periodic setting

Theorem (multidimensional): $\mathcal{W}_\theta$ converges as $\varepsilon \to 0$ to $\mathbb{W}_{\text{hom}}$, where

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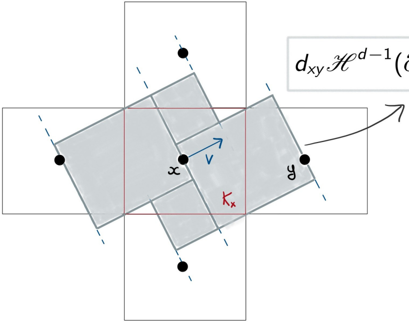
- $\mathbb{W}_{\text{hom}} = \mathbb{W}_2$ if and only if the mesh is isotropic: in the periodic setting, it reads

$$\frac{1}{2} \sum_{y \sim x} d_{xy} \mathscr{H}^{d-1}(\partial K_x \cap \partial K_y) n_{xy} \otimes n_{xy} = |K_x| \mathrm{id}, \quad \forall x \in \mathcal{X}.$$



$$d_{xy} \mathscr{H}^{d-1}(\partial K_x \cap \partial K_y)(n_{xy} \cdot v)^2$$

Possible future directions

- Discrete-to-continuum limits of (generalised) gradient flows.
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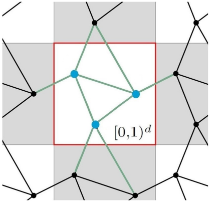

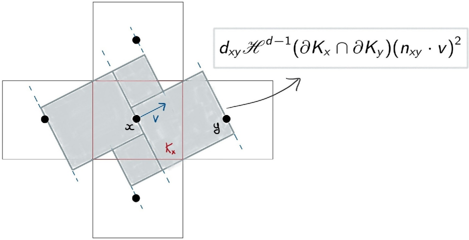

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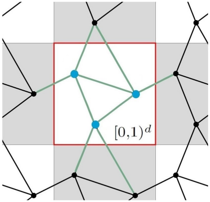

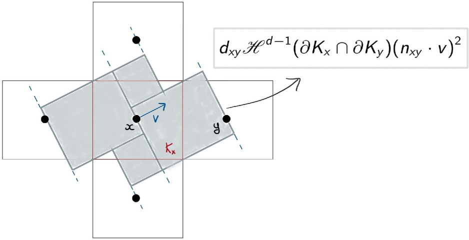

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- $f_{\text{hom}}(\mu, \xi) = \dfrac{\|\xi\|^2_{\text{hom}}}{\mu} \leq \dfrac{|\xi|^2}{\mu}$, where $\|\cdot\|_{\text{hom}}$ is a norm (possibly not Riemannianian!)

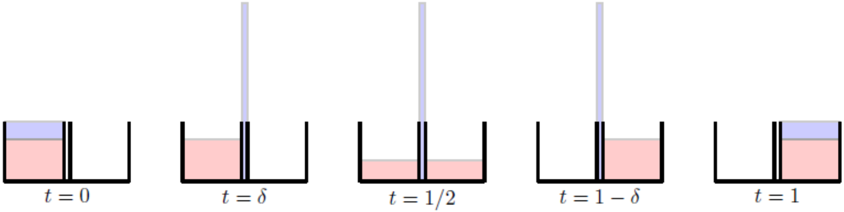

Figure: Strongly oscillating measures on the graph scale can be cheaper.