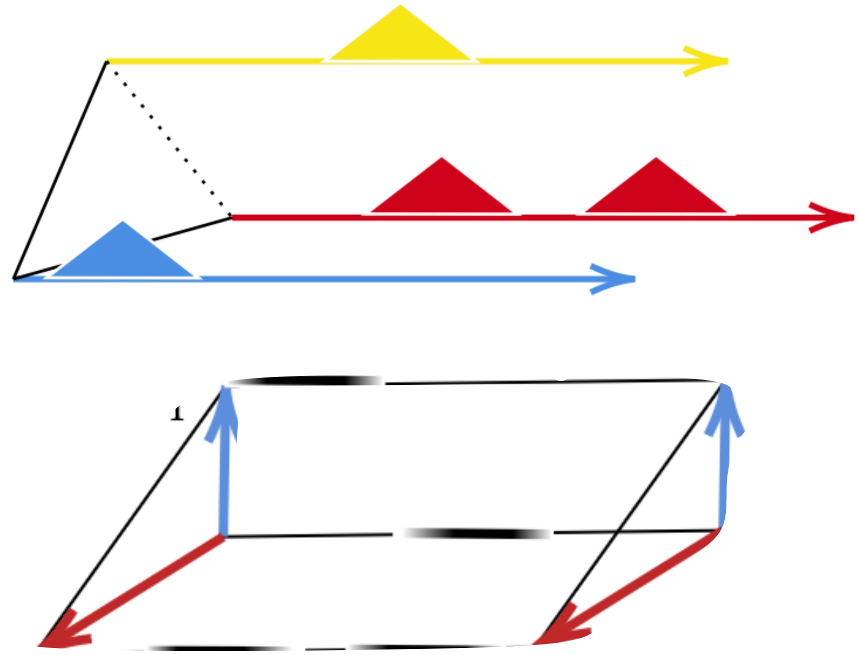

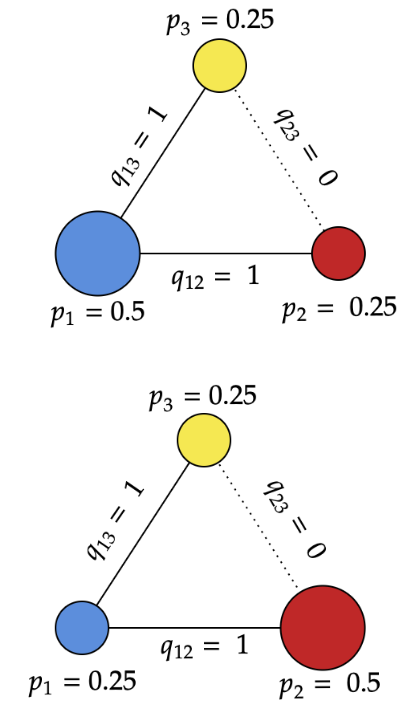

Vector Valued Optimal Transport:

From Dynamic to Static Formulations

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Dynamics of Density Operators
IPAM
April 28, 2025

Plan

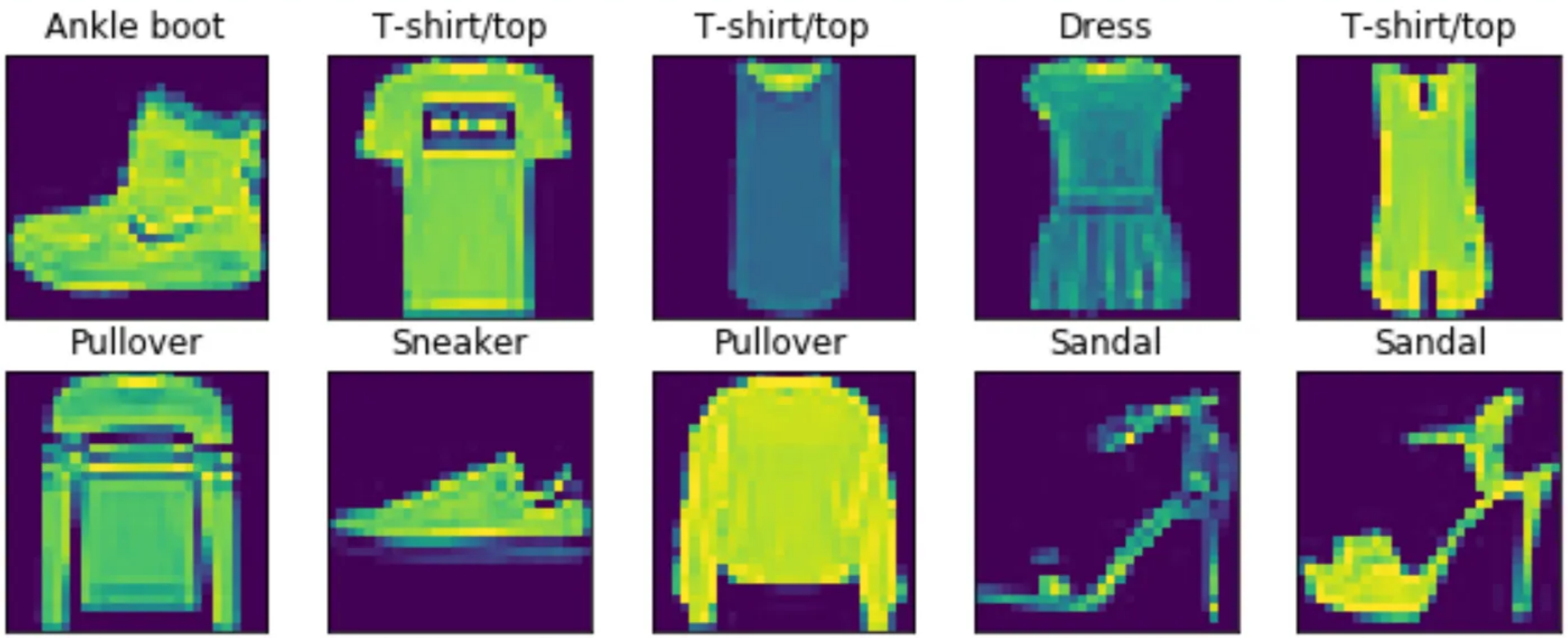
1. Motivation for vector valued OT

2. Previous work on vector valued and graph OT

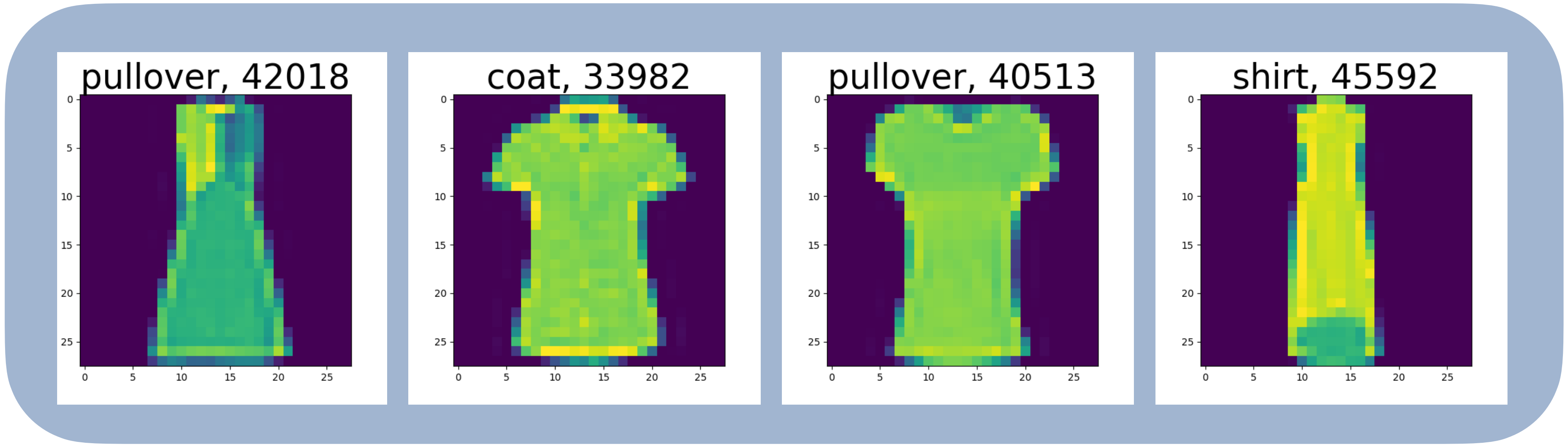
3. New dynamic and static (semi)-metrics

4. Metric comparison

Motivation: image classification



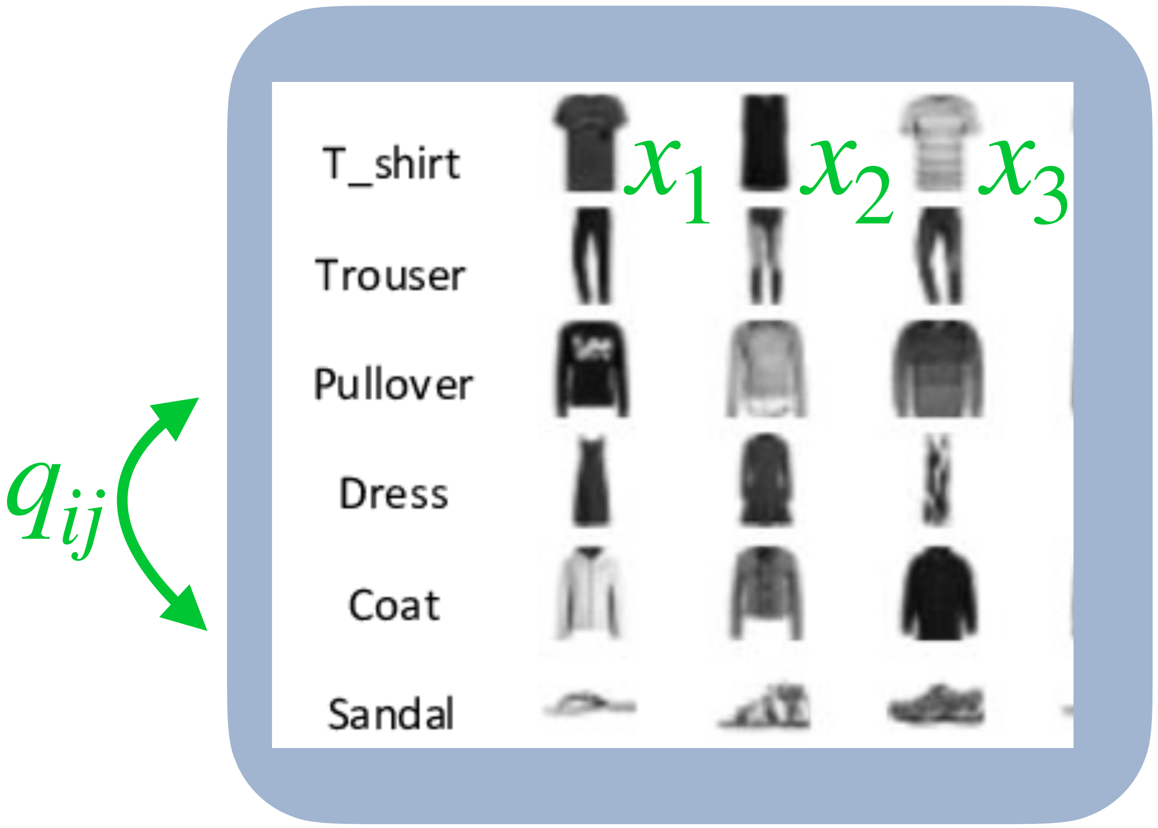
Mild misclassifications in Fashion MNIST— for example…



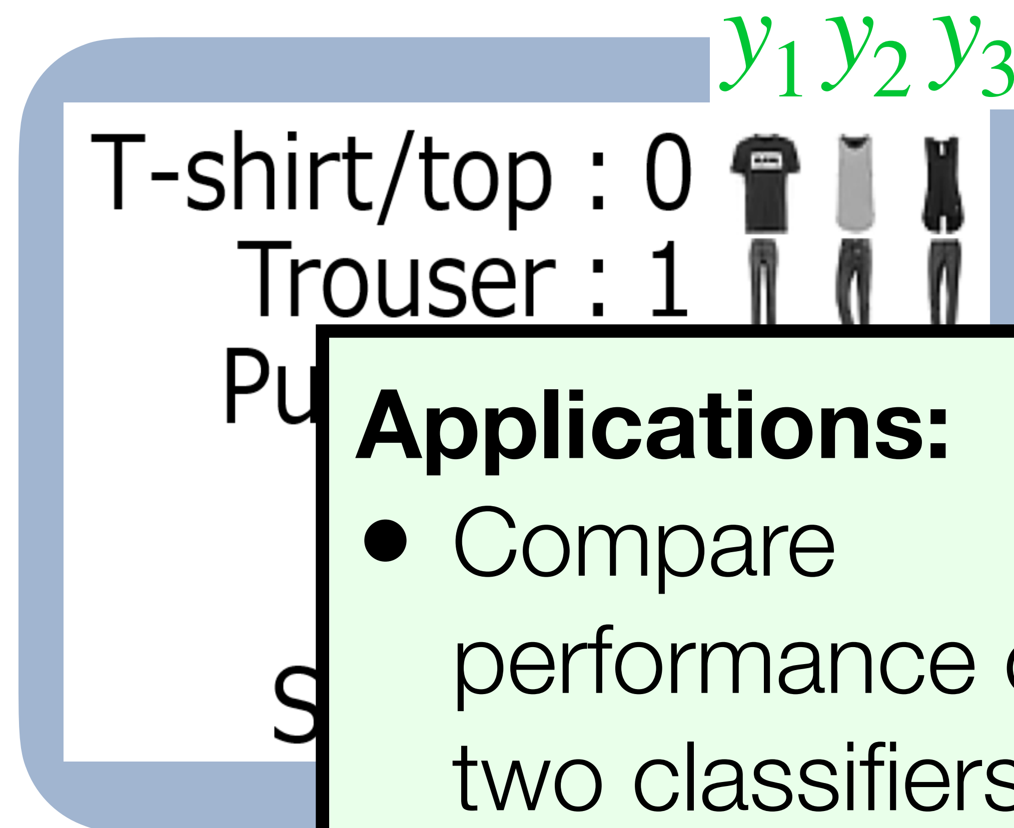
[Müller, Markert 2019]

Motivation: image classification

Labeled Dataset #1



Labeled Datas



Applications:

- Compare performance of two classifiers
- Compare structure of two labeled datasets (ATLAS/CMS)

How different are these datasets?

Represent images as points $x_k, y_l \in \mathbb{R}^d$

Similarity between images $= ||x_k - y_l||$

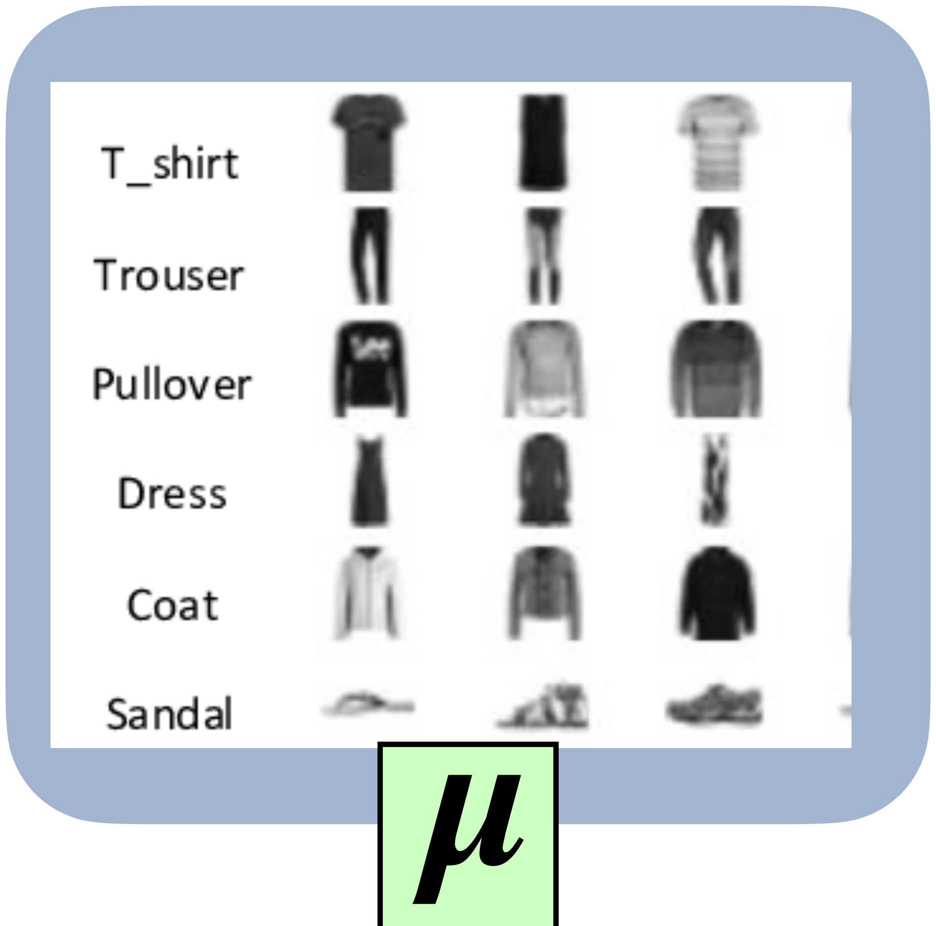
Dissimilarity between label i and label $j = q_{ij}$

Datasets are similar if their images & labels are similar.

Motivation: image classification

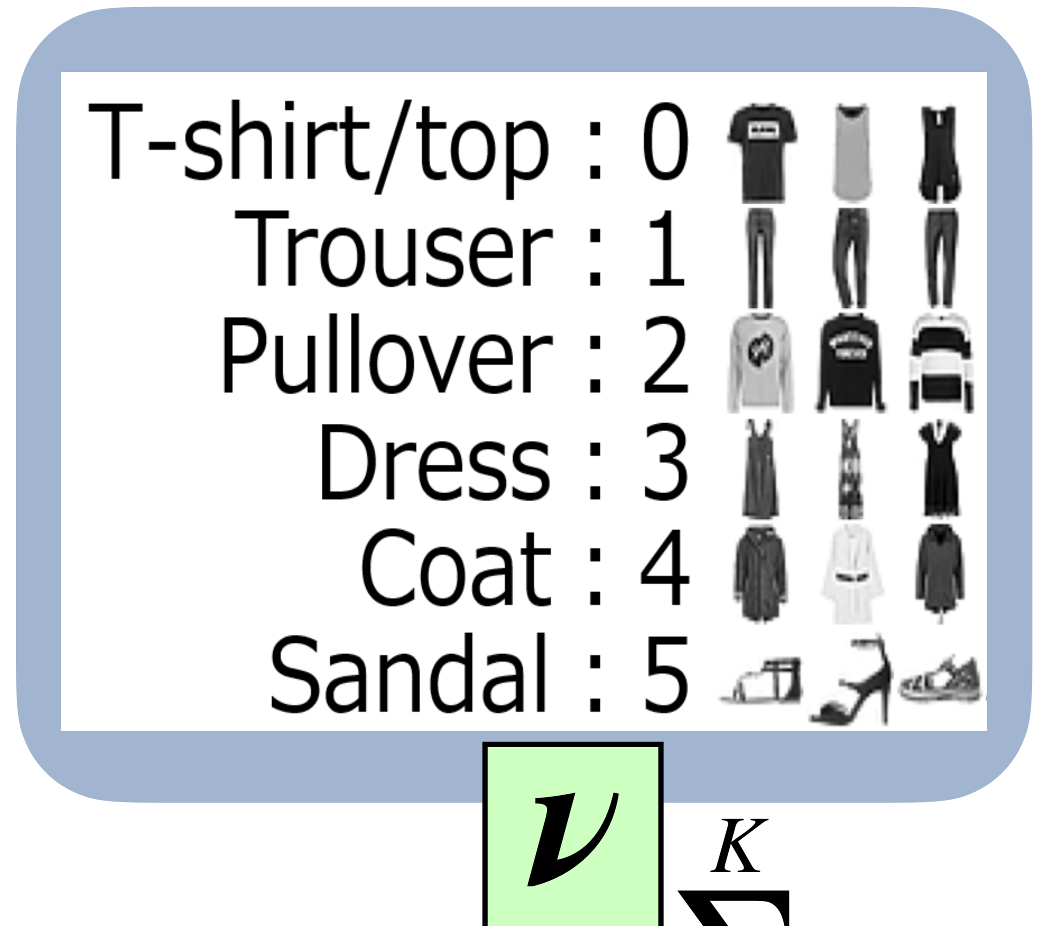
Labeled Dataset #1

$$\begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \mu_4 \\ \mu_5 \\ \mu_6 \end{bmatrix}$$



Labeled Dataset #2

$$\begin{bmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \\ \nu_4 \\ \nu_5 \\ \nu_6 \end{bmatrix}$$



Represent collection of images with label i as $\mu_i = \sum_{k=1}^{K} \delta_{x_k} m_k$

Represent datasets as vector valued measures $\boldsymbol{\mu} = [\mu_i]_{i=1}^{n}$

Datasets are similar if $\boldsymbol{d}(\boldsymbol{\mu}, \boldsymbol{\nu}) \ll 1$ for some distance **d**.

Motivation: gradient flows

Given a target vector valued measure $\boldsymbol{\mu}$, a loss functional $\mathscr{L}$, and a constraint set C, find a minimizer of

$$\min_{\rho \in C} \mathscr{L}(\boldsymbol{\rho}, \boldsymbol{\mu}) \,.$$

Given a distance **d** between vector valued measures, could flow to critical points via **gradient descent**. In discrete time,

$$\boldsymbol{\rho}_\tau^{n+1} = \operatorname{argmin}_{\rho \in C} \mathscr{L}(\boldsymbol{\rho}, \boldsymbol{\mu}) + \frac{1}{2\tau} \boldsymbol{d}^2(\boldsymbol{\rho}, \boldsymbol{\rho}_\tau^n),$$

which, for nice $\mathscr{L}$, is stable wrt perturbations in **d**.

For classification or gradient flows, what is an appropriate notion of distance **d** between vector valued measures?

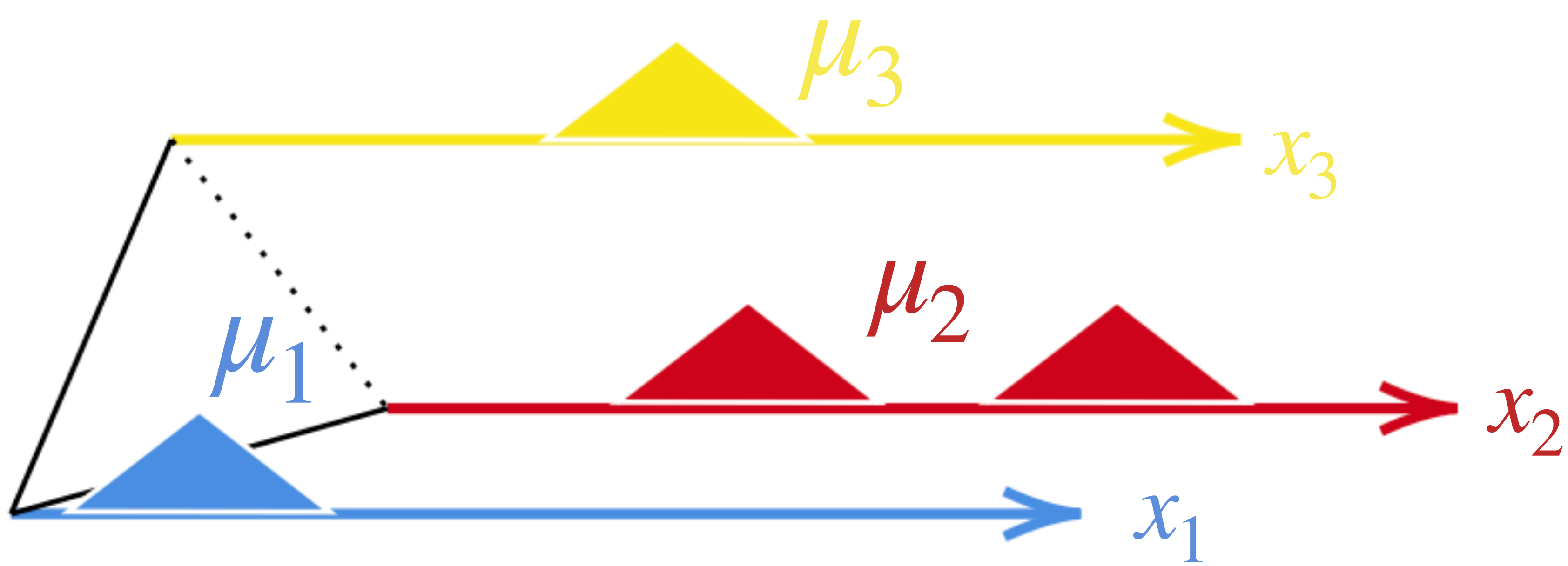
Vector valued measures

Fix $\boldsymbol{\Omega} \subseteq \mathbb{R}^d$ closed. Let $\boldsymbol{G}$ denote an $\boldsymbol{n}$ node graph.

Consider vector valued measures with total mass one:

$$\mathscr{P}(\Omega \times G) := \left\{ \boldsymbol{\mu} = [\mu_i]_{i=1}^n : \mu_i \in \mathscr{M}(\Omega), \underbrace{\sum_{i=1}^n \mu_i}_{=: \bar{\mu}} \in \mathscr{P}(\Omega) \right\}$$

For example, when $\boldsymbol{\Omega} = \mathbb{R}$ and $\boldsymbol{G}$ has three nodes:



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Previous work on vector valued OT

There are several existing notions of distance on $\mathscr{P}(\Omega \times G)$.

[Chen, Georgiou, Tannenbaum '18]: define dynamic distance via a product space structure on $(W_G, \mathscr{P}(G))$ & $(W_2, \mathscr{P}(\mathbb{R}^d))$

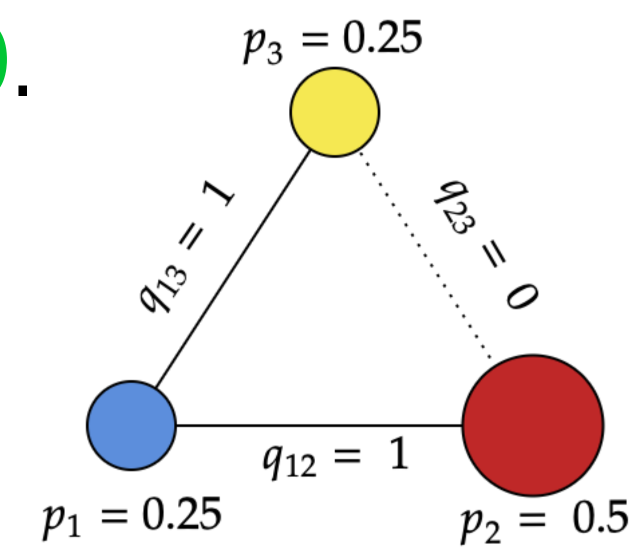
[Bacon '20]: define static distance via Kantorovich formulation; transport plans γ_{ij} move mass from μ_i to ν_j at cost $c_{ij}(x, y)$; prove strong duality; compatibility of c_{ij} to ensure metric.

Also W_1-type metrics [Todeschi, Metvier, Mirebeau '25], [Ryu, Chen, Li, Osher '18].

We seek a W_2-type distance on $\mathscr{P}(\Omega \times G)$ that unites dynamic and static perspectives, with a (formal) Riemannian structure for gradient flows and linearization.

Graph Wasserstein metric

Let G denote an n node weighted graph, where the weight of the edge connecting node i to node j is $q_{ij} \geq 0$.



$$\mathscr{P}(G) = \left\{ p = \sum_{i=1}^{n} p_i \delta_i : p_i \geq 0, \sum_{i=1}^{n} p_i = 1 \right\}$$

$$W_G^2(p, \tilde{p}) := \min \frac{1}{2} \sum_{i,j=1}^{n} \int_0^1 |v_{ij,t}|^2 \theta(p_{i,t}, p_{j,t}) q_{ij} dt$$

$$\text{such that} \quad \partial_t p_t + \nabla_G \cdot (\check{p}_t v_t) = 0,\ p_0 = p,\ p_1 = \tilde{p}$$

$$\check{p}_{ij} v_{ij} := \theta(p_i, p_j) v_{ij}$$

Examples: $\theta(p_i, p_j) = (p_i + p_j)/2,$ $\sqrt{p_i p_j},$ or $\displaystyle\int_0^1 p_i^{1-s} p_j^s ds$

Graph Wasserstein metric

Thm [Maas '11]: For $\mathscr{G}$ connected, $(\mathscr{P}_{>0}(G), W_G)$ is a smooth Riemannian manifold.

Rmk: The manifold is not complete, and the geodesic between two points in the interior can touch the boundary [Gangbo, Li, Mou '19], so branching is possible.

To see role of q_{ij}, absorb weights into velocity: for $q_{ij} > 0$,

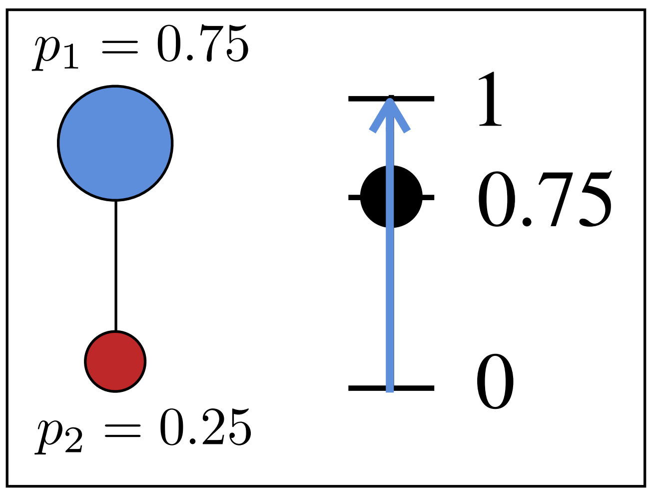
$$W_G^2(p, \tilde{p}) = \min \frac{1}{2} \sum_{i,j=1}^{n} \int_0^1 |v_{ij,t}|^2 \theta(p_{i,t}, p_{j,t}) q_{ij}^{-1} dt$$

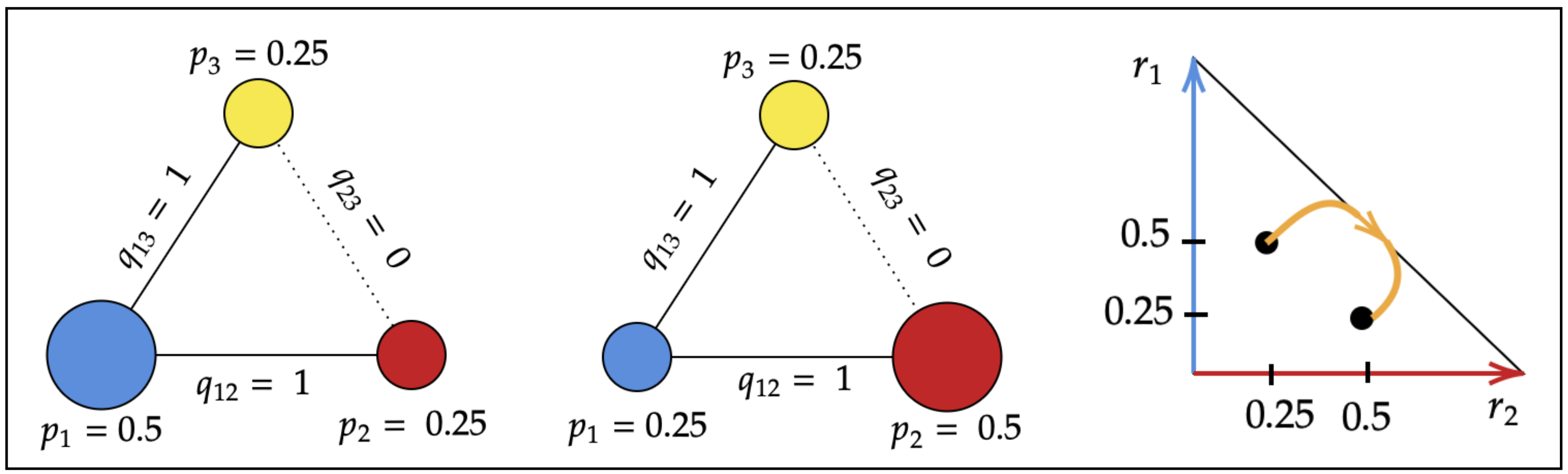
$$\text{such that} \quad \partial_t p_t + \nabla_{[n]} \cdot (\check{p}_t v_t) = 0, \; p_0 = p, \; p_1 = \tilde{p}$$

Induced geometry on simplex

Via the isometry $\boldsymbol{p} : \Delta^{n-1} \to \mathscr{P}(G) : r \mapsto \left[r_1, r_2, \ldots, 1 - \Sigma_i r_i\right]$,

$$\Delta^{n-1} = \left\{ r \in \mathbb{R}_+^{n-1} : \sum_{i=1}^{n} r_i \leq 1 \right\} \cong \mathscr{P}(G)$$





Induced distance: $d_{\Delta^{n-1}}(r, \tilde{r}) = W_G(\boldsymbol{p}(r), \boldsymbol{p}(\tilde{r}))$.

Prop: [c.f. Maas, Erbar '12]
$(\Delta^{n-1}, d_{\Delta^{n-1}})$ is topologically equivalent to $(\Delta^{n-1}, \|\cdot\|_{\mathbb{R}^{n-1}})$;
on $(\Delta^{n-1})^{\circ}$, it is a smooth Riemannian manifold.

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Continuity equation

$$\theta(\rho_i, \rho_j) := \theta\left(\frac{d\rho_i}{d\bar{\rho}}, \frac{d\rho_j}{d\bar{\rho}}\right)\bar{\rho}$$

Given $\boldsymbol{\Omega} \subseteq \mathbb{R}^d$ closed, convex … graph, we consider the following continuity equation on $\boldsymbol{\Omega} \times G$:

For velocities $\boldsymbol{u}_t(x) = [u_{i,t}(x)]_{i=1}^n$ and $\boldsymbol{v}_t(x) = [v_{ij,t}(x)]_{i,j=1}^n$,

$$\partial_t \boldsymbol{\rho} + \nabla \odot (\boldsymbol{\rho} \odot \boldsymbol{u}) + \nabla_G \cdot (\check{\boldsymbol{\rho}} \boldsymbol{v}) = 0$$

$$(\boldsymbol{\rho} \odot \boldsymbol{u})_i(x) = \rho_i(x) u_i(x) \qquad (\check{\boldsymbol{\rho}} \boldsymbol{v})_{ij}(x) = \theta(\rho_i(x), \rho_j(x)) v_{ij}(x)$$

For $\boldsymbol{v}$ symmetric, ith component of $\boldsymbol{\rho}_t(x) = [\rho_{i,t}(x)]_{i=1}^n$ satisfies

$$\partial_t \rho_{i,t} + \nabla \cdot (u_{i,t} \rho_{i,t}) = \sum_{j=1}^n \theta(\rho_{i,t}, \rho_{j,t}) v_{ij,t} q_{ij}$$

Let $\mathscr{C}(\boldsymbol{\rho}, \tilde{\boldsymbol{\rho}})$ denote the solutions satisfying $\boldsymbol{\rho}_0 = \boldsymbol{\rho}$, $\boldsymbol{\rho}_1 = \tilde{\boldsymbol{\rho}}$.

Dynamic metric

Given a solution of the continuity eqn, we consider the action

$$\|(\boldsymbol{u},\boldsymbol{v})\|_{\boldsymbol{\rho}}^2 := \sum_{i=1}^{n}\int_\Omega |u_i|^2\rho_i + \sum_{i,j=1}^{n}\int_\Omega |v_{ij}|^2\theta(\rho_i,\rho_j)q_{ij}$$

This leads to the dynamic distance:

$$W_{\Omega\times G}^2(\boldsymbol{\mu},\boldsymbol{\nu}) = \inf\int_0^1 \|(\boldsymbol{u}_t,\boldsymbol{v}_t)\|_{\boldsymbol{\rho}_t}^2 dt$$

$$\text{such that } (\boldsymbol{\rho},\boldsymbol{u},\boldsymbol{v}) \in \mathscr{C}(\boldsymbol{\mu},\boldsymbol{\nu})$$

Thm: [C., García Trillos, Nikolic '25]: $W_{\Omega\times G}$ is a metric on $\mathscr{P}_2(\Omega\times G)$ and a minimizer exists.

Dynamic metric comparison

Continuity equation: $\partial_t \boldsymbol{\rho} + \nabla \cdot (\boldsymbol{\rho} \odot \boldsymbol{u}) + \nabla_G \cdot (\check{\boldsymbol{\rho}} \boldsymbol{v}) = 0$

<u>C., García Trillos, Nikolic</u>

$$(\check{\boldsymbol{\rho}} \boldsymbol{v})_{ij} = \theta(\rho_i, \rho_j) v_{ij}$$

<u>Chen, Georgiou, Tannenbaum</u>

$$(\check{\boldsymbol{\rho}} \boldsymbol{v})_{ij} = \rho_i (v_{i,j})_+ - \rho_j (v_{ij})_-$$

Action: $\|(\boldsymbol{u}, \boldsymbol{v})\|_{\boldsymbol{\rho}}^2 := \sum_i \int |u_i|^2 \rho_i + (\mathrm{II})$

$$(\mathrm{II}) = \sum_{i,j=1}^{n} \int_\Omega |v_{ij}|^2 \theta(\rho_i, \rho_j) q_{ij}$$

$$(\mathrm{II}) = \sum_{i,j=1}^{n} \int_\Omega (v_{ij})_+^2 \rho_i q_{ij}$$

Thm [Chen, Georgiou, Tannenbaum '18], [Esposito, Patacchini, Schlichting, Slepčev '21]: The CGT formulation is not symmetric and leads to a **Finslerian structure**.

From dynamic to static

Potential analogy with Hellinger-Kantorovich?

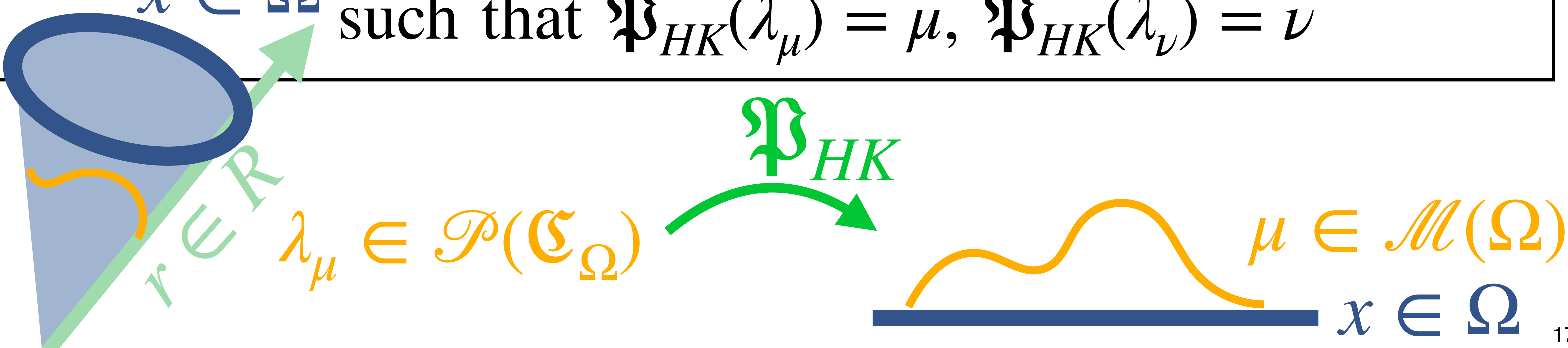
$$HK^2(\mu,\nu) = \inf \int_0^1 \int_\Omega (|v_t|^2 + 4\xi_t^2)\rho_t dt$$

$$\text{such that } \partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 4\rho_t \xi_t, \quad \rho_0 = \mu, \rho_1 = \nu$$

Thm [Liero, Mielke, Savaré '16]: Given the projection operator, $\mathfrak{P}_{HK} : \mathscr{P}(\mathfrak{C}_\Omega) \to \mathscr{M}(\Omega) : \lambda \mapsto \pi_\Omega \#(r^2 d\lambda(x,r))$, we have

$$HK(\mu,\nu) = \inf W_{\mathfrak{C}_\Omega}(\lambda_\mu, \lambda_\nu)$$

$$\text{such that } \mathfrak{P}_{HK}(\lambda_\mu) = \mu,\ \mathfrak{P}_{HK}(\lambda_\nu) = \nu$$



Static

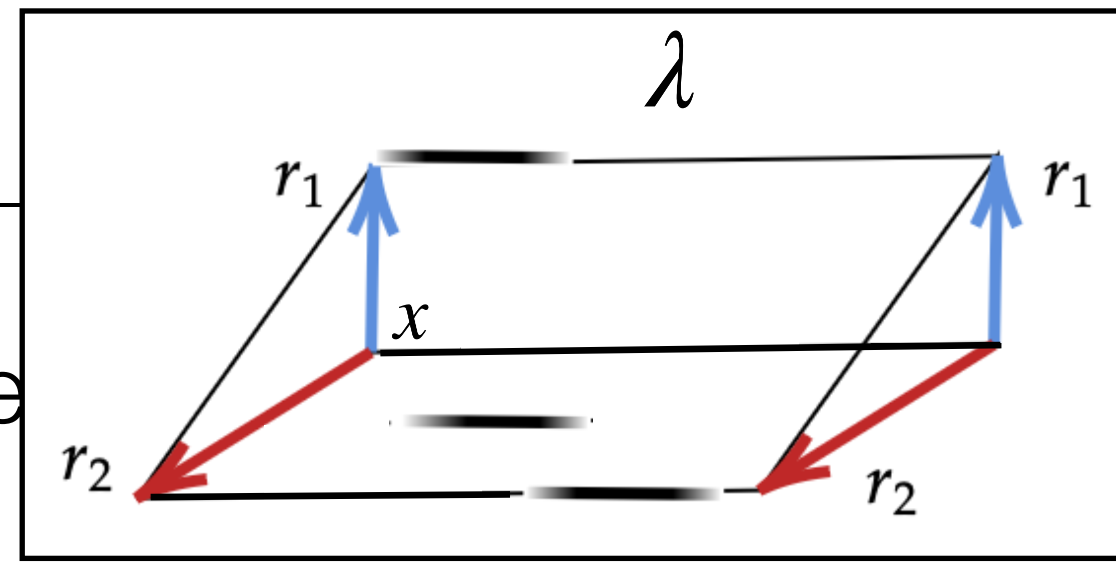
$$\int_{\mathbb{R}^d} \eta(x)d\mu_n(x) = \int_{\mathbb{R}^d\times\Delta^{n-1}} \left(1-\sum_{i=1}^{n} r_i\right)\eta(x)d\lambda(x,r)$$

Motivated

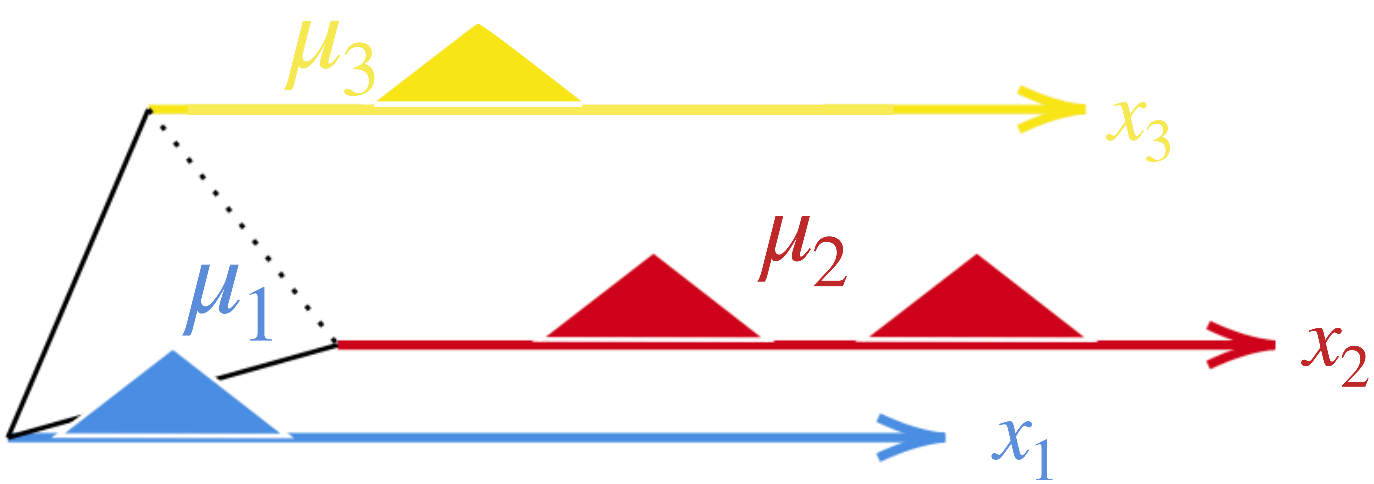
$$\mathfrak{P} : \mathscr{P}(\mathbb{R}^d \times \Delta^{n-1}) \to \mathscr{P}(\mathbb{R}^d \times G) : \lambda \mapsto \pi_{\mathbb{R}^d}\#(\boldsymbol{p}(r)\lambda(x,r))$$

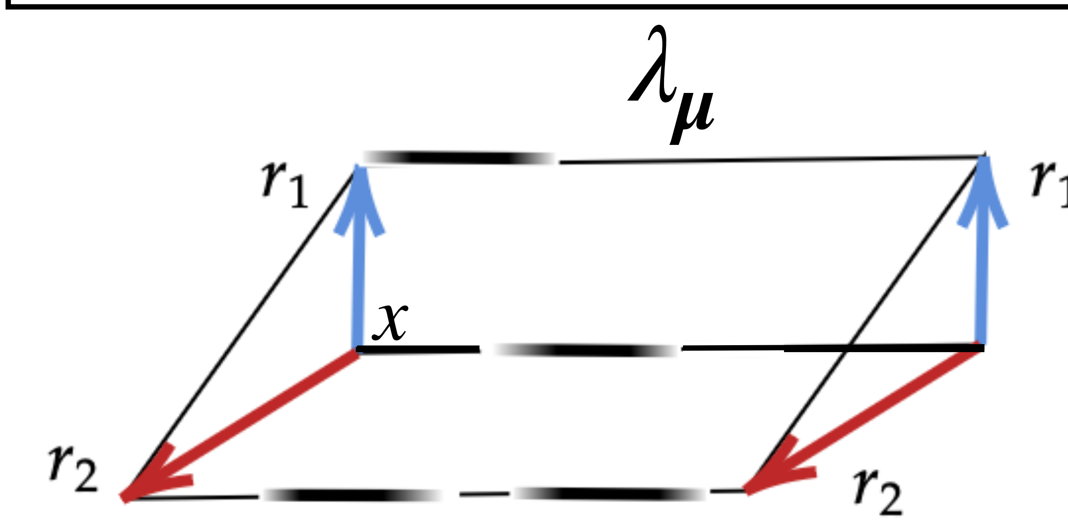
In other words, $\boldsymbol{\mu} = \mathfrak{P}\lambda$ iff for $i = 1,\ldots,n-1$, $\eta \in C_b(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} \eta(x)d\mu_i(x) = \int_{\mathbb{R}^d\times\Delta^{n-1}}$$



Call $\lambda_{\boldsymbol{\mu}}(x,r) := \sum_{i=1}^{n} \mu_i(x) \otimes \delta_{e_i}(r)$ the





Static (semi) met

$D_{\mathbb{R}^d \times G}$ fails the triangle inequality

$$D_{\mathbb{R}^d\times G}(\boldsymbol{\mu},\boldsymbol{\nu}) := \inf\left\{W_{\mathbb{R}^d\times\Delta^{n-1}}(\lambda_1,\lambda_2) : \mathfrak{P}\lambda_1 = \boldsymbol{\mu},\ \mathfrak{P}\lambda_2 = \boldsymbol{\nu}\right\}$$

$$W_{2,\mathscr{W}}(\boldsymbol{\mu},\boldsymbol{\nu}) := W_{\mathbb{R}^d\times\Delta^{n-1}}(\lambda_{\boldsymbol{\mu}},\lambda_{\boldsymbol{\nu}})$$

Prop [C., García Trillos, Nikolic '25]: On $\mathscr{P}_2(\mathbb{R}^d \times G)$, $D_{\mathbb{R}^d\times G}$ is a semi-metric, $W_{2,\mathscr{W}}$ is a metric, and $D_{\mathbb{R}^d\times G} \le W_{2,\mathscr{W}}$.

Prop [C., García Trillos, Nikolic '25]:

$$W^2_{2,\mathscr{W}}(\boldsymbol{\mu},\boldsymbol{\nu}) = \min \sum_{i,j=1}^{n} \iint \|x-\tilde{x}\|^2 + W_G^2(\delta_j,\delta_i)\,d\gamma_{ij}(x,\tilde{x})$$

$$\text{s.t. } \gamma_{ij} \in \mathscr{P}(\mathbb{R}^{2d}),\ \mu_i = \sum_{j=1}^{n} \pi_1 \# \gamma_{ij},\ \nu_j = \sum_{i=1}^{n} \pi_2 \# \gamma_{ij}$$

c.f. [Erbar, Maas '12] on graph, [Bacon '20] for cost $c_{ij}(x,\tilde{x})$

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Comparison of metrics

How are these various (semi) metrics related?

Thm [C., García Trillos, Nikolic '25]: For $\boldsymbol{\mu}, \boldsymbol{\nu} \in \mathscr{P}(\Omega \times G)$,

$$W_{\Omega \times G}(\boldsymbol{\mu}, \boldsymbol{\nu}) \leq D_{\mathbb{R}^d \times G}(\boldsymbol{\mu}, \boldsymbol{\nu}) \leq W_{2,\mathscr{W}}(\boldsymbol{\mu}, \boldsymbol{\nu})$$

Cor [C., García Trillos, Nikolic '25]: Suppose $\Omega \subseteq \mathbb{R}^d$ is bounded. For $C_q \sim \max_i \sum_j q_{ij}$ and $C_d \sim \operatorname{diam}(\Omega \times \Delta^{n-1})$,

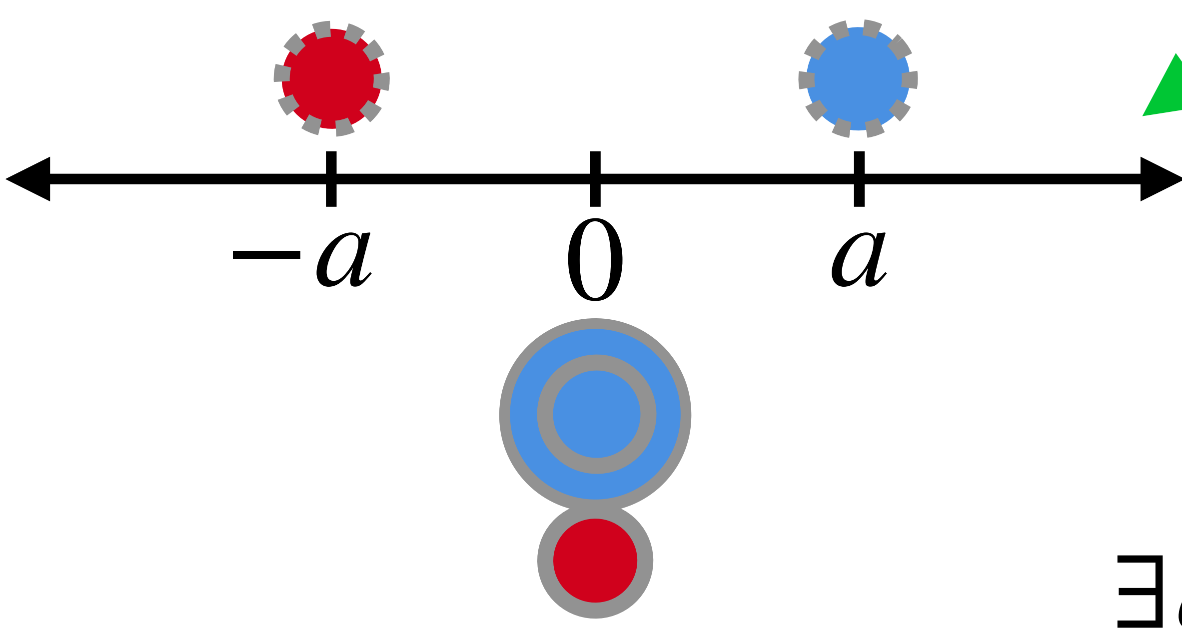
$$\min\{1, C_q^{-1/2}\} d_{BL}(\boldsymbol{\mu}, \boldsymbol{\nu}) \leq \dots \leq \max\{1, C_d^{3/2} n^{1/4}\} d_{BL}^{1/2}(\boldsymbol{\mu}, \boldsymbol{\nu})$$

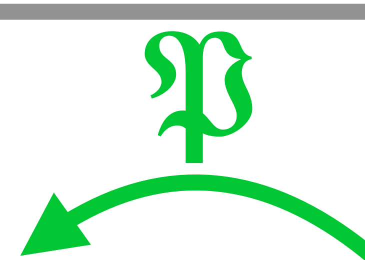
In particular, on a bounded domain, all are topologically equiv.

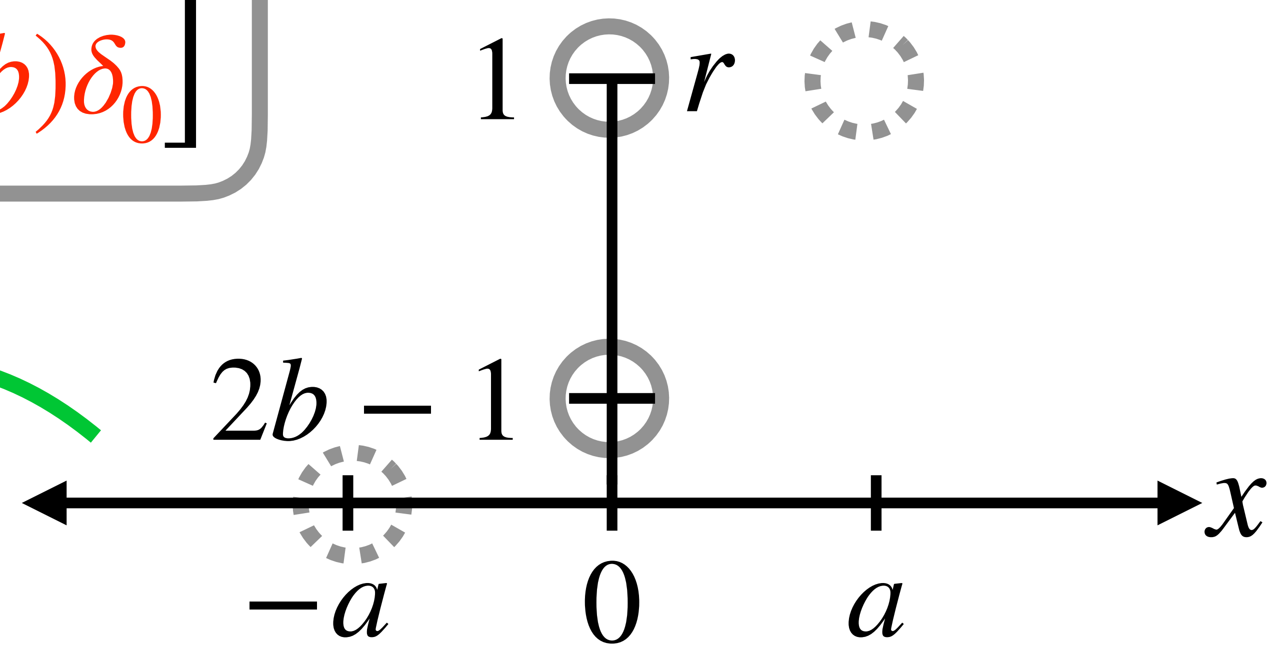
Example

$$\boldsymbol{\mu} = \frac{1}{2}\begin{bmatrix} \delta_a \\ \delta_{-a} \end{bmatrix}$$

$$\boldsymbol{\nu} = \begin{bmatrix} b\delta_0 \\ (1-b)\delta_0 \end{bmatrix}$$







$$W_{\mathbb{R}\times G}(\boldsymbol{\mu},\boldsymbol{\nu}) \leq a + d_{[0,1]}(1/2, b)$$

$\exists a, b$ s.t.

$$<$$

$$D_{\mathbb{R}\times G}(\boldsymbol{\mu},\boldsymbol{\nu}) = \sqrt{a^2 + \frac{1}{2} d^2_{[0,1]}(2b-1, 0)}$$

Example

$$\boldsymbol{\mu} = \frac{1}{2}\begin{bmatrix} \delta_a \\ \delta_{-a} \end{bmatrix}$$

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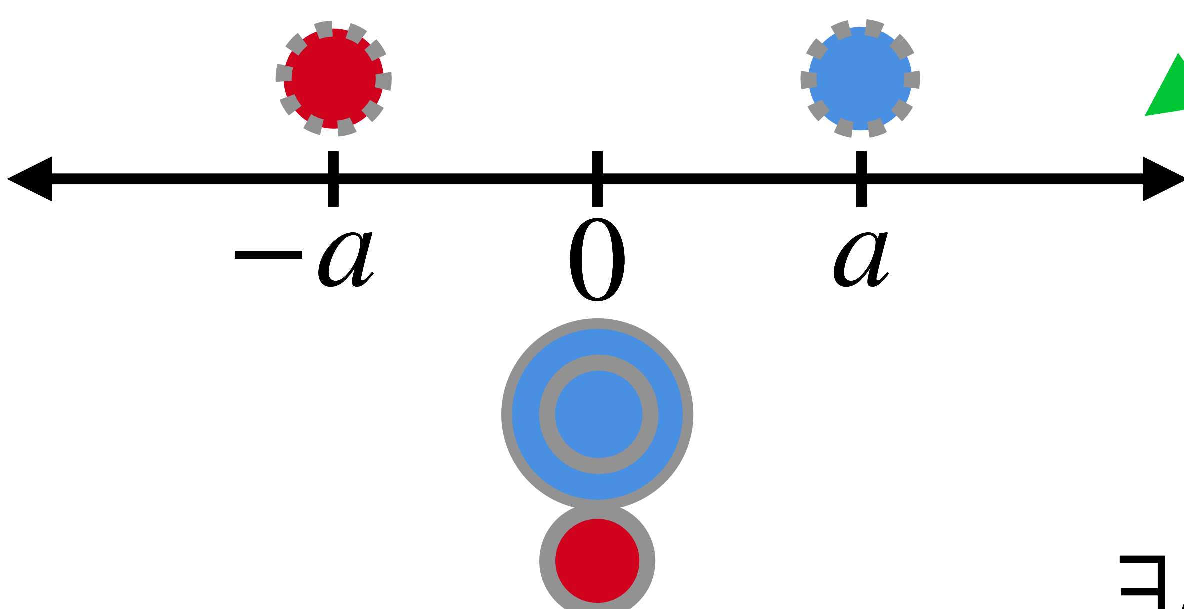

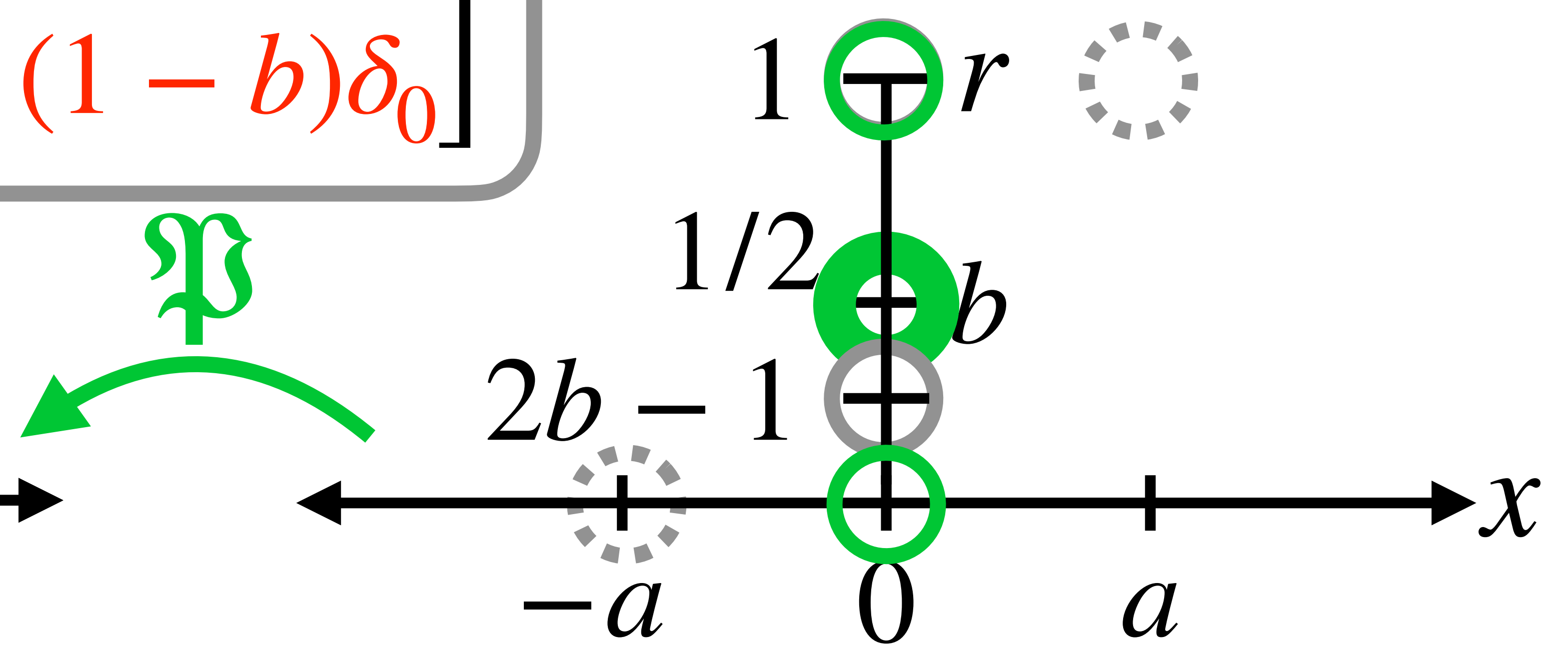

$$W_{\mathbb{R}\times G}(\boldsymbol{\mu},\boldsymbol{\nu}) \leq a + d_{[0,1]}(1/2, b)$$

$\exists a, b$ s.t. $<$

$$D_{\mathbb{R}\times G}(\boldsymbol{\mu},\boldsymbol{\nu}) = \sqrt{a^2 + \frac{1}{2} d^2_{[0,1]}(2b-1, 0)}$$

Which metric to use?

Dynamic metric: **gradient flows**; for $\mathscr{L}(\boldsymbol{\rho}, \boldsymbol{\mu}) := \sum_{i=1}^{n} KL(\rho_i \,|\, \mu_i)$,

$$\partial_t \rho_{i,t} = \Delta \rho_{i,t} - \nabla \cdot (\nabla \log(\mu_i) \rho_{i,t}) + \sum_{j=1}^{n} \theta(\rho_{i,t}, \rho_{j,t}) \log\left(\frac{\rho_{i,t}/\mu_i}{\rho_{j,t}/\mu_j}\right) q_{ij}$$

Static metric: **classification and linearization**

$$d^2_{LOT}(\boldsymbol{\mu}, \boldsymbol{\nu}) := \int_{\mathbb{R}^d \times \Delta^{n-1}} \|T_{\boldsymbol{\mu}}(x, r) - T_{\boldsymbol{\nu}}(x, r)\|^2 d\lambda_{\text{ref}}(x, r)$$

Caveat: existence of $T_{\boldsymbol{\mu}}$ satisfying $T_{\boldsymbol{\mu}} \# \lambda_{\text{ref}} = \lambda_{\boldsymbol{\mu}}$ open, since $\mathbb{R}^d \times \Delta^{n-1}$ may be a branching space [Cavallett, Mondino '17]

Thank you!

Gradient flows

Energy:

$$E(\boldsymbol{\mu}) = \int_{\mathbb{R}^d} f(\boldsymbol{\mu}(x))dx + \sum_{i=1}^{n} \int_{\mathbb{R}^d} V_i(x)\mu_i(x)dx$$

$$+ \frac{1}{2} \sum_{i,j=1}^{n} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \mu_i(x) W_{ij}(x-y) \mu_j(y) dx dy,$$

Gradient flows:

$$\partial_t \mu_i(x) = \nabla \cdot \left(\mu_i(x) \left(\nabla \partial_i f(\boldsymbol{\mu}(x)) + \nabla V_i(x) + \sum_{k=1}^{n} \nabla W_{ik} * \mu_k(x) \right) \right)$$

$$- \sum_{j=1}^{n} \left(\partial_i f(\boldsymbol{\mu}(x)) - \partial_j f(\boldsymbol{\mu}(x)) + V_i(x) - V_j(x) + \sum_{k=1}^{n} (W_{ik} - W_{jk}) * \mu_k(x) \right)$$

$$\cdot \theta\left(\mu_i(x), \mu_j(x)\right) q_{ij},$$

Graph operators

$$\nabla_{\mathcal{G}} : \mathbb{R}^n \to \mathbb{R}^{n \times n}(\mathbb{R}) : \phi \mapsto [\phi_j - \phi_i]_{i,j=1}^n$$

$$\mathrm{div}_{\mathcal{G}} : \mathbb{R}^{n \times n} \to \mathbb{R}^n : v \mapsto \Big[-\frac{1}{2} \sum_j (v_{ij} - v_{ji}) q_{ij} \Big]_{i=1}^n$$