Entropic Optimal Transport and Wasserstein Barycenters in Random Graphs

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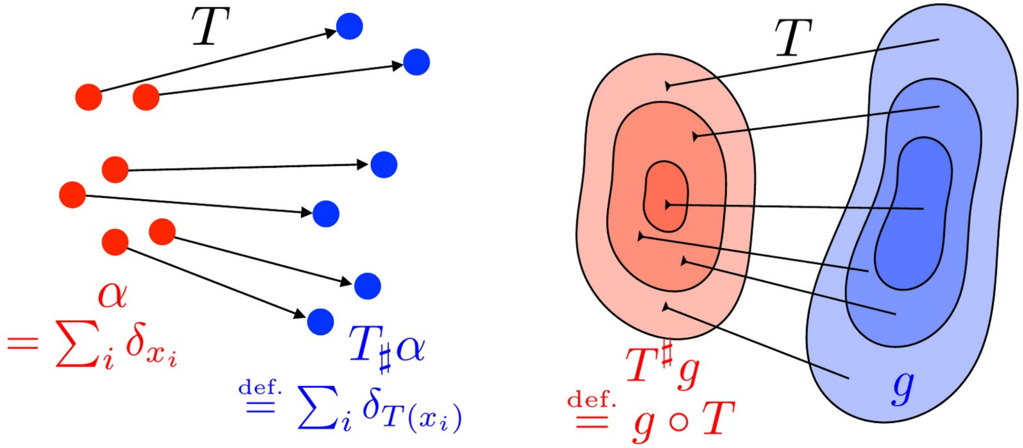
CNRS, Gipsa-lab, IRISA

Joint work with Marc Theveneau

(Ecole polytechnique)

(Optimal) Transport in Graphs

Optimal Transport (OT): "optimal" way to transport "mass" between several locations. Defines a (family of) metric(s) between probability distributions.



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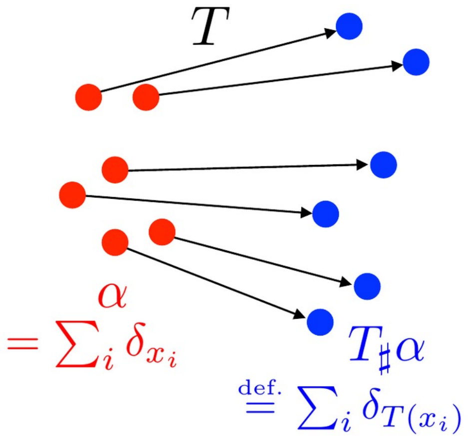

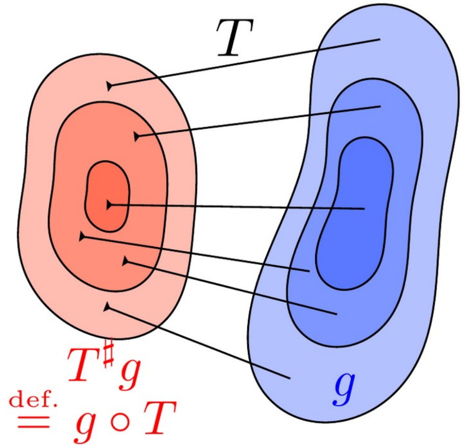

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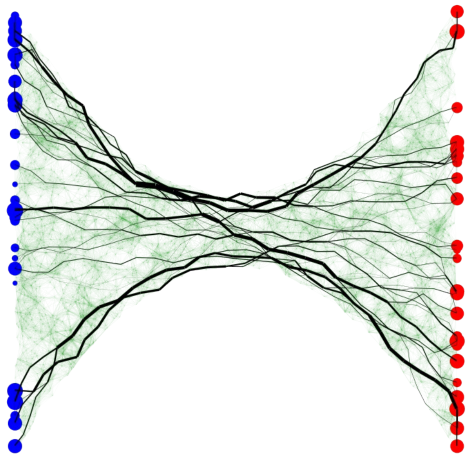

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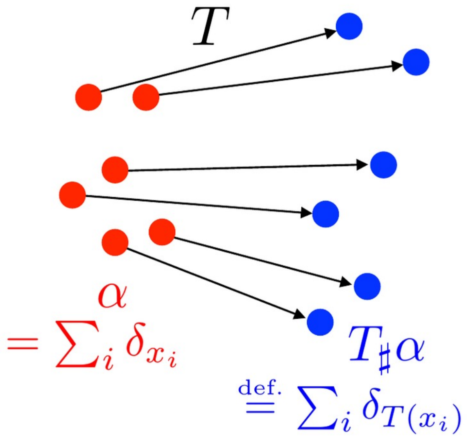

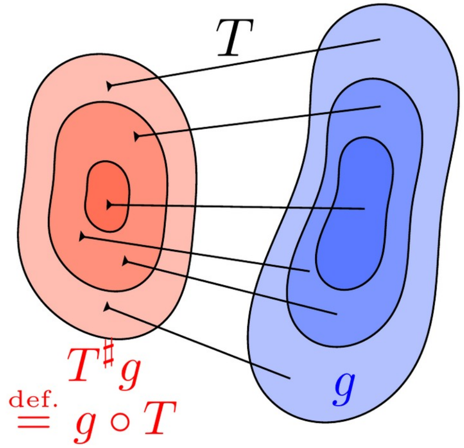

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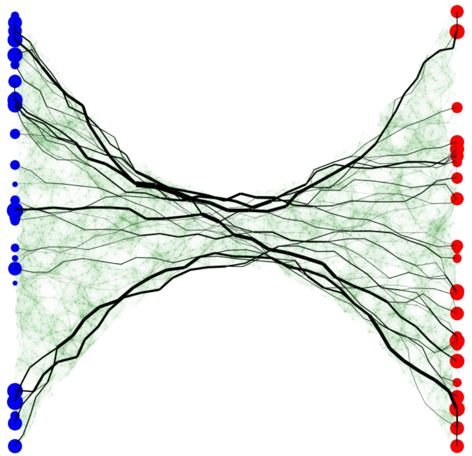

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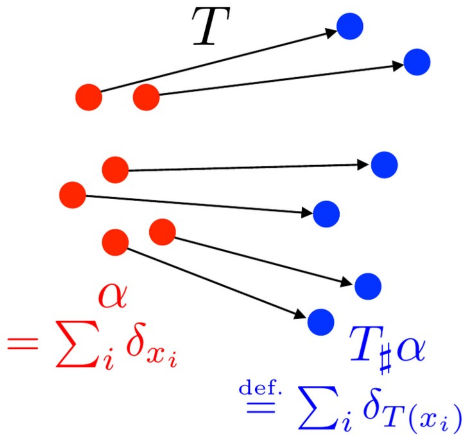

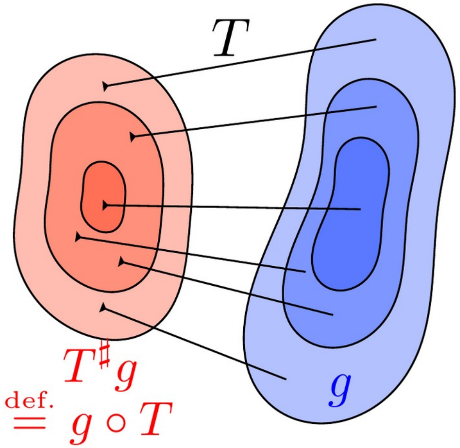

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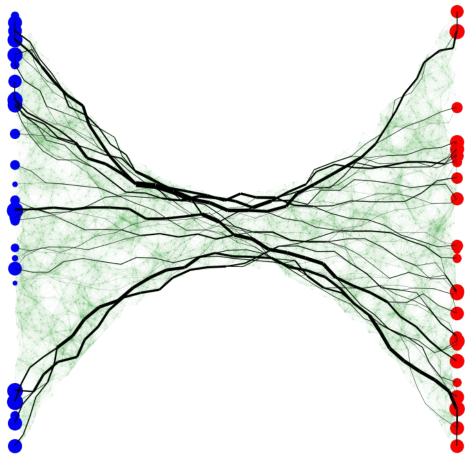
- Here, target nodes are **given** (user- or algorithm-chosen)



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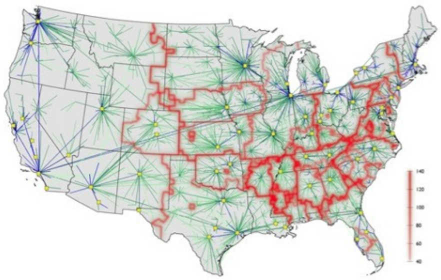

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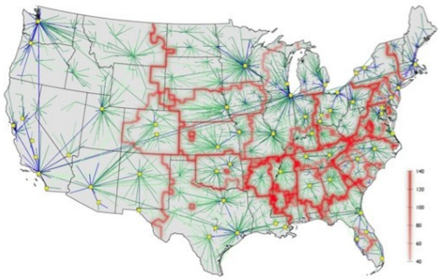

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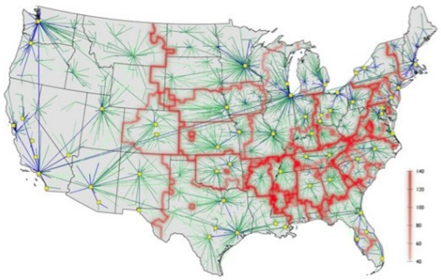

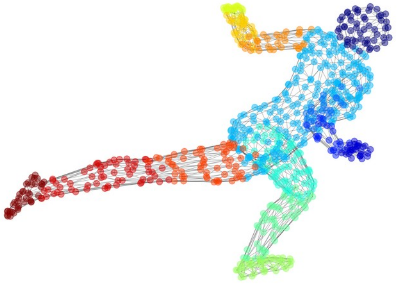
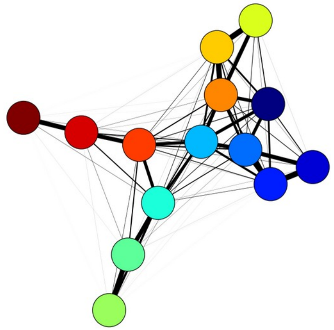

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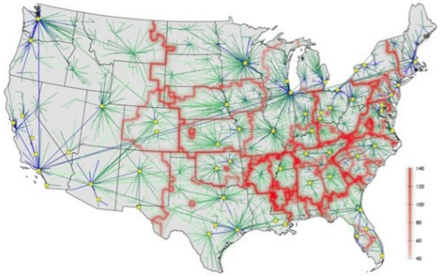
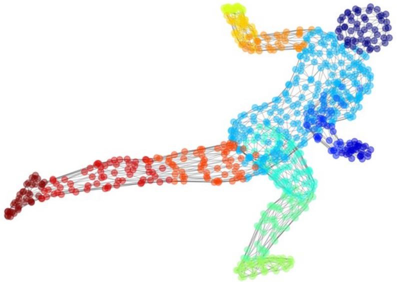
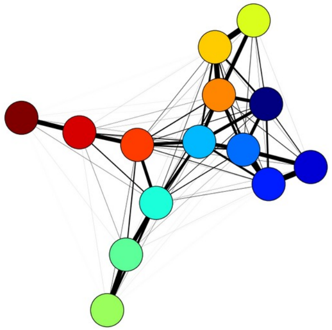
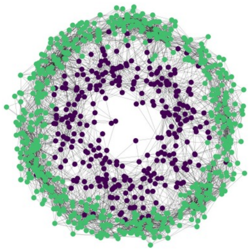
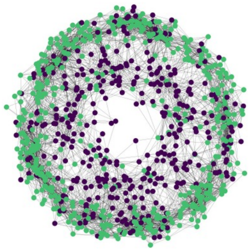
- What is a good criterion to evaluate the "quality" of clustering algorithms?



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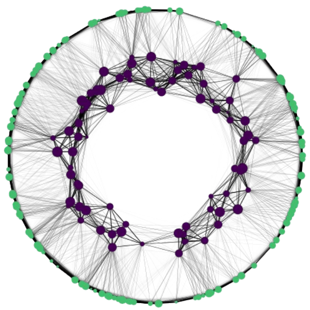

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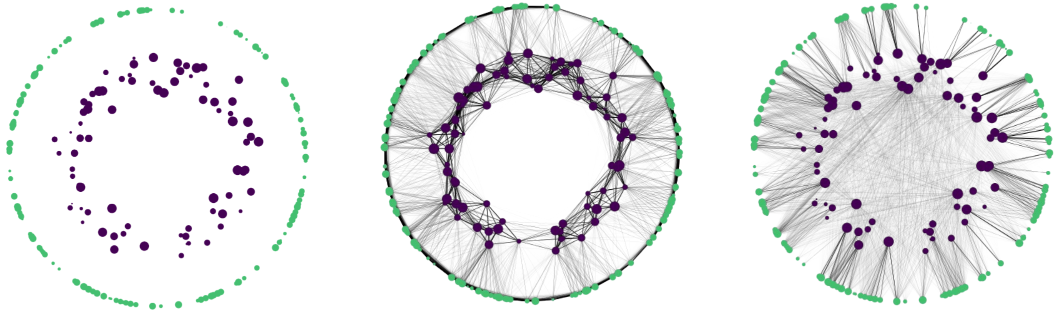

Entropic-regularized OT: [Cuturi 2013]

$$\mathcal{W}_\epsilon^C(\alpha, \beta) = \min_{P \in \Pi(\alpha,\beta)} \langle C, P \rangle + \epsilon KL(P|\alpha \otimes \beta)$$

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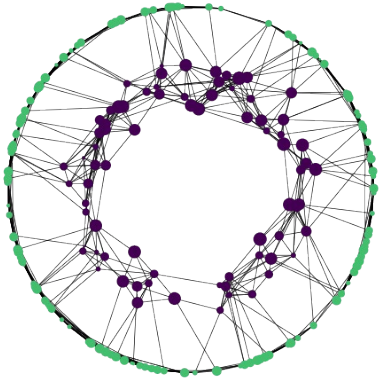

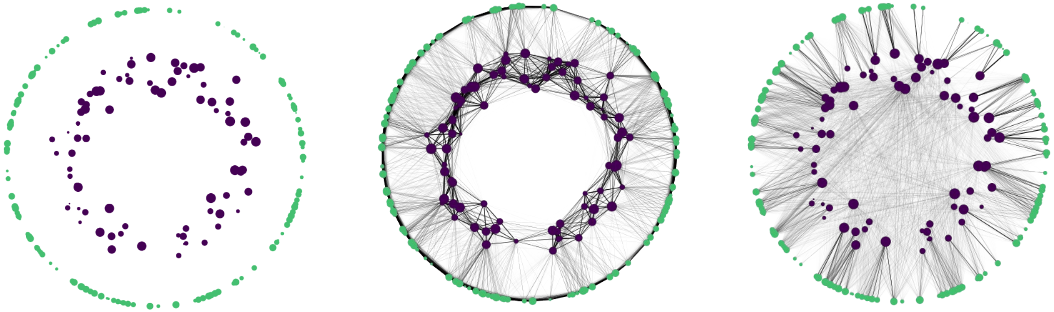

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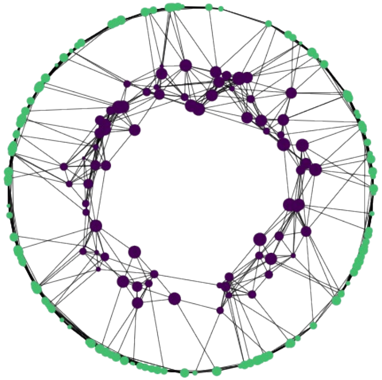

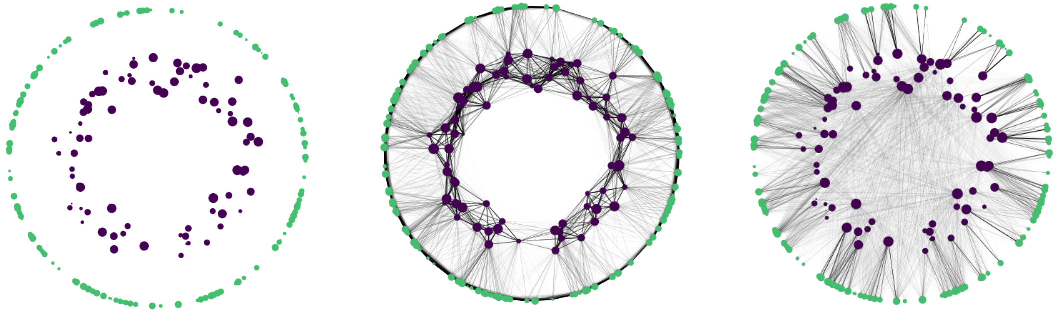

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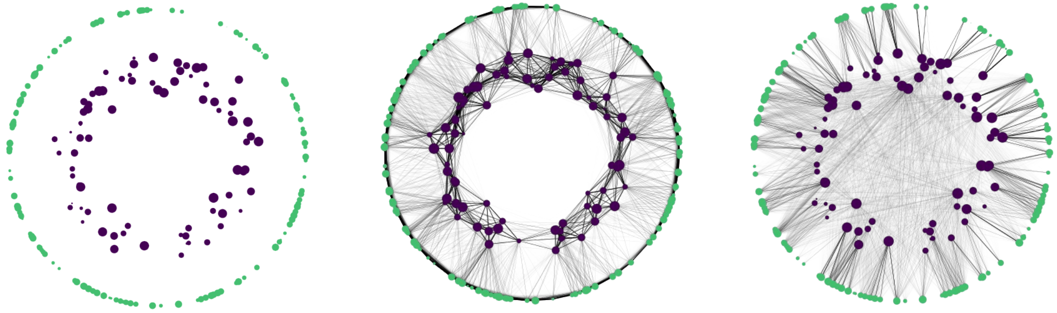

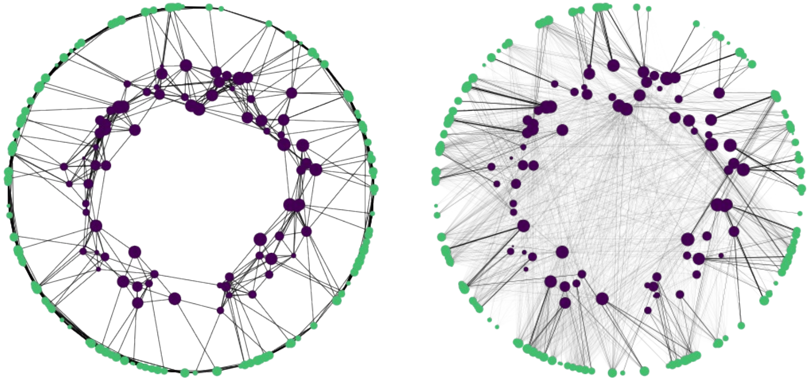

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- Estimate $\hat{C}$
- **How close is** $\mathcal{W}_\epsilon^{\hat{C}}(\alpha, \beta)$ **?**

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1. Stability of OT to inexact cost
2. Application to RG with “local” kernels
3. Application to RG with “non-local” kernel
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Stability to inexact cost

Stability to inexact cost matrix?

Immediate: $\forall \epsilon \geq 0 \quad |\mathcal{W}_\epsilon^C(\alpha, \beta) - \mathcal{W}_\epsilon^{\hat{C}}(\alpha, \beta)| \leq \sup_P |\langle P, C - \hat{C} \rangle| \leq \|C - \hat{C}\|_\infty$

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- Invariant to translating $C, \hat{C}$
- Exponential in ϵ
- First bound stronger, second bound more "usable"
- Proof: classical, bound the dual potentials

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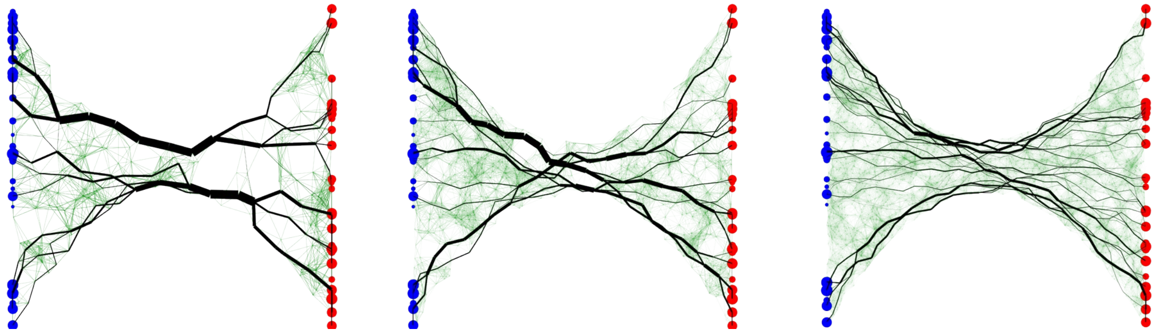

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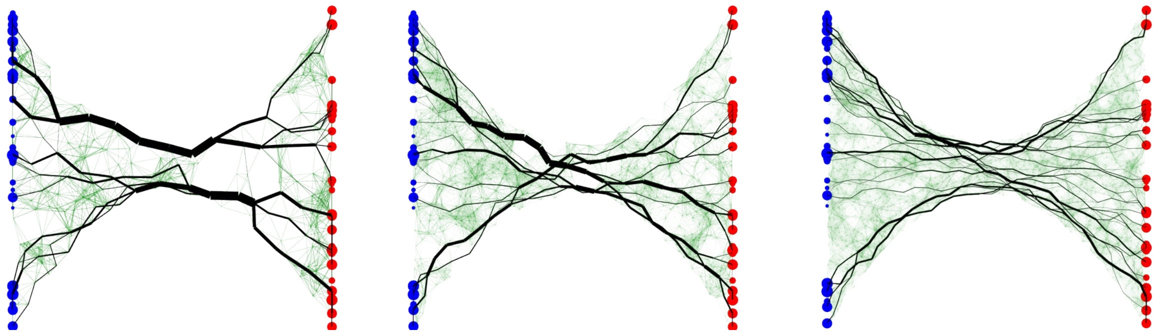

- Still invariant by cost shift
- Includes both norms
- Slower rate than convergence of the metric itself

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RGs with "**local kernels**": close nodes are connected, radius decreases when #nodes increases

*Known: **weighted shortest paths** converge to geodesic distance*

[Bernstein et al. 2000]

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- Fixed $\{x_1, \ldots, x_{n+m}\} \subset \mathcal{M}_k$
- Nodes $\{x_{n+m+1}, \ldots, x_N\} \overset{iid}{\sim} \nu$ with $N \to \infty$
- Kernel $w_N(x,y) = 1_{\|x-y\| \leq h_N}$ with $\frac{\log(1/h_N)}{N h_N^k} \to 0$

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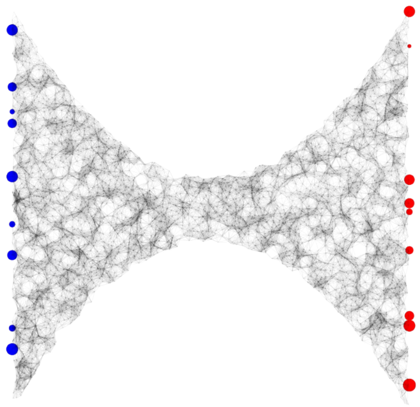

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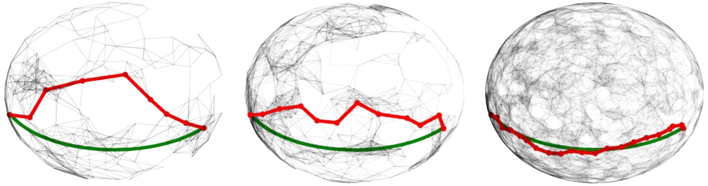

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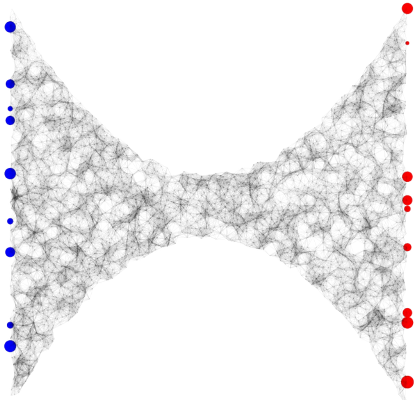

Theorem (K.): if ν has a lower-bounded density, whp

$$h_N \mathrm{SP}(v_i, v_{n+j}) = d_\mathcal{M}(x_i, x_{n+j}) + \mathcal{O}\left(\left(\frac{\log 1/h_N}{N h_N^k}\right)^{\frac{1}{k}}\right)$$

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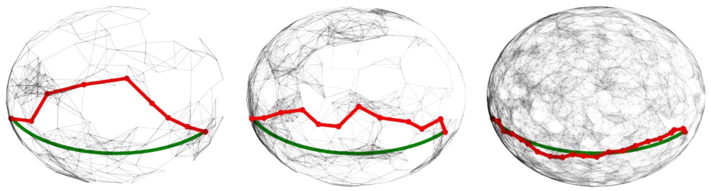

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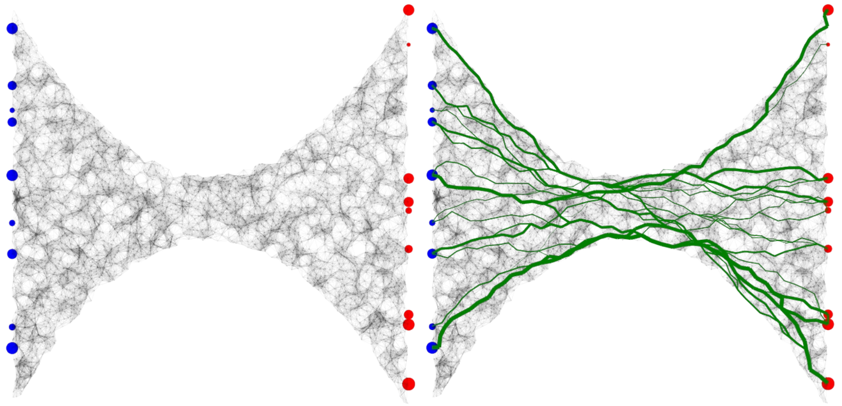

Corollary

$C_{ij} = f(d_{\mathcal{M}}(x_i, x_{n+j}))$

leads to

$\|\hat{C}_{\mathrm{SP}} - C\|_\infty \to 0$

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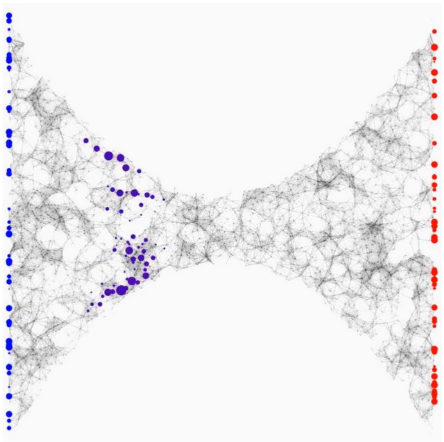
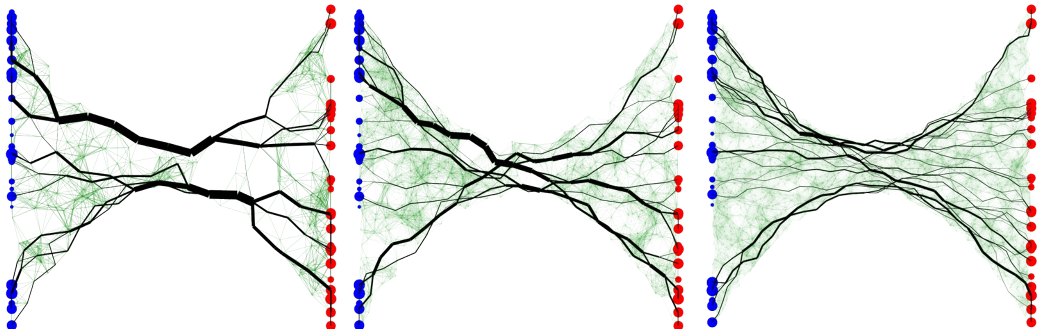
Illustration

Some numerical illustrations...





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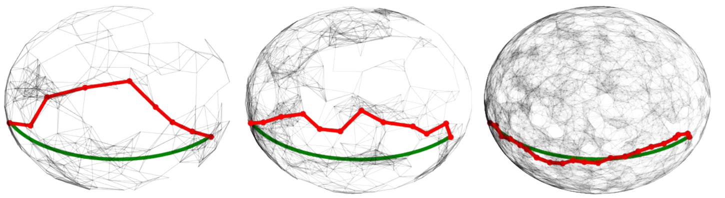
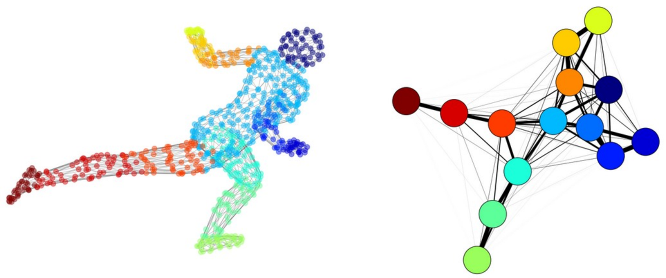
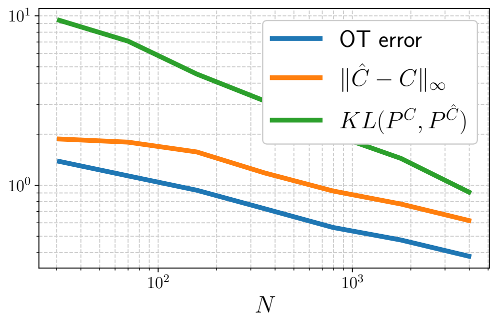


Convergence of shortest path



MDS embedding



Convergence rates

Outline

1. Stability of OT to inexact cost
2. Application to RG with “local” kernels
3. Application to RG with “non-local” kernel
4. Wasserstein Barycenters *(w/ Marc Theveneau)*

USVT estimator

RGs with "nonlocal kernels": fixed kernel, multiplying factor decreases when #nodes increases

- Nodes $\{x_1, \ldots, x_{n+m}\}$
  with $n \sim m \to \infty$
- Kernel $w_n(x,y) = \rho_n w(x,y)$
  with $\rho_n \gtrsim (\log n)/n$
  and psd kernel
- Cost $c(x,y) = f(w(x,y))$
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[Lei&Rinaldo 2015]

Pbm: $\frac{1}{n}\|A/\rho_n - W\| \lesssim (n\rho_n)^{-\frac{1}{2}}$

but $\frac{1}{n}\|A/\rho_n - W\|_F \not\to 0$

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Universal Singular Value Thresholding (USVT)

[Chatterjee 2015]

- Diagonalize $A = \sum_i \sigma_i a_i a_i^\top$

$$\hat{W}_\gamma = \mathrm{cut}_{[w_{\min}, w_{\max}]}(\rho_n^{-1} \textstyle\sum_{\sigma_i \geq \gamma\sqrt{\rho_n n}} \sigma_i a_i a_i^\top)$$

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Corollary:

$$|\mathcal{W}_\epsilon^{\hat{C}_{\gamma_r}}(\alpha,\beta) - \mathcal{W}_\epsilon^{C}(\alpha,\beta)| \lesssim e^{2(L-\ell)/\epsilon}(\rho_n n)^{-1/4}$$

$$\mathrm{KL}(P^C | P^{\hat{C}}) \lesssim \epsilon^{-1/2} e^{4(L-\ell)/\epsilon}(\rho_n n)^{-1/8}$$

"Fast" rate

When $w(x,y) = e^{-\frac{\|x-y\|^p}{\sigma}}$, the matrix W is **directly** the "Sinkhorn" matrix $K = e^{-C/\sigma}$

when $\epsilon = \sigma$ **and** $c(x,y) = \|x-y\|^p$

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Theorem (K.):

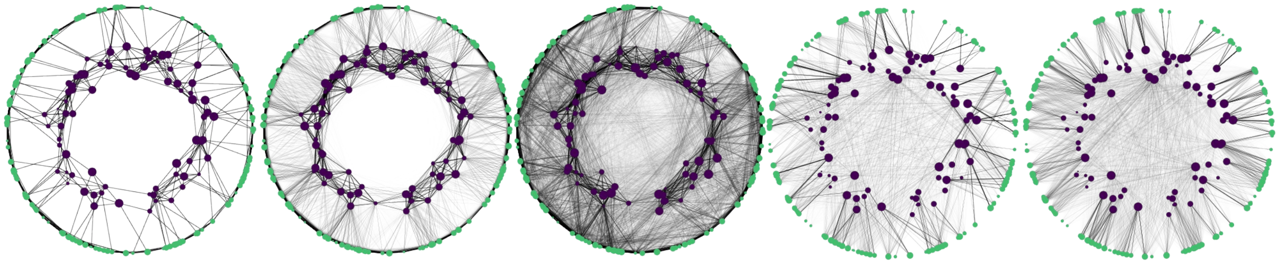
Defining $\mathcal{L}_\epsilon^K(\alpha,\beta) = \max_{f,g} f^\top\alpha + g^\top\beta - \epsilon(e^{\frac{f}{\epsilon}} \odot \alpha)^\top K(e^{\frac{g}{\epsilon}} \odot \beta) + \epsilon$

the dual OT cost with matrix K , whp

(plus some bounding conditions on the potentials)

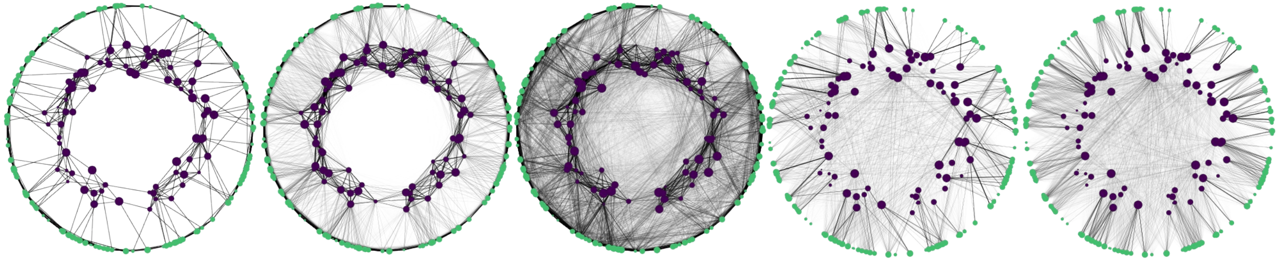
$$|\mathcal{L}_\sigma^{A/\rho_n}(\alpha,\beta) - \mathcal{W}_\sigma^C(\alpha,\beta)| \lesssim (n\rho_n)^{-1/2}$$

Illustration



Observation, true kernel, USVT, true OT plan, estimated OT plan.

Illustration



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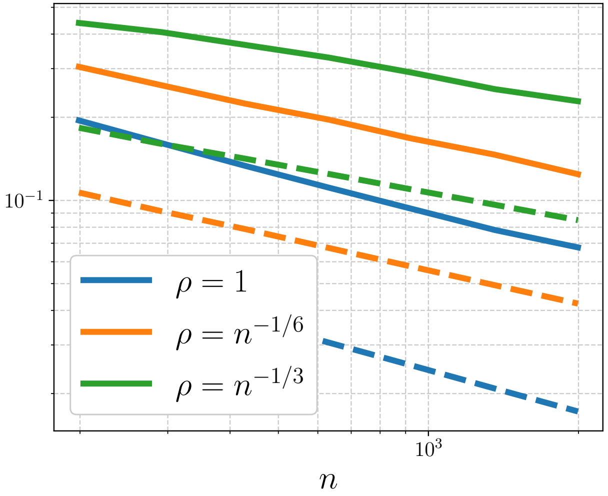
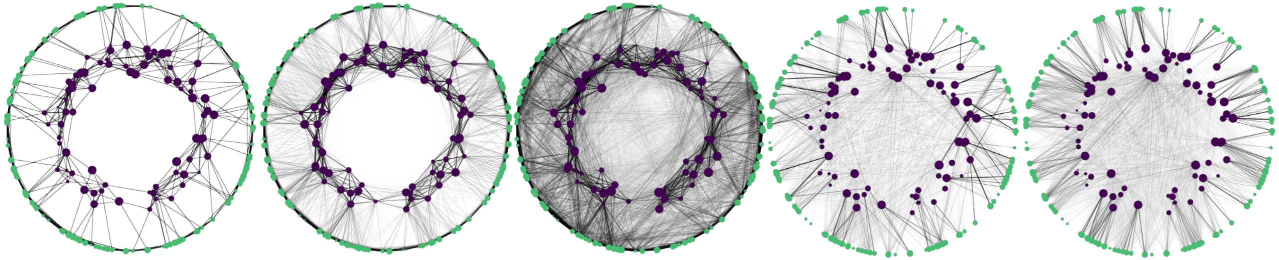


Convergence of OT distance.

Dotted: fast estimator

Illustration



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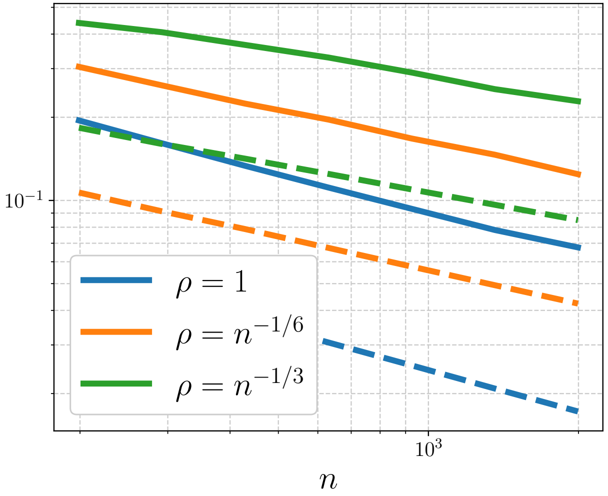

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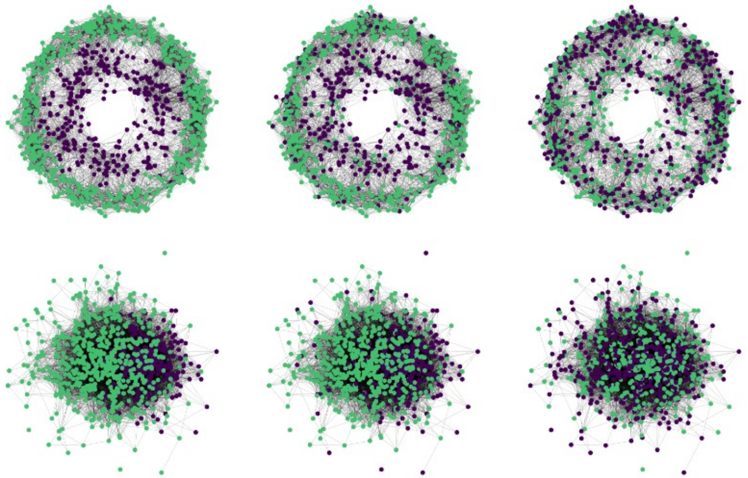

	Cond.	Cut	Cov.	Perf.	Mod.	OT
Circ.	0.78	0.95	0.96	0.91	0.96	**0.97**
GMM	0.71	0.95	0.95	0.92	0.95	**0.97**

***Clustering quality**: correlation between quality metrics and increasingly noisy clustering*

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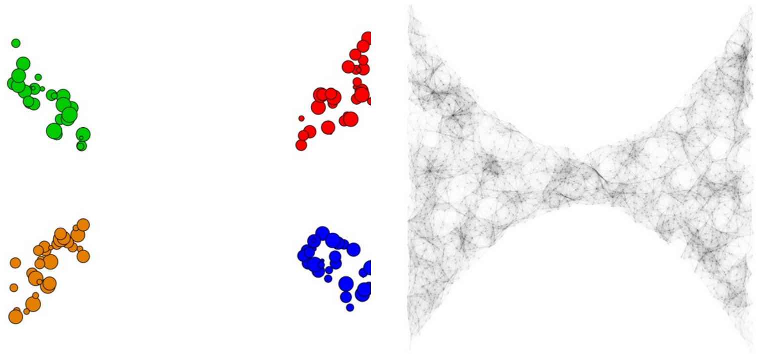
Entropic Wasserstein Barycenters

S distributions	S cost matrices **to a common space**
$\beta_s \in \Delta_{m_s}^+$	$C_s \in \mathbb{R}_+^{n \times m_s}$



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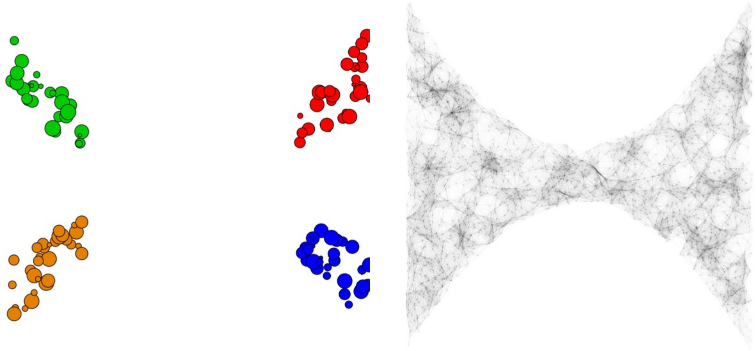
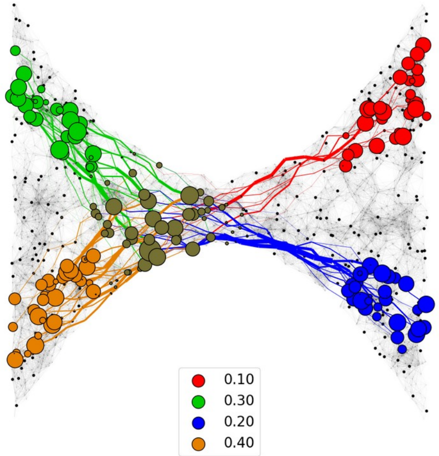


Wasserstein Barycenters [Agueh Carlier 2011]

Given nonnegative weights $\sum_s \lambda_s = 1$

$$\alpha^C = \arg \min_{\alpha \in \Delta_n^+} B^C(\alpha) = \sum_s \lambda_s \mathcal{W}_\epsilon^{C_s}(\alpha, \beta_s)$$

NB: a variant of ***Sinkhorn's algorithm*** *only uses* $K_s = e^{-C_s/\epsilon}$



WB stability to inexact cost

Immediate: $\forall \epsilon \geq 0 \quad |B_\epsilon^C(\alpha_\epsilon^C) - B_\epsilon^{\hat{C}}(\alpha_\epsilon^{\hat{C}})| \leq \sum_s \lambda_s \|C_s - \hat{C}_s\|_\infty$

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We are more interested in the stability of the barycenters α^C !

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Theorem (T,K): If $\ell \leq C_{sij}, \hat{C}_{sij} \leq L$

$\forall \epsilon > 0$

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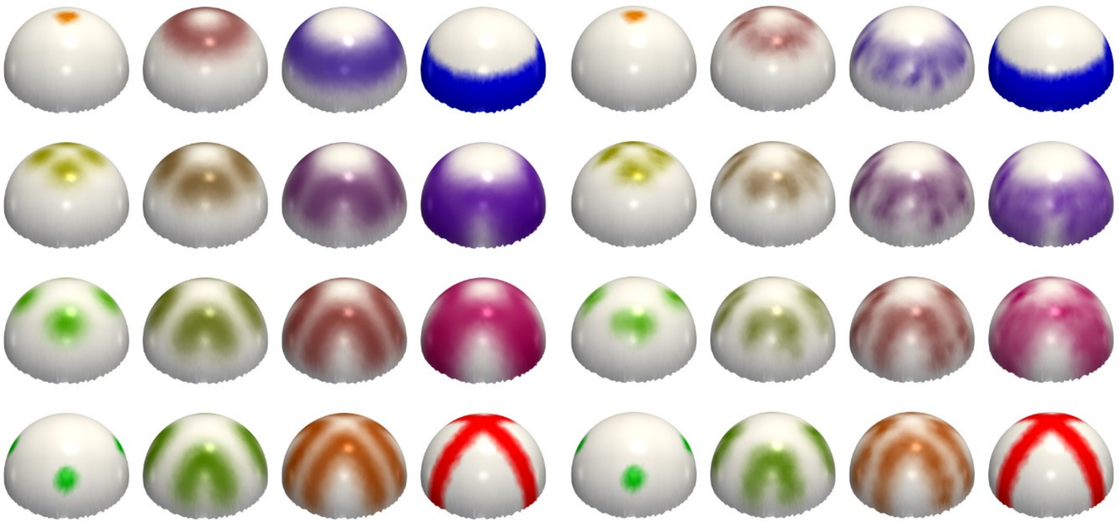
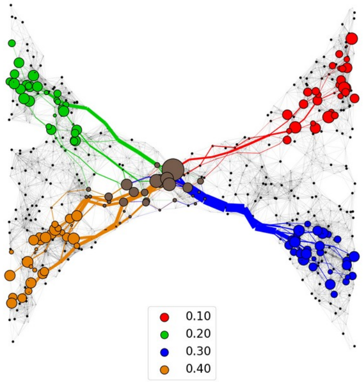
- Invariant to translating $C, \hat{C}$
- Exponential in ϵ
- Only supremum norm, Frobenius still open
- Proof: classical, bound the dual potentials
- More recent results with different approach: see Chizat 2023

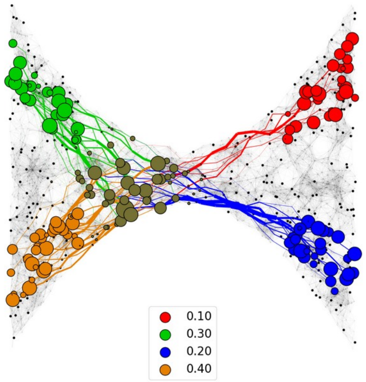
Illustration

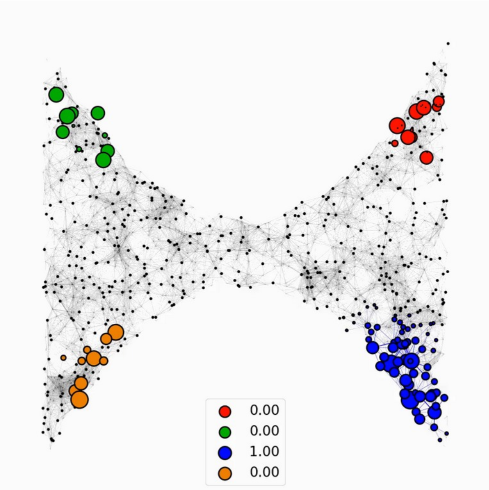
Immediately lead to convergence for **local kernels on manifolds** (non-local still open)

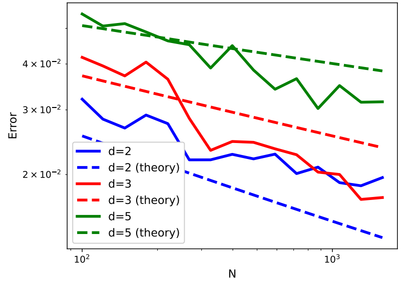


(a) Barycenters with the true geodesics (known for the sphere). (b) Barycenters with the shortest paths in a random graph.









Conclusion

- OT and WB can be done when the cost matrix is not known exactly
- *Maybe "reinventing the wheel" a bit, but* interesting results in the context of random graphs
- First steps, many **outlooks**:
  - More integrated, data-driven way of estimating the cost?
  - WB with non-local kernels
  - Other applications?

Keriven N. **Entropic Optimal Transport in Random Graphs.** a*rXiv:2201.03949*
Theveneau M., Keriven N. **Stability of Entropic Wasserstein Barycenters and application to random geometric graphs.** arXiv:2210.10535

nkeriven.github.io