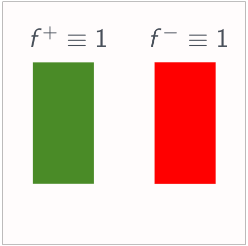
Numerical solution of Optimal Transport Problem on graphs

Enrico Facca, Michele Benzi
8^{th} ECM - June 22^{nd}, 2021

SCUOLA NORMALE SUPERIORE

L^1-Optimal Transport Problem (continuous)

$\Omega \subset \mathbb{R}^n$ f^+, f^- two non-negative densities with $\int_\Omega f^+ = \int_\Omega f^-$



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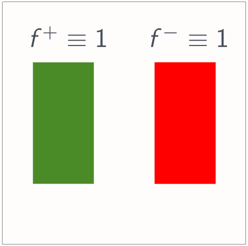

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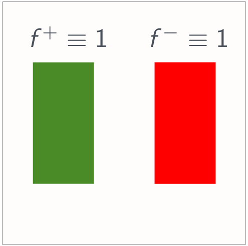

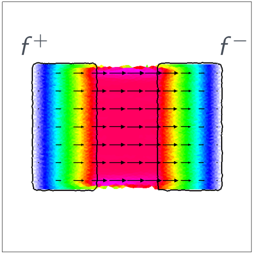

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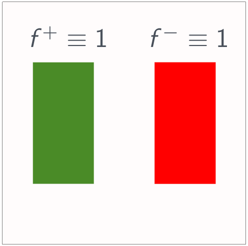

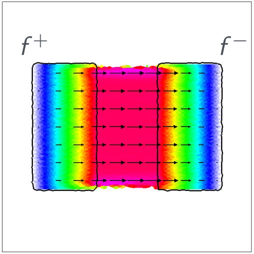

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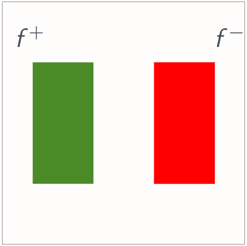

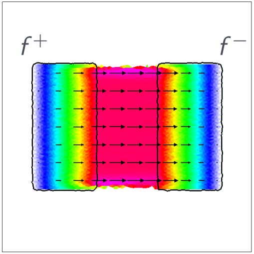

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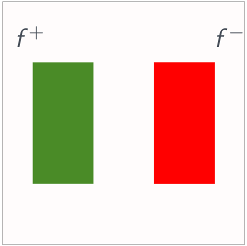

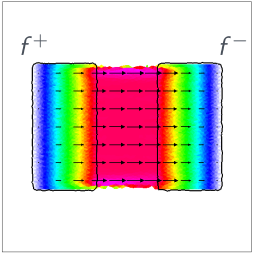

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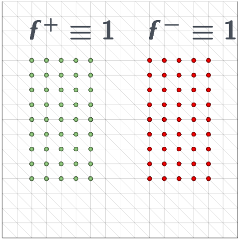

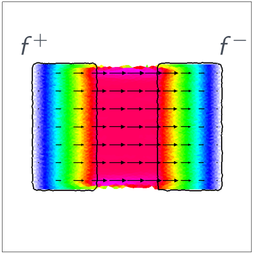

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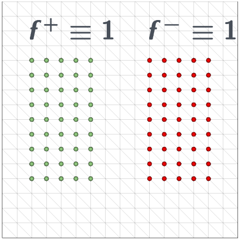

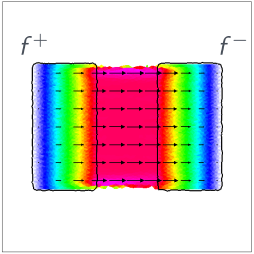

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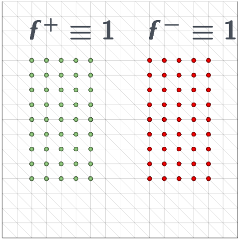

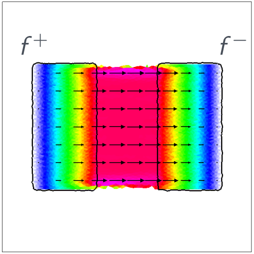

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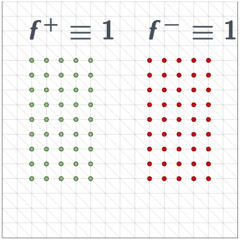

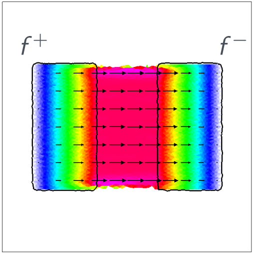

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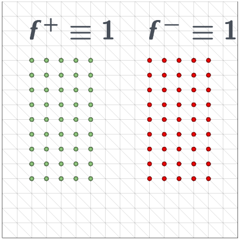

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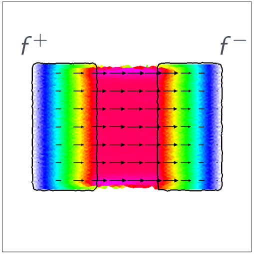

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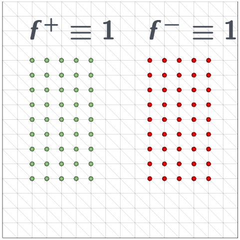

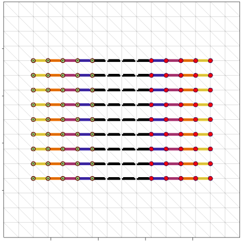

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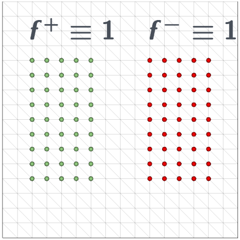

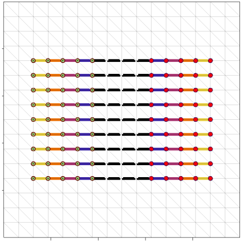

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Wasserstein-1 distance in Inverse Problems

$$\min_{\theta} \|\text{Model}(\theta) - \text{Observ.}\|_{L^2} \qquad \theta = \text{Parameters}$$

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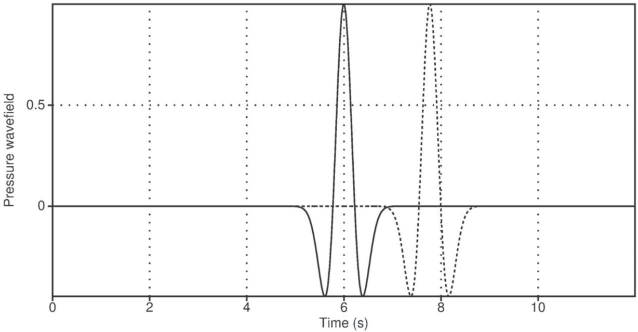

L. Métivier, R. Bros- sier,Q. Mérigot, E. Oudet, J. Virieux, *Measuring the misfit between seismograms using an optimal transport distance: application to full waveform inversion*, Geophysical Journal International, 2016

Wasserstein-1 distance in Inverse Problems

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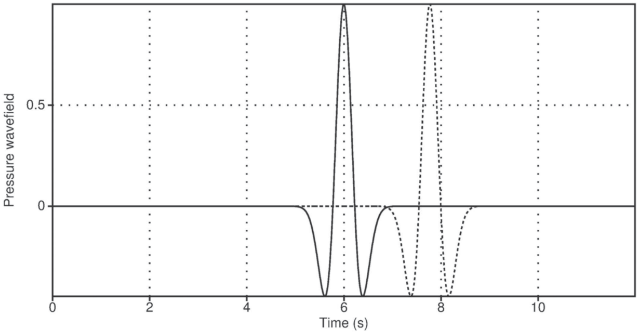
$$\frac{\partial}{\partial f^+} W^1(f^+, f^-) = u(\mu^*)$$



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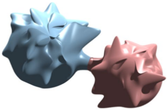
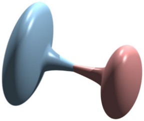
Oliver-Ricci Flow

Reimannian Manifold (M, g)

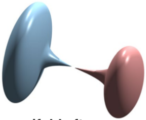
$$\partial_t g = -\text{Ricci}(g)$$



(a) initial manifold



(b) manifold after Ricci flow



(c) manifold after surgery

Ni, CC., Lin, YY., Luo, F. et al. Community Detection on Networks with Ricci Flow. Sci Rep 9, (2019).

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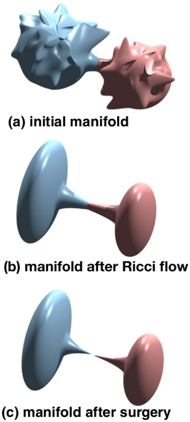
Weighted Graph$(\mathcal{G}, \boldsymbol{w})$

$$\partial_t w = -????$$



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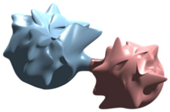

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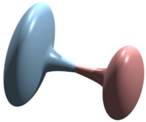
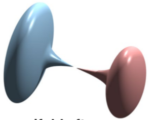


(b) manifold after Ricci flow

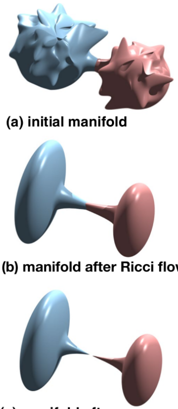


(c) manifold after surgery

Ni, CC., Lin, YY., Luo, F. et al. Community Detection on Networks with Ricci Flow. Sci Rep 9, (2019).

Oliver-Ricci Flow

Reimannian Manifold (M, g)	Weighted Graph$(\mathcal{G}, \boldsymbol{w})$
$\partial_t g = -\text{Ricci}(g) \approx \text{Ricci}(W^1)$	$\partial_t w = -\ \text{Ricci}(W^1)$



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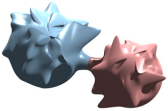

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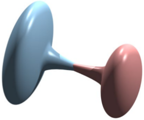

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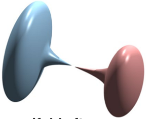

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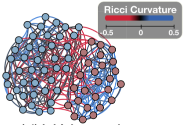
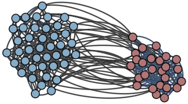
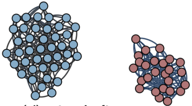


(a') initial network



(b') network after Ricci flow



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Take home message: the problem

- The Optimal Transport Problem of moving continuous densities f^+ and f^- with cost equal to Euclidean Distance

$$\min_{\mu:\Omega\to\mathbb{R}^+} \left\{ \mathcal{L}(\mu) := \int_\Omega \mu \frac{|\nabla u(\mu)|^2}{2} + \int_\Omega \frac{\mu}{2} \right\}$$

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$$\min_{\boldsymbol{\mu}\in\mathbb{R}^{|\mathcal{E}|}_{\geq 0}} \left\{ \mathcal{L}(\boldsymbol{\mu}) := (\boldsymbol{w}\odot\boldsymbol{\mu})^T \frac{|\nabla u(\boldsymbol{\mu})|^2}{2} + \frac{\boldsymbol{\mu}^T\boldsymbol{w}}{2} \right\}$$

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$$\inf_{\boldsymbol{\mu}} \left\{ \mathcal{L}(\mu) = (\boldsymbol{w} \odot \boldsymbol{\mu})^T \frac{|\nabla u(\boldsymbol{\mu})|^2}{2} + \frac{\boldsymbol{\mu}^T \boldsymbol{w}}{2} \ : \ \boldsymbol{\mu} \geq 0 \right\}$$

- **Gradient Descent Dynamics**
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- **Bio-inspired Dynamics (Mirror gradient descent)**
  $\partial_t \boldsymbol{\mu}(t) = -\boldsymbol{\mu}(t) \nabla_{\boldsymbol{\mu}} \mathcal{L}(\boldsymbol{\mu}(t))$ $\boldsymbol{\mu}(t) \geq \exp^{-t} \min \boldsymbol{\mu}(0)$
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Time Discretization

$$\text{DAE} \begin{cases} \mathbf{div}\, \mathrm{diag}\left(\boldsymbol{\sigma}^2/2\right) \boldsymbol{\nabla} \cdot \boldsymbol{u}(t) = \boldsymbol{f} \\ \boldsymbol{\sigma}'(t) = -\nabla_{\boldsymbol{\sigma}} \mathcal{L}(\Psi(\boldsymbol{\sigma}(t))) \\ \boldsymbol{\sigma}(0) = \boldsymbol{\sigma}^0 > 0 \end{cases} \qquad t^{k+1} = t^k + \Delta t^k$$

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  One weighted Laplacian system $\mathbf{div}\, \mathrm{diag}\left(\tilde{\mu}\right) \boldsymbol{\nabla} \boldsymbol{x} = \boldsymbol{b}$ per iteration
  Time step size limitation
- **Implicit Euler + Inexact Newton**

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More than 1 inexact weighted Laplacian system per iteration
Larger time step size

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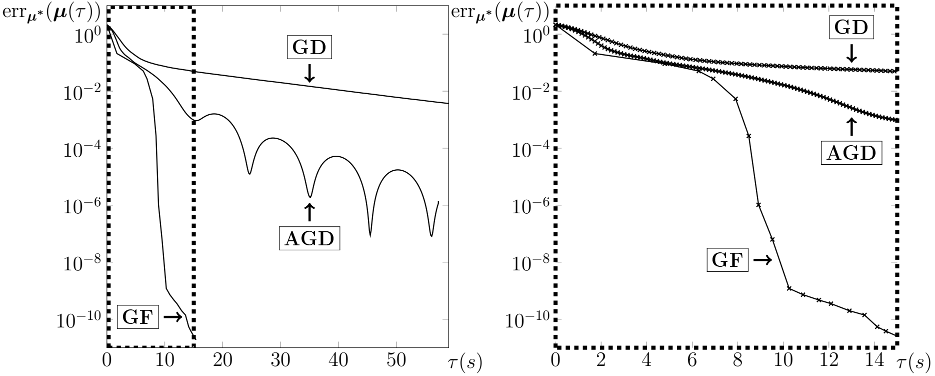
Comparison - Errors vs CPU-time



$\approx 10^5$ nodes/edges

Computational Cost - Scaling with graphs' size

"Grid-like" graphs (only "local" connection)

Graphs $\mathcal{G}$	$\lvert\mathcal{V}\rvert$	$\lvert\mathcal{E}\rvert$	Time steps	Newton steps	AGMG Iters.	CPU (s)	Errors $\text{err}_{\boldsymbol{u}^*}(\hat{\boldsymbol{u}})$
$\mathcal{G}_0$	$1.1 \cdot 10^3$	$3.1 \cdot 10^3$	9	29	335	0.0963	3.3e-15
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$\mathcal{G}_2$	$1.7 \cdot 10^4$	$4.9 \cdot 10^4$	7	26	399	0.902	9.0e-14
$\mathcal{G}_3$	$6.6 \cdot 10^4$	$2.0 \cdot 10^5$	7	28	456	4.43	3.3e-15
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$\mathcal{G}_5$	$1.1 \cdot 10^6$	$3.1 \cdot 10^6$	8	34	646	136	5.0e-14

#Newton-step $\approx \mathcal{O}(1)$ CPU $\approx \mathcal{O}(|\mathcal{E}|^{0.11})$

AGMG=**AG**gregation-based algebraic **M**ulti**G**rid (Notay et al.)

"Watts-Strogatz " graphs

#Newton-step $\approx \mathcal{O}(|\mathcal{E}|^{0.31})/\mathcal{O}(|\mathcal{E}|^{0.36})$ CPU $\approx \mathcal{O}(|\mathcal{E}|^{1.14})/\mathcal{O}(|\mathcal{E}|^{1.51})$

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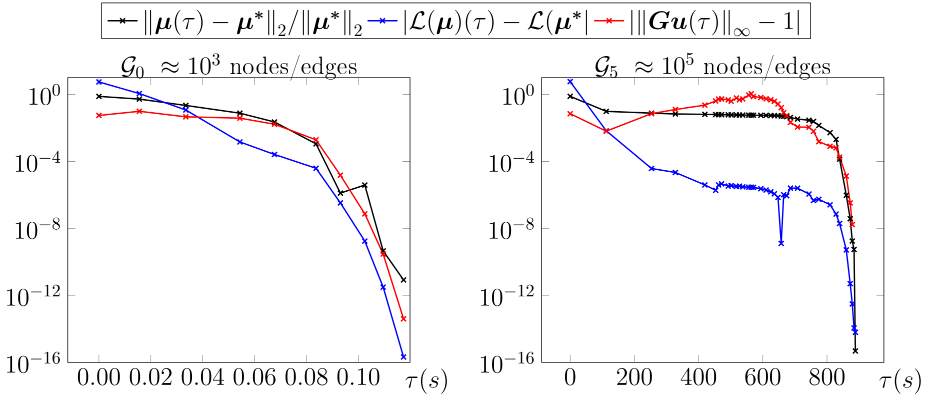
Computational Cost - Errors evolution



Take home messages on the numerical solution

- Using the $\boldsymbol{\mu} = \boldsymbol{\sigma}^2/2$ positiveness is preserved and purely Gradient Descent approaches can be used
- Explicit (or 1^{st}-order) schemes (GD or AGD) are cheap but requires many iterations to converge
- Implicit Euler + Inexact Newton (2^{nd}-order schemes) more expensive requires less time iterations
- "And the winner is": **Implicit Euler + Inexact Newton**
- The weighted Laplacian systems are solved efficiently by algebraic Multigrid Solvers (AGMG and LAMG)
- Selection of "active" edges can drastically improve efficiency

The paper: E. Facca and M. Benzi, "Fast iterative solution of the optimal transport problem on graphs" SIAM J. Sci. Comput. (2021).

The code : `https://gitlab.com/enrico_facca/dmk_solver`

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