A Sparse Algorithm for Optimal Transport

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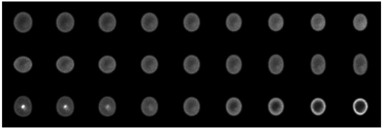
Applications of Numerical Optimal Transport



Versatile Tool

- computer vision & machine learning: histogram comparison [Rubner et al., 2000; Pele and Werman, 2009], ground metric learning [Wang and Guibas, 2012; Cuturi and Avis, 2014]
- imaging: interpolation [Maas et al., 2014], shape matching [Schmitzer and Schnörr, 2015], deformation analysis [Wang et al., 2012], denoising [Lellmann et al., 2014]
- optics [de Castro et al., 2014; Feng et al., 2015; Brix et al., 2015], physics [Frisch et al., 2002; Brenier, 2011], bakery logistics. . .

✗ computationally demanding

Solvers & Related Work

Discrete Solvers

- Hungarian method [Kuhn, 1955], Auction algorithm [Bertsekas, 1979], network simplex [Ahuja et al., 1993]

✓ numerically 'simple & robust', work on any cost-function

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Continuous Solvers

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✓ elegant theory, need only handle transport map

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Approximations and Tricks

- approximations: cost thresholding [Pele and Werman, 2009], tangent space [Wang et al., 2012], entropy smoothing [Cuturi, 2013]
- multi-scale [Mérigot, 2011; Schmitzer and Schnörr, 2013], sparse iterations [Mérigot and Oudet, 2014; Schmitzer, 2015; Oberman and Ruan, 2015]

(Discrete) Optimal Transport in a Nutshell

Transport Plans / Couplings

$$\Pi(\mu,\nu) = \{\pi \in \mathrm{Prob}(X \times Y) \colon \mathrm{Proj}_{X\sharp}\pi = \mu,\ \mathrm{Proj}_{Y\sharp}\pi = \nu\}$$

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subject to $\alpha(x) + \beta(y) \leq c(x,y)$ for all $(x,y) \in X \times Y$.

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PD Optimality Condition: $\pi(x,y) > 0 \Rightarrow \alpha(x) + \beta(y) = c(x,y)$

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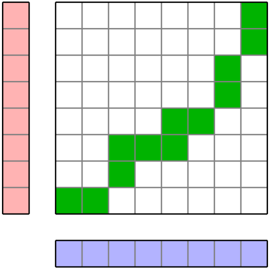
Restricted Problem: $\mathcal{N} \subset X \times Y$

Multi-Scale Scheme



Intuition & Experience

- only small subset $\mathcal{N} \subset X \times Y$ relevant

How to select $\mathcal{N}$?

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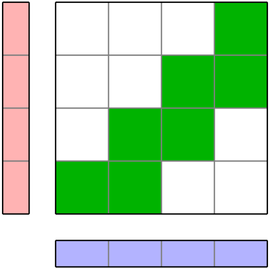

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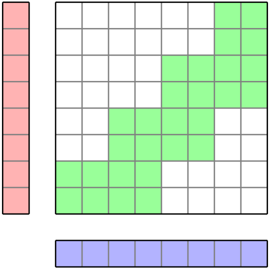

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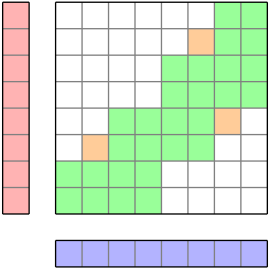

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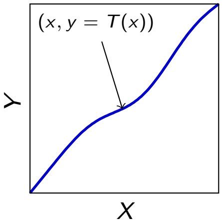
How to guarantee global optimality?

- a priori estimates? ✗ very difficult
- a posteriori: quick verification, 'smart' updates of $\mathcal{N}$

Polar Factorization & Local Optimality



Continuous Setting

- $X = Y = \mathbb{R}^n$, $c(x, y) = \|x - y\|^2$
- Optimal coupling induced by map $T : \mathbb{R}^n \to \mathbb{R}^n$: $\pi = (\mathrm{id}, T)_\sharp \mu$
- $T = \nabla\varphi$ for a convex potential $\varphi : \mathbb{R}^n \to \mathbb{R}$

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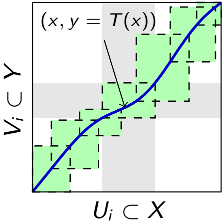

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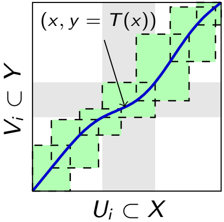

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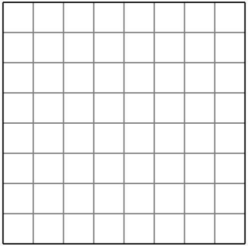
Discrete Equivalents:

- 1D: 'trivial': Monge property, 2D: not so much...

Short-Cuts



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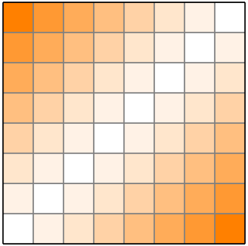

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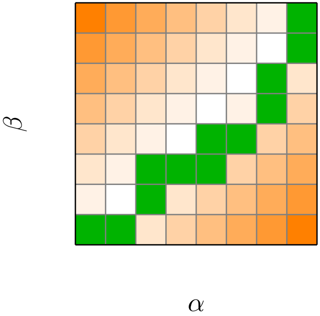

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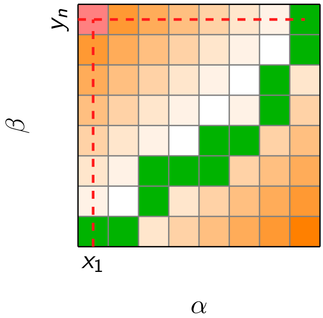

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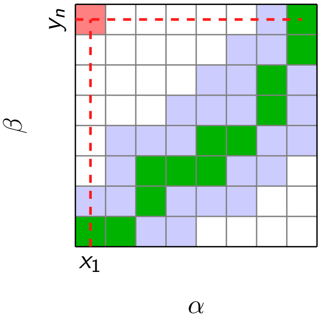

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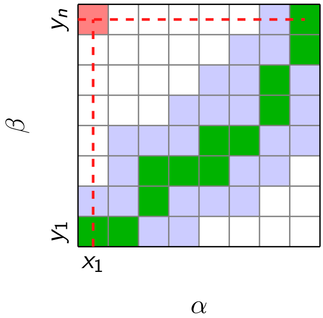

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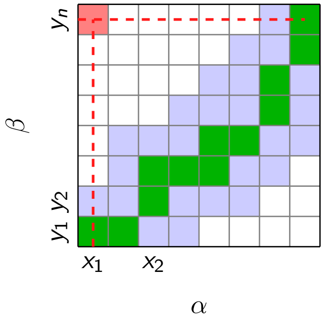

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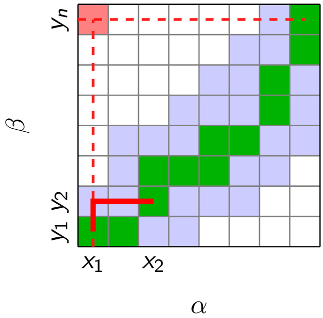

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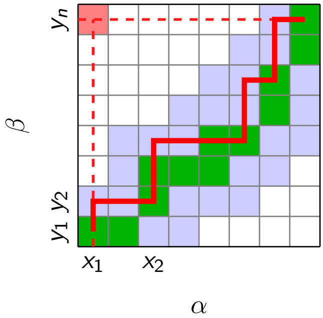

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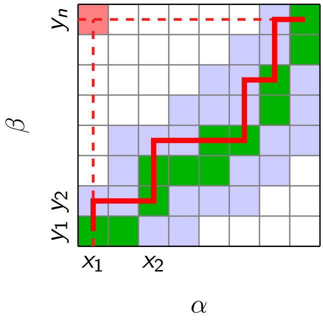

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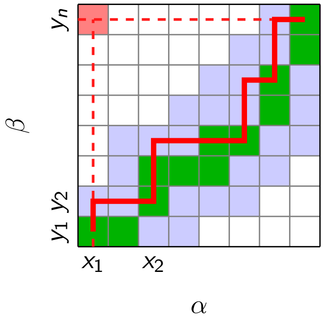

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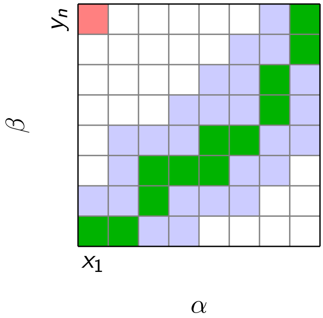
- continuum, $c(x, y) = \|x - y\|^2$: points along straight line are short-cuts

Shielding Condition



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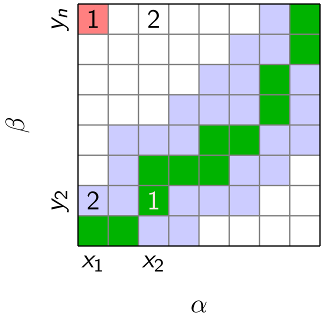

- $\underbrace{c(x_1, y_n) + c(x_2, y_2)}_{1} \geq \underbrace{c(x_1, y_2) + c(x_2, y_n)}_{2}$

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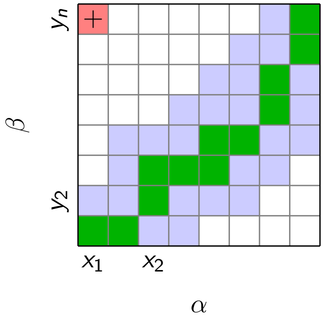

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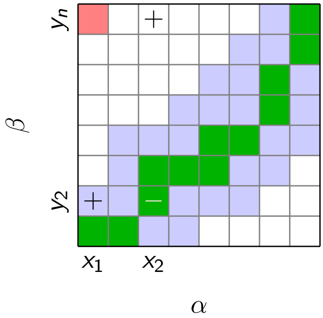

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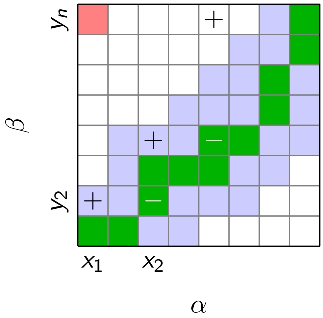

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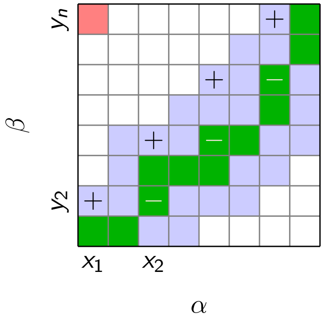

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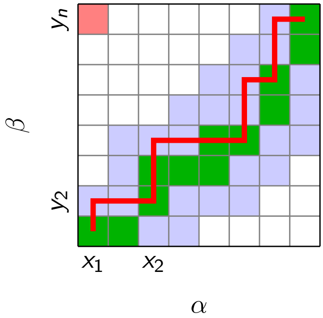

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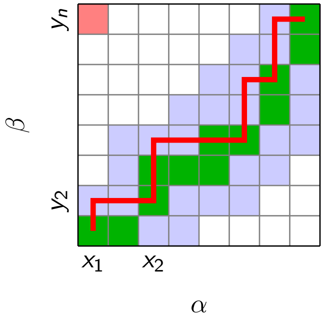

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- shielding neighbourhood: always find a shielding cell

✓ existence of short-cuts follows

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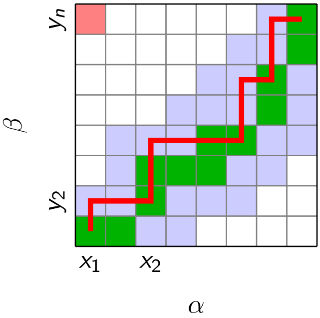

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✓ Local optimality + shielding neighbourhood ⇒ global optimality

A Sparse Algorithm

Ingredients

- sparse optimal transport solver $F : \mathcal{N} \mapsto \pi$
- construction of shielding neighbourhood $G : \pi \mapsto \mathcal{N}$

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$$\pi_{k+1} = F(\mathcal{N}_k)$$
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until π_k is already locally optimal on $\mathcal{N}_k$.

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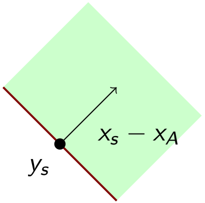
Properties of Algorithm

- Calling F is fast when $\mathcal{N}_k$ is sparse. Any solver can be used as black box.
- When π_1 / $\mathcal{N}_1$ are good initial guesses: need only few iterations $\Rightarrow$ multi-scale scheme
- Design of G must exploit geometric structure of cost-function

G for Squared Euclidean Distance



Shielding Condition for $c(x, y) = \|x - y\|^2$

$$\langle y_B - y_s, x_s - x_A \rangle > 0$$

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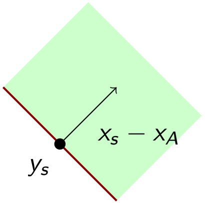

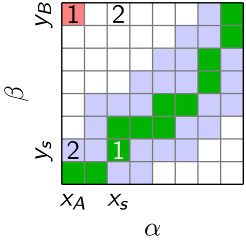

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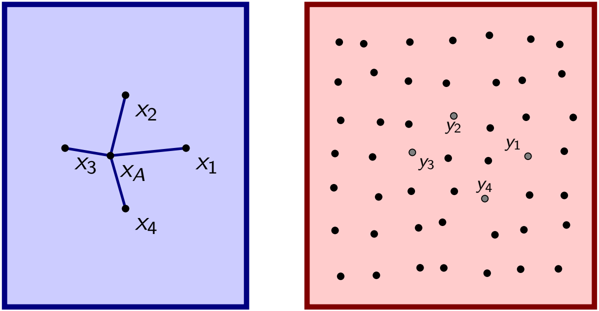

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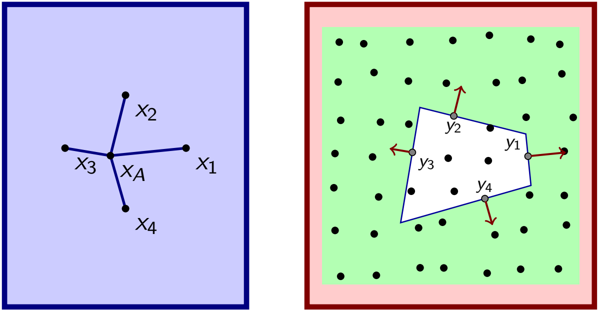

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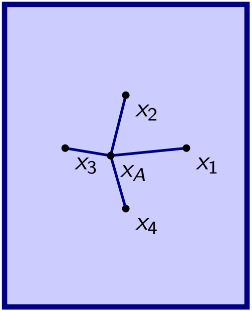

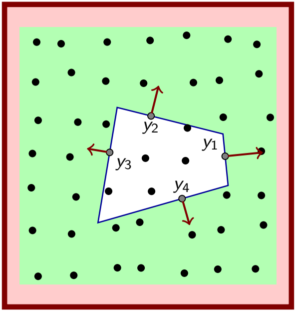

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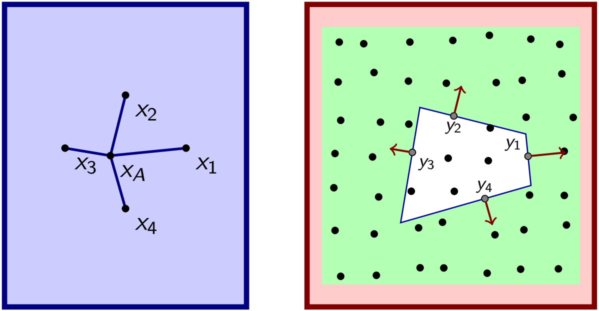
✓ regular grids, ✓ point-clouds with tree structure

G for Squared Euclidean Distance



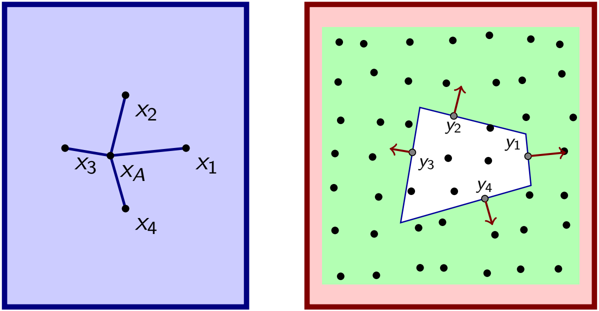
Shielding Condition for $c(x, y) = \|x - y\|^2$

$$\langle y_B - y_s, x_s - x_A \rangle > 0$$

✓ regular grids, ✓ point-clouds with tree structure

- mass assignment regular* $\Rightarrow |\mathcal{N}| = \mathcal{O}(|X|) \ll \mathcal{O}(|X \times Y|)$

G for Squared Euclidean Distance



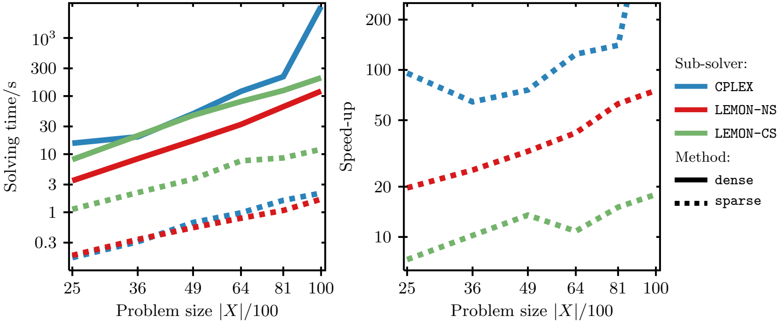
Shielding Condition for $c(x, y) = \|x - y\|^2 + \varepsilon(x, y)$

$$\langle y_B - y_s, x_s - x_A \rangle > 0$$

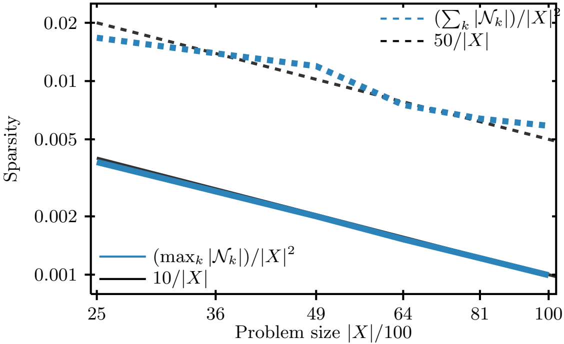
✓ regular grids, ✓ point-clouds with tree structure

- mass assignment regular* $\Rightarrow |\mathcal{N}| = \mathcal{O}(|X|) \ll \mathcal{O}(|X \times Y|)$
- can deal with noise
- more general costs …

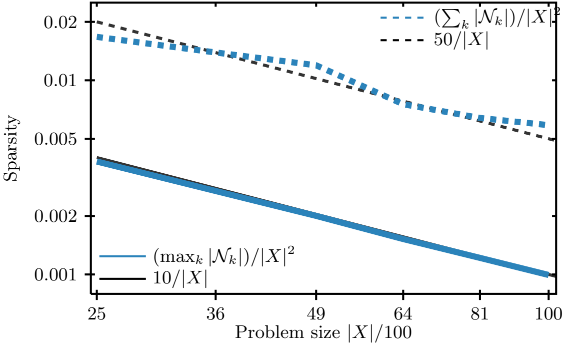
Numerical Results: Speed-up



Numerical Results: Sparsity

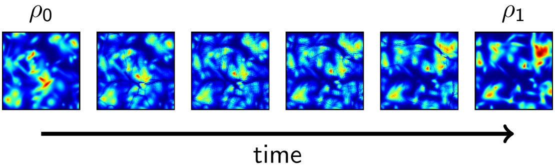


Numerical Results: Sparsity

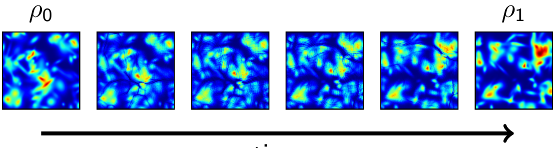


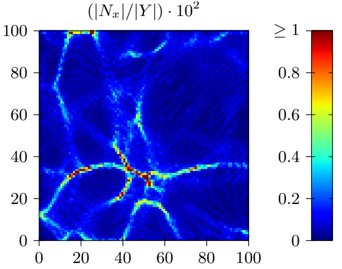
- 95% quantile of iteration numbers: 8

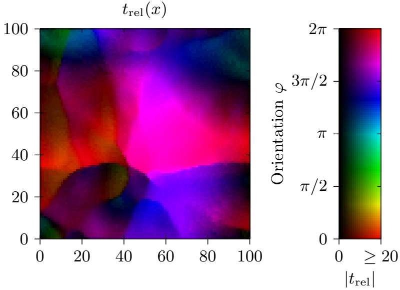
Numerical Results: Sparsity II



Numerical Results: Sparsity II

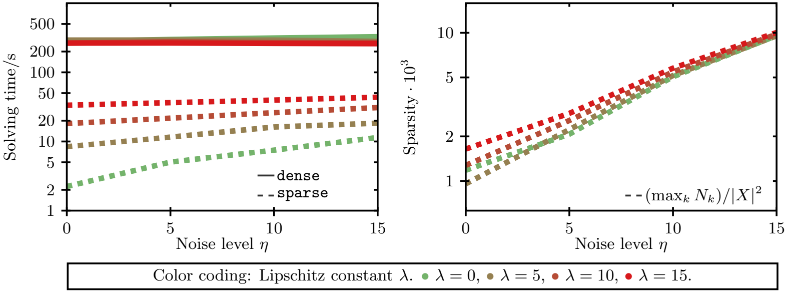






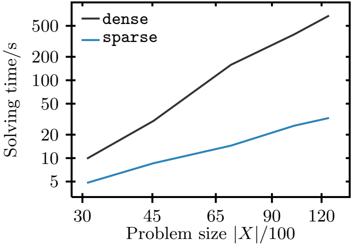
- $N_x = \{y \in Y : (x, y) \in \mathcal{N}\}$
- t_{rel}: Barycentric projection of relative transport map

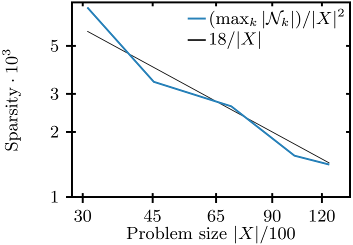
Numerical Results: Noisy Costs



- noise: random (η) + Lipschitz component (λ)
- slower with increasing noise (expected), ✓ no immediate breakdown

Shielding Neighbourhoods for More General Costs

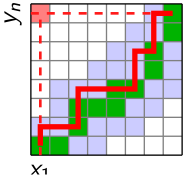




Preliminary Results

- ✗ more complicated,
  ✓ point-clouds with tree structure (⇒ multi-scale scheme)
- intuition: ✓ strictly convex costs, ✓ squared geodesic distance on sphere
- numerics: • speed, ✓ sparsity

Summary & Outlook



Summary

- ✓ verify global optimality locally ⇔ analogy to continuum
- ✓ basis for efficient sparsification of dense problems ⇒ combinatorial algorithms become applicable
- ✓ speed-up and saves memory

Open Questions

- closer look at other cost functions
- computational complexity
- code!

ArXiv: B. Schmitzer 'A Sparse Multi-Scale Algorithm for Dense Optimal Transport' 10/2015

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