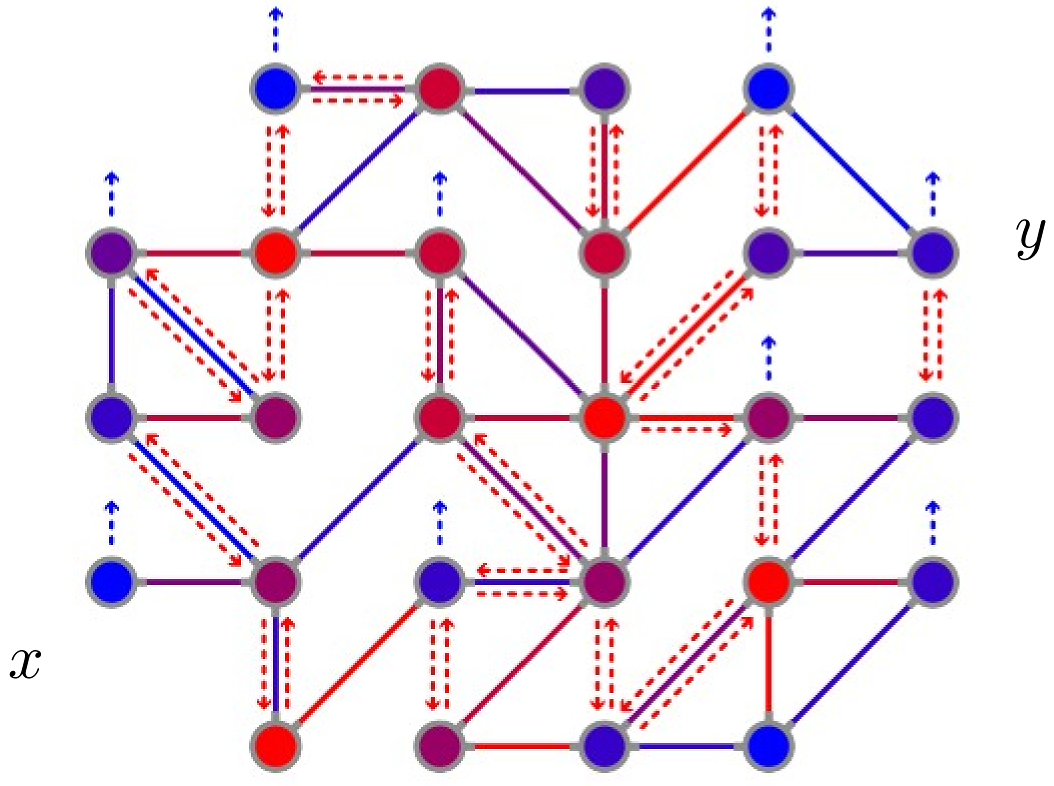
Graph, Geometry, Optimal Control and Optimal Transport

A Layman's Perspective

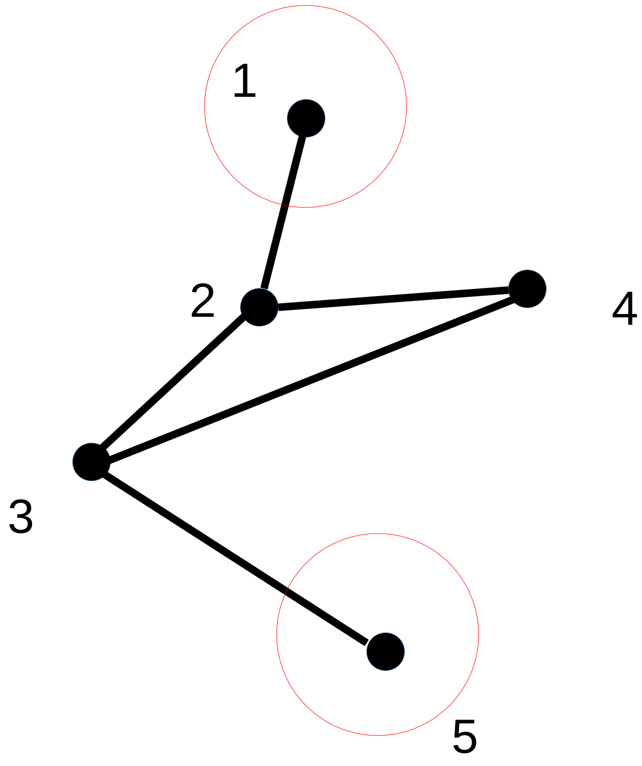
Dongjun Wu

Graph distance



David et. al. 2023

Graph distance



$$A=\begin{bmatrix}-1 & 1 & 0 & 0 & 0\\ 1 & -3 & 1 & 1 & 0\\ 0 & 1 & -3 & 1 & 1\\ 0 & 1 & 1 & -2 & 0\\ 0 & 0 & 1 & 0 & -1\end{bmatrix}, \quad \delta = \begin{bmatrix}1\\0\\0\\0\\0\end{bmatrix}$$

$$A\delta = \begin{bmatrix}-1\\1\\0\\0\\0\end{bmatrix}, A^2\delta = \begin{bmatrix}2\\-4\\1\\1\\0\end{bmatrix}, A^3\delta = \begin{bmatrix}*\\*\\*\\*\\1\end{bmatrix}$$

$A\delta,\ A^2\delta,\ \cdots$ until $(A^n\delta)_5 \neq 0$

Graph distance

$A\delta,\ A^2\delta,\ \cdots$ until $(A^n\delta)_5 \neq 0$

$$(I - tA)u_t = \delta$$

$$u_t = (I - tA)^{-1}\delta = \sum_{k=0}^{\infty} t^k A^k \delta$$

$$(u_t)_5 = t^n (A^n\delta)_5 + o(t^n)$$

$$\log(u_t)_5 = n \log t + \log(A^n\delta)_5$$
$$\approx n \log t$$

$$n = \lim_{t \to 0+} \frac{\log(u_t)_5}{\log t}$$

Put $u_0 = \delta$

$$u_t = u_0 + tAu_t$$

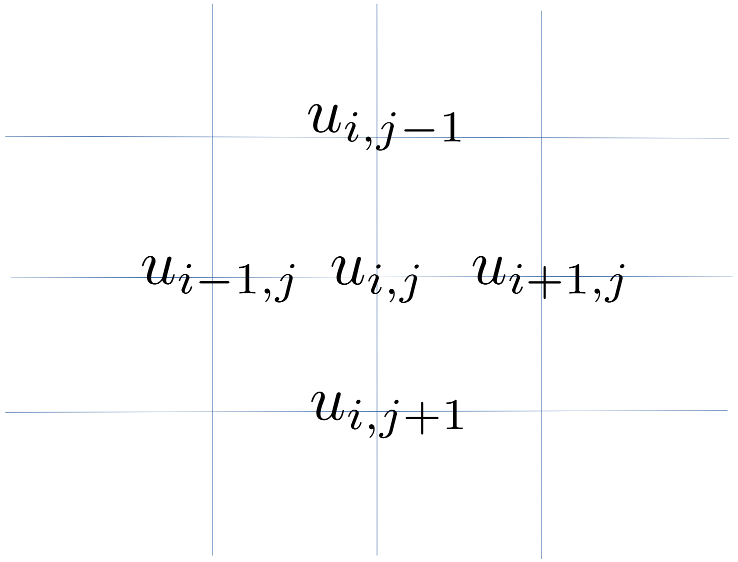
$$\frac{\partial u_t}{\partial t} = Au_t$$

P-S. Laplace 1749 – 1827

Why is Laplacian Laplacian?

Laplacian and Laplacian

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \sim Au$$



$$A = \begin{bmatrix} -2 & 1 & 0 & \cdots & 1 & 0 & \cdots & & \\ 1 & -4 & 1 & 0 & \cdots & 1 & 0 & 0 & \cdots \\ 0 & 1 & -4 & 1 & 0 & \cdots & 1 & 0 & 0 \\ \vdots & \vdots & & \ddots & & & & & \end{bmatrix}$$

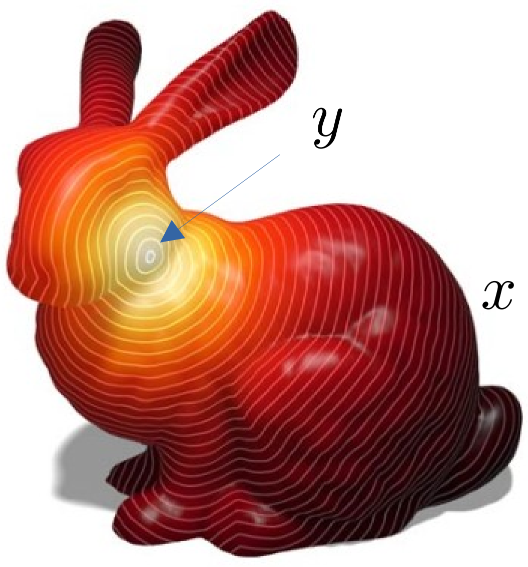
(-) *Laplacian matrix*!

$$\Delta:\ 0 = \lambda_0 > \lambda_1 > \cdots$$

(-) Graph Laplacian: $0 = \lambda_0 > \lambda_1 > \cdots > \lambda_n$

Bunny in Heat

$$\frac{\partial u_t}{\partial t} = A u_t, \; u_0 = \delta \quad \rightsquigarrow \quad \frac{\partial u}{\partial t} = \Delta u, \quad u(0) = \delta_y$$



$$u(t,x,y) = \frac{1}{\sqrt{(4\pi t)^2}} \exp\left\{ -\frac{\|x-y\|^2}{4t} \right\}$$

$$\|x-y\| = \lim_{t \to 0+} \sqrt{-4t \log u(t,x,y)}$$

Holds on *Riemannian manifolds*! $\quad \Delta \leftarrow \Delta_g$

Varadhan’s formula

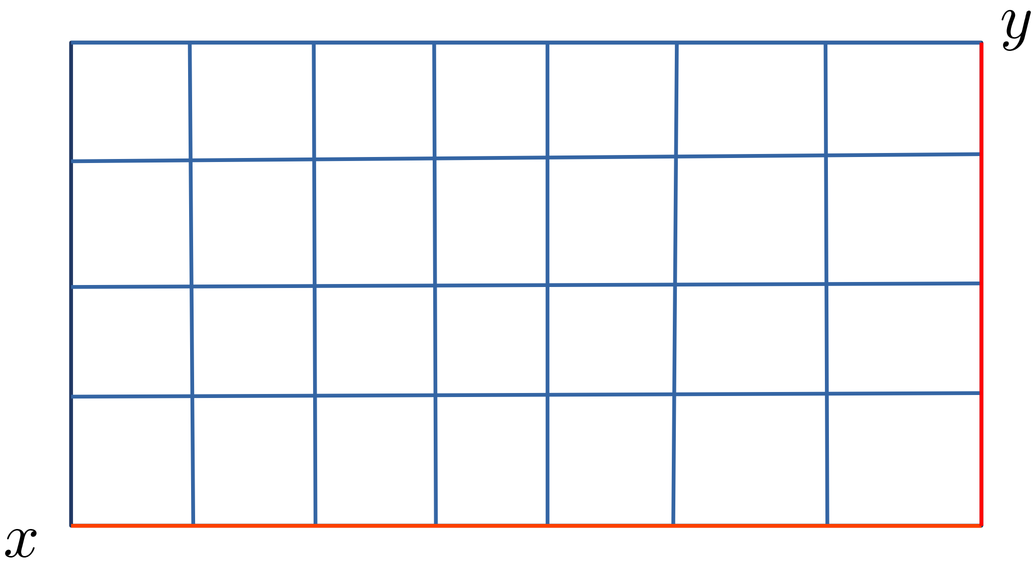
Discrete ⚔ Continuous

$$\frac{\partial u_t}{\partial t} = A u_t,\ u_0 = \delta_y,$$

$$d(x,y) = \lim_{t \to 0+} \frac{\log (u_t)_x}{\log t}$$

$$\frac{\partial u}{\partial t} = \Delta u, \quad u(0) = \delta_y,$$

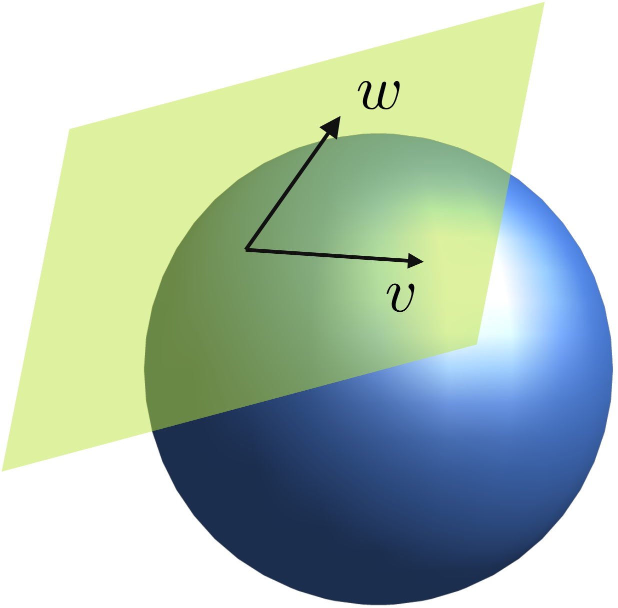
$$d(x,y) = \lim_{t \to 0+} \sqrt{-4t \log u(t,x,y)}$$



$$d_G(x,y) = \sqrt{2} d_{\mathbb{R}^2}(x,y)$$

Discretize-then-Optimize
or
Optimize-then-Discretize

Geometry on graph



Difficulty: graph distance is *not* geodesic …

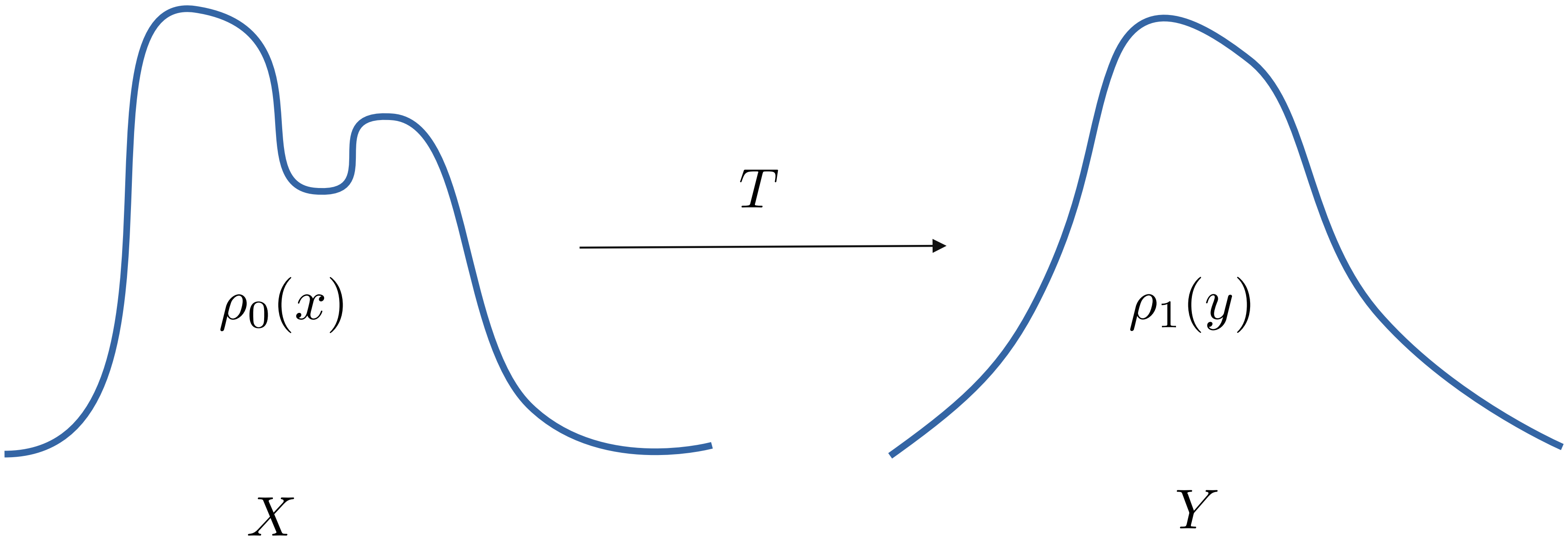
$$d(x(t), x(s)) \leq c|t-s|$$

No smooth structure ☹

Analogies, embeddings … can be made

Optimal Transport

Gaspard Monge 1746 - 1818



$$\min_T \int_X c(x, T(x)) d\rho_0(x)$$

Define distance between prob. dist.

$c(x,y)$ is the unit cost from x to y

$$c(x,y) = \|x - y\|^p \Rightarrow W_p(\rho_0, \rho_1)$$

OT as Optimal Control

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

$$\min_T \int_X \|x - T(x)\|^2 d\rho_0(x)$$ s.t. $$T_\# \rho_0 = \rho_1$$

$$\min_u \int_0^1 \int_X \rho(t,x) |u|^2 dx dt$$

s.t. $\partial_t \rho + \nabla \cdot \rho u = 0, \ \rho(0,\cdot) = \rho_0, \ \rho(1,\cdot) = \rho_1$

Benamou and Brenier 2000

OT as Stochastic Control

$$\min_u \mathbb{E}\left[\int_0^1 \|u(t,x)\|^2 dt\right]$$

$$dX_t = u(t, X_t)dt + \sqrt{\epsilon} dB_t,\ \ X_0 \sim \rho_0,\ \ X_1 \sim \rho_1$$

$\Updownarrow$

$$\min \int_0^1 \rho(t,x)\|u(t,x)\|^2 dxdt$$

$$\partial_t \rho + \nabla \cdot \rho u - \epsilon \Delta \rho = 0,\ \ \rho(0,\cdot) = \rho_0,\ \ \rho(1,\cdot) = \rho_1$$

Optimal transport

$$\min_u \int_0^1 \int_X \rho(t,x)|u|^2 dxdt$$

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$

$$\rho(0,\cdot) = \rho_0,\ \ \rho(1,\cdot) = \rho_1$$

T. Mikami et. al. 2008,
Y. Chen et. al. 2017,
(TAC best paper award)

$\epsilon \to 0$

“vanishing viscosity”

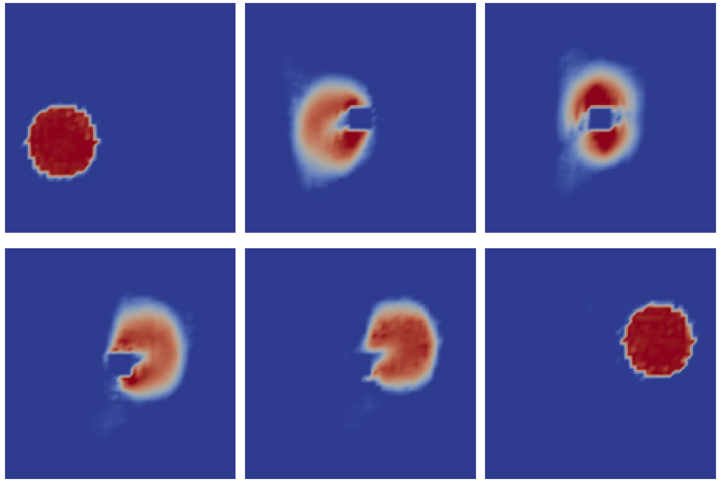
A digression about my work ...

$$\min_u \int_0^1 \int_X \rho(t,x)|u|^2 dx dt$$

s.t. $\partial_t \rho + \nabla \cdot \rho v = 0,\ \rho(0,\cdot) = \rho_0,\ \rho(1,\cdot) = \rho_1$

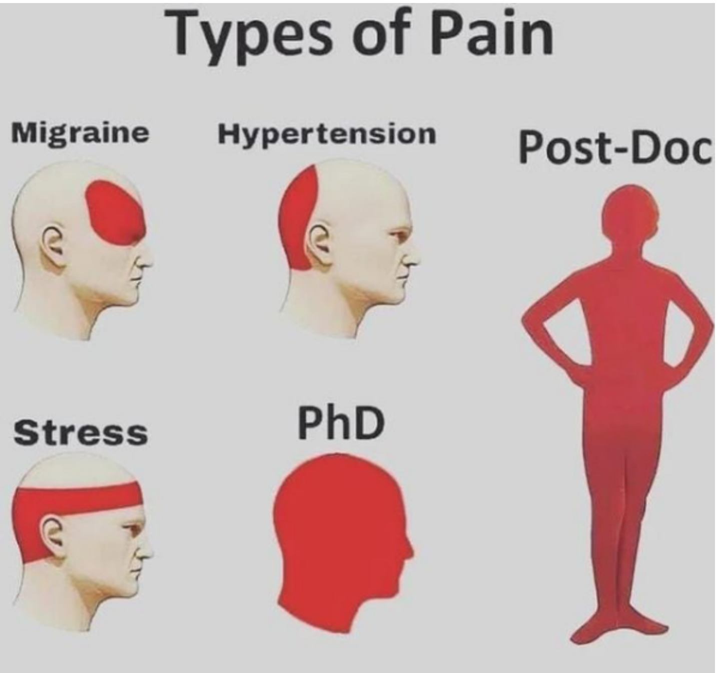
$$v = f(x) + g(x)u,\ u \in U,\ I(\rho) \leq 0$$

Input and density constraints



D. Wu and A. Rantzer 2024

A digression about my work ...



Curvature, input & density constraints
State space: mesh space

Lavenant et. al. 2018

A digression about my work ...

OT on Lie group

$$dR = R(\Omega + \Omega_0)dt + udt + \sum_i R\Omega_i dB_t^i$$

$$dX = (AX + Bu)dt + \sum_i D_i X dB_t^i, \; X_0 \sim \rho_0, \; X_1 \sim \rho_1$$

Controlling covariance

Back to geometry on graph

No Riemannian geometry exists on graph

But certain curvature can still be defined

Ricci curvature of metric spaces

Yann Ollivier

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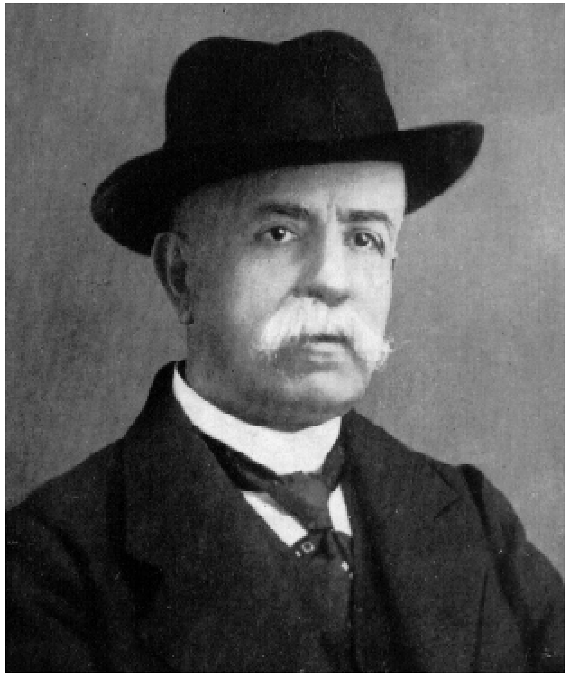
Received 21 September 2007; accepted after revision 6 October 2007

Presented by Étienne Ghys

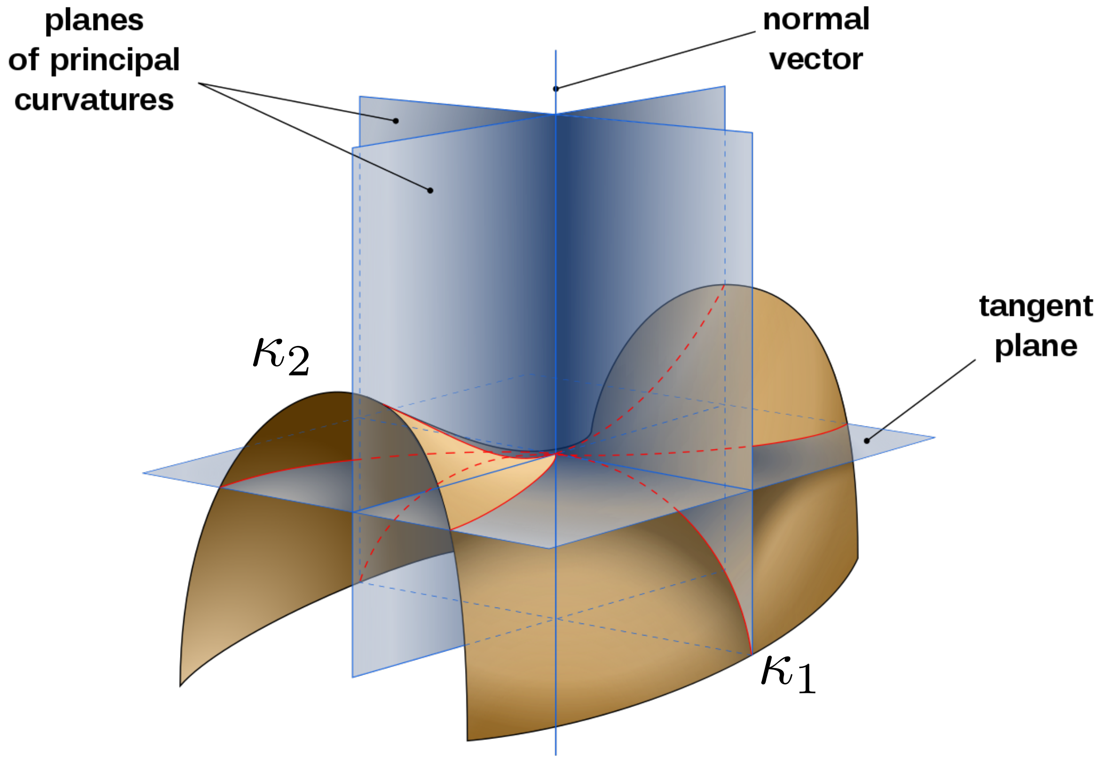
Abstract

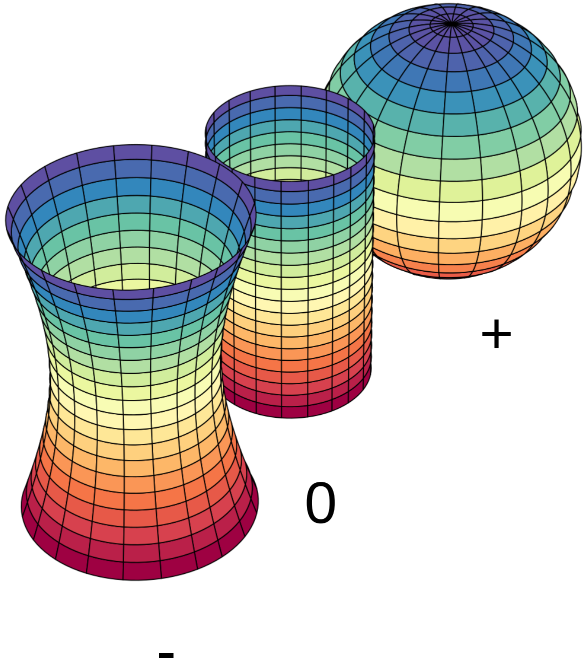
We define a notion of Ricci curvature in metric spaces equipped with a measure or a random walk. For this we use a local contraction coefficient of the random walk acting on the space of probability measures equipped with a transportation distance. This notions allows to generalize several classical theorems associated with positive Ricci curvature, such as a spectral gap bound (Lichnerowicz theorem), Gaussian concentration of measure (Lévy–Gromov theorem), logarithmic Sobolev inequalities (a result of Bakry–Émery theory) or the Bonnet–Myers theorem. The definition is compatible with Bakry–Émery theory, and is robust and very easy to implement in concrete examples such as graphs. ***To cite this article: Y. Ollivier, C. R. Acad. Sci. Paris, Ser. I 345 (2007).***

Ricci curvature



Gregorio Ricci-Curbastro 1853-1925
(discoverer of Tensor Calculus)



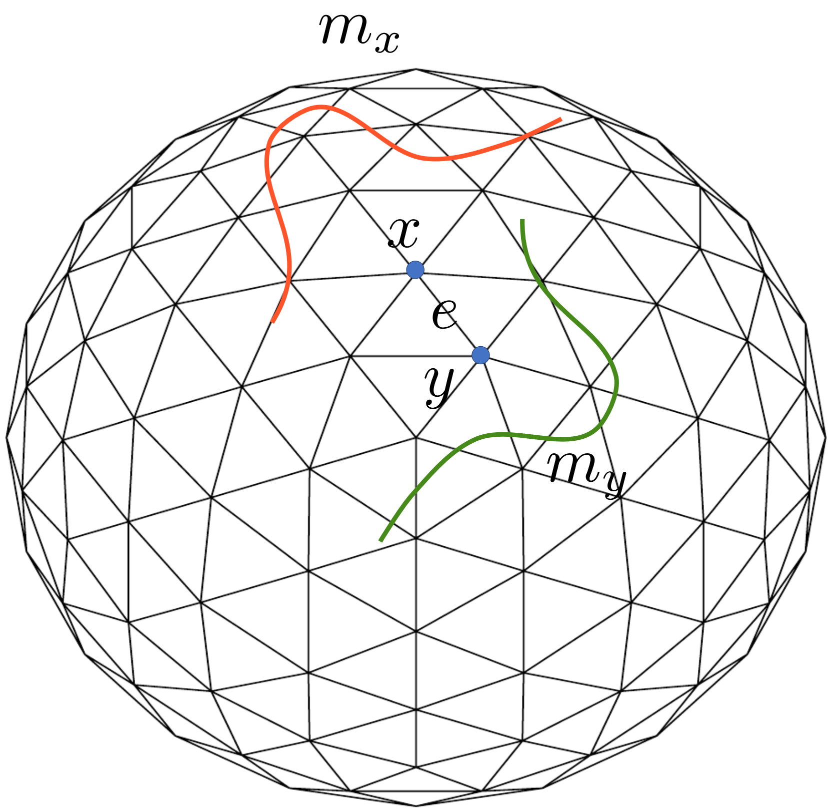


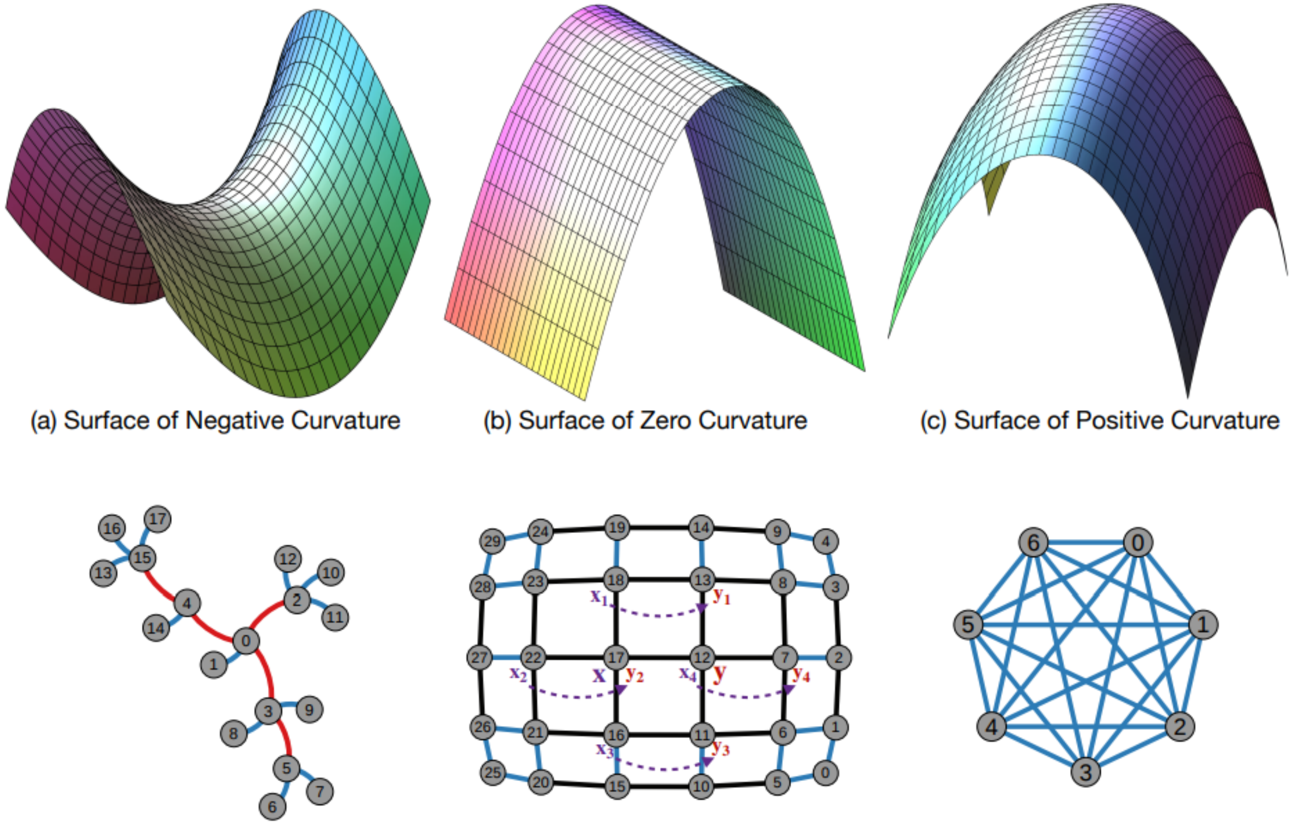
$$K_{\text{Gauss}} = \kappa_1 \kappa_2$$

$$\text{Ric}(v) = \text{tr}(x \mapsto R(x,v)v))$$

Ricci curvature on graph

$$\mathrm{Ric}(\overrightarrow{xy}) \approx 1 - \frac{W_1(m_x, m_y)}{d(x,y)}$$





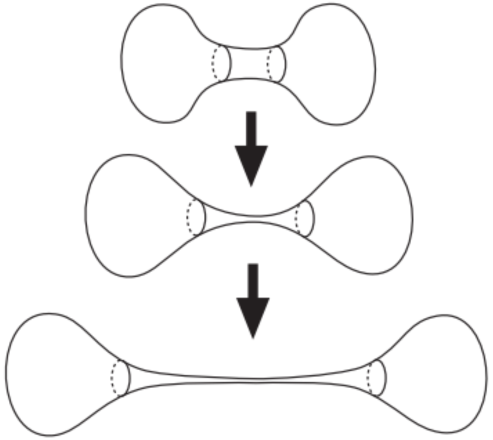
(a) Surface of Negative Curvature
(b) Surface of Zero Curvature
(c) Surface of Positive Curvature
(d) Negative Curvature
(e) Zero Curvature
(f) Positive Curvature

Ni et. al. 2019 *Scientific reports*

Ricci flow

Richard S. Hamilton

$$\frac{\partial g_t}{\partial t} = -2\mathrm{Ric}^{g_t}$$



Grigori S. Perelman

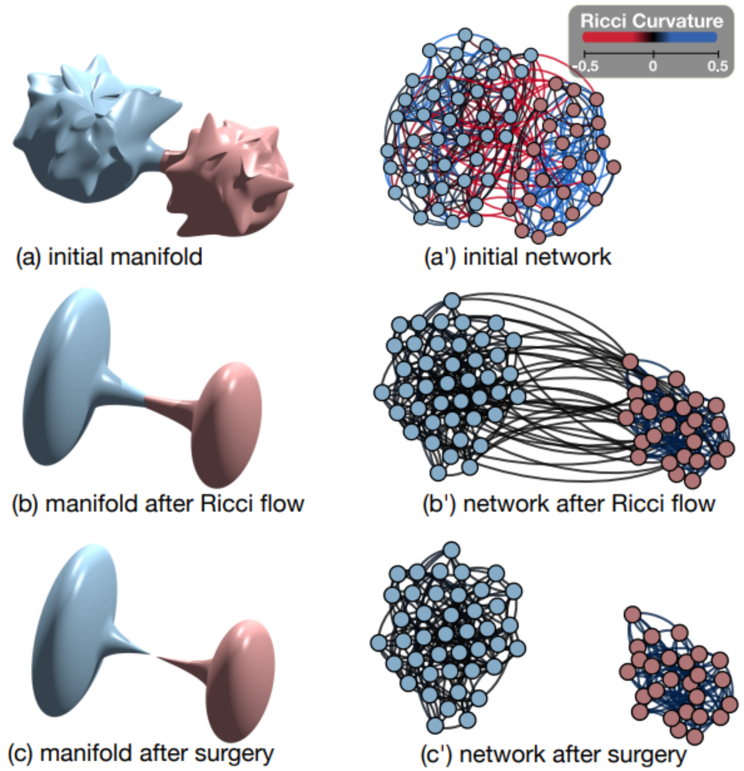
Surgery

Ricci flow with surgery on three-manifolds

Grisha Perelman*

February 1, 2008

This is a technical paper, which is a continuation of [I]. Here we verify most of the assertions, made in [I, §13]; the exceptions are (1) the statement that a 3-manifold which collapses with local lower bound for sectional curvature is a graph manifold - this is deferred to a separate paper, as the proof has nothing to do with the Ricci flow, and (2) the claim about the lower bound for the volumes of the maximal horns and the smoothness of the solution from some time on, which turned out to be unjustified, and, on the other hand, irrelevant for the other conclusions.



Ni et. al. 2019 *Scientific reports*

One more word on Geometry & Control

Roger W. Brockett 1938 - 2023

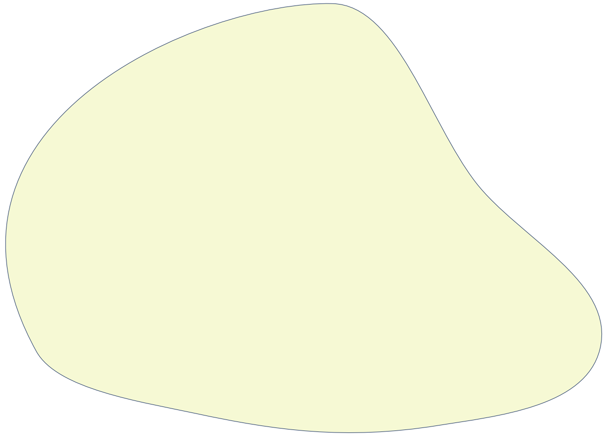
sub-Riemannian geometry $\Longleftrightarrow$ OC of non-holonomic sys.

$$\dot{x} = u_1$$
$$\dot{y} = u_2$$
$$\dot{z} = u_1 y - u_2 x$$

$$\min_u \int \sqrt{u_1^2 + u_2^2} dt,$$

$$(x_0, y_0) \text{ fixed}$$

$$\dot{x} = u_i f_i(x)$$



- Dido’s problem
- Isoperimetric problem
- Heisenberg geometry

An OT solver to Dido

C $\qquad\qquad$ B

$$\mu = \frac{1}{\pi r^2}\Big|_C$$

$$\mathrm{vol} C = \mathrm{vol} B = 1$$

$$\exists T_{\#}\mu = \nu,\ T = \nabla\phi$$

$$\nu = \frac{1}{\pi r^2}\Big|_B$$

$$\det \nabla T(x) = \frac{\mu(x)}{\nu(T(x))} = 1 \leq \frac{1}{2}\mathrm{div} T(x)$$

$$1 = \mathrm{vol}(C) \leq \int_C \frac{1}{2}\mathrm{div} T = \frac{1}{2}\int_{\partial C} T \cdot d\ell \leq \frac{1}{2}\ell(C)$$

$$\longrightarrow \quad \ell(C) \geq \ell(B)$$

- Dido’s problem
- Isoperimetric problem
- Heisenberg geometry

Conclusion

- Various connections between graph, geometry, OT, OC
- Try dynamics even if the problem is static, e.g., heat flow, dynamic OT, Ricci flow
- Continuous model sometimes provides more insight
- Discretization may lead to unpredictable behaviors
- A lot to explore regarding graph geometry!

www.control.lth.se

LUND UNIVERSITY

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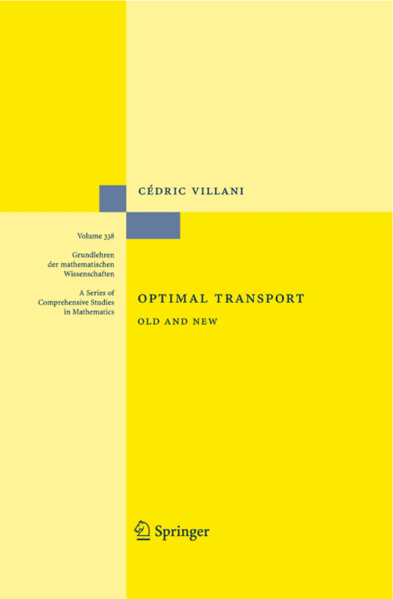
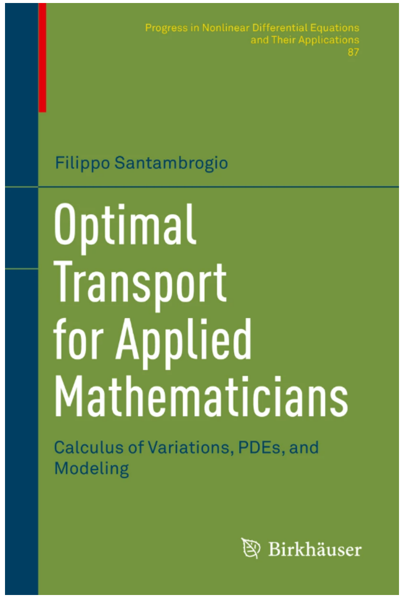
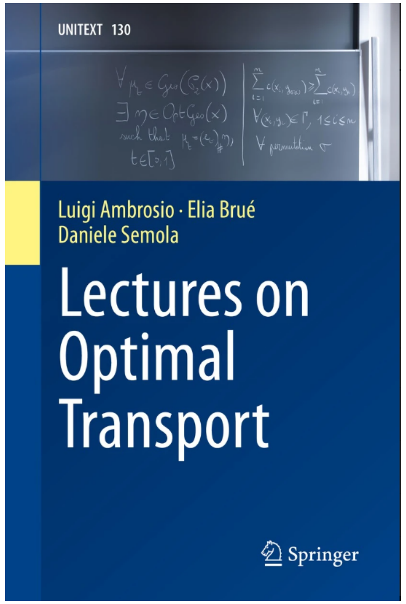
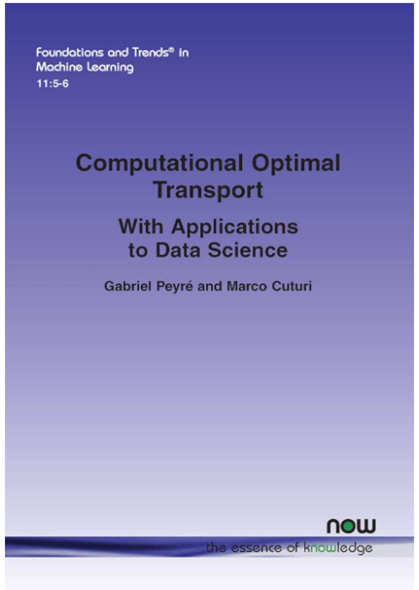
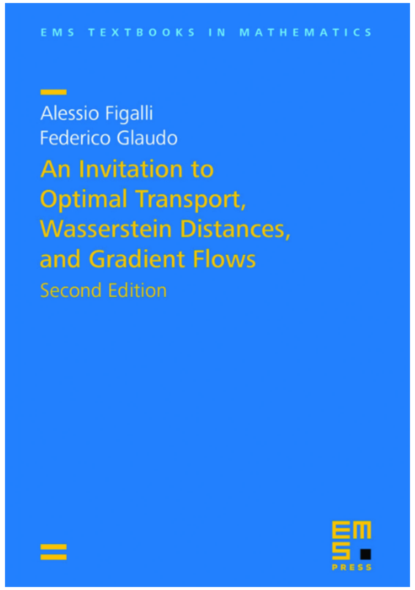
Resources

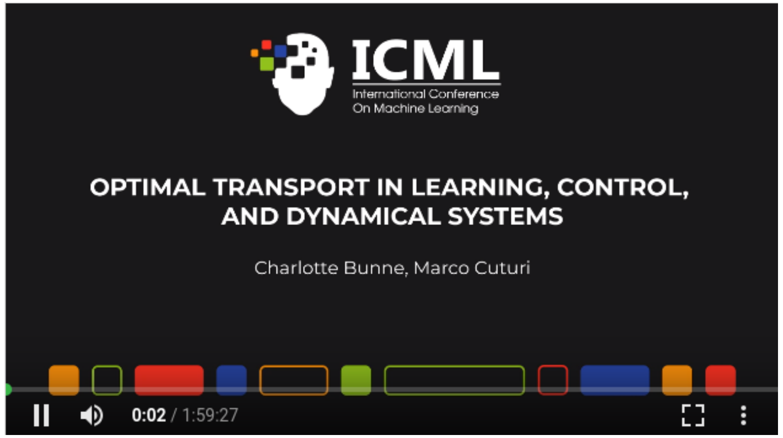












(google Charlotte Bunne)

“The aim of science is to make difficult things understandable in a simpler way; the aim of poetry is to state simple things in an incomprehensible way. The two are incompatible.”

— Paul A.M. Dirac