# Optimal Mass Transport

# and (matrix) density flows

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Optimal Transport meets
Probability, Statistics and Machine Learning
BIRS, Oaxaca

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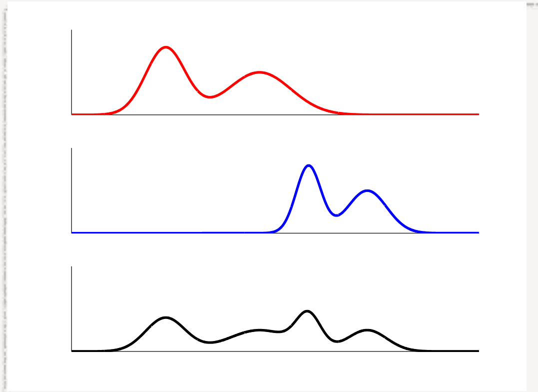
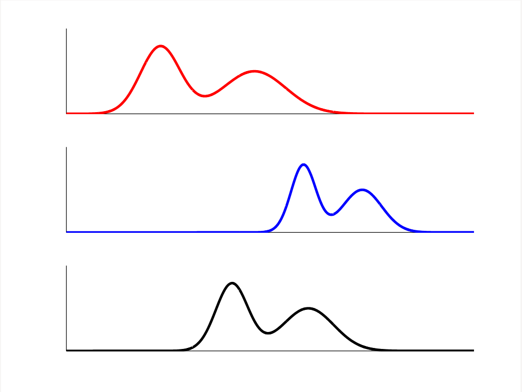
# Motivation
# interpolation of densities



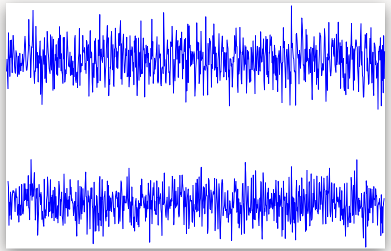
Arithmetic mean



Transportation mean

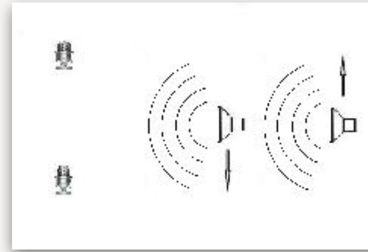
- push/pop?
- artifacts?
- etc

Time-series

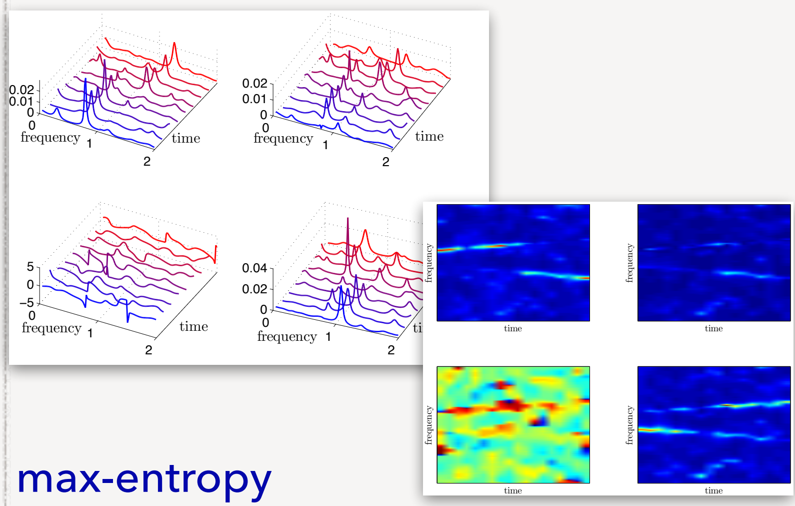


positioning
via
relative intensity
& doppler shift

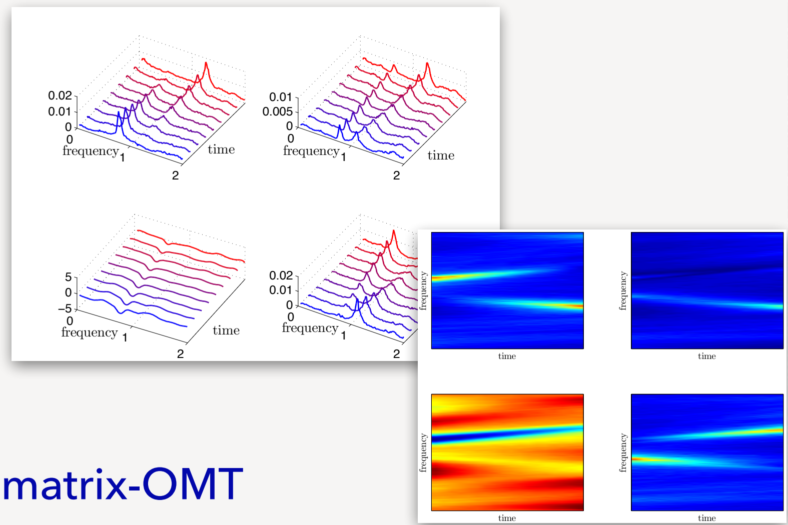
Physical arrangement



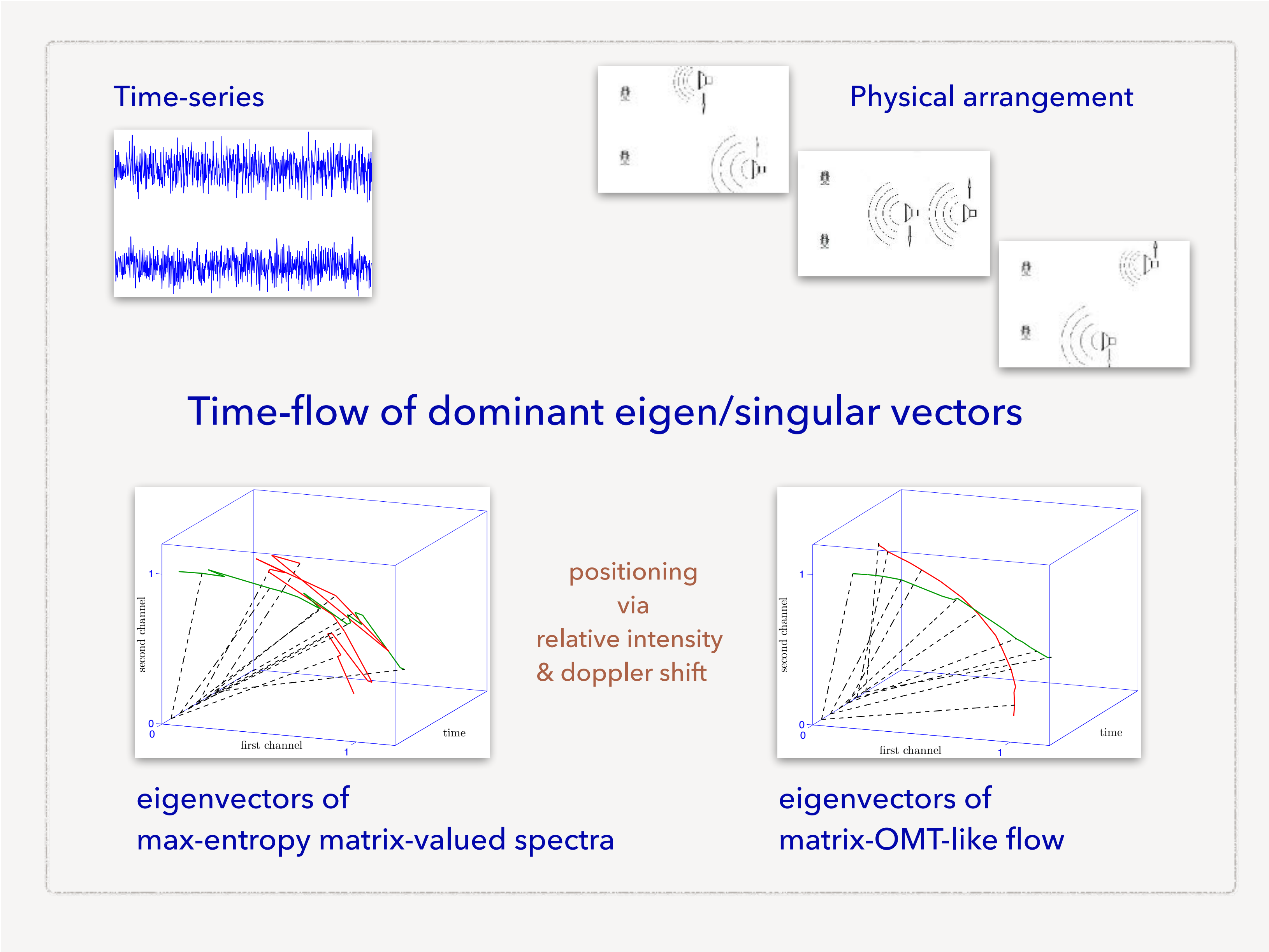
# Matrix-valued power spectra




max-entropy
matrix-valued spectra




matrix-OMT
power spectral flow




Kantorovich-like formulation in product-space:

Ning, Georgiou, Tannenbaum, On matrix-valued Monge-Kantorovich OMT, 2015

# OMT in quantum theory

Eric Carlen & Jan Maas
"An Analog of the 2-Wasserstein Metric..Fermionic Fokker-Planck..
Gradient Flow for the Entropy," Comm. Math. Phys. 2014

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arXiv:
Eric Carlen & Jan Maas

"Gradient flow and entropic inequalities...," Sept 2016

Markus Mittnenzweig & Alexander Mielke

"An entropic gradient structure for Lindblad...," Sept 2016.

Yongxin Chen, TTG & Allen Tannenbaum

"Matrix OMT: a Quantum Mechanical approach," Oct 2016

# Our goal

- extend the **Benamou-Brenier** framework to transport of
  - Hermitian matrices (Quantum density matrices)
  - matrix-valued distributions

I.e., formulate for matrices...

$$\inf \int \int_0^1 \rho(t,x) \|v(t,x)\|^2 \, dt \, dx$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) \; = \; 0,$$

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

# Quantum continuity equation

Starting point: Lindblad equation (in "diagonal form" $L_k = L_k^*$)

$$\begin{aligned}\dot{\rho} &= -[iH, \rho] \\ &\quad + \sum_{k=1}^{N} (L_k \rho L_k - \frac{1}{2}\rho L_k L_k - \frac{1}{2} L_k L_k \rho),\end{aligned}$$

Notation:

$\mathcal{H}$ and $\mathcal{S}$ the set of $n \times n$ Hermitian and skew-Hermitian matrices

$\mathcal{H}_+$ and $\mathcal{H}_{++}$ nonnegative and positive-definite matrices

$\mathcal{D}_+ := \{\rho \in \mathcal{H}_{++} \mid \mathrm{tr}(\rho) = 1\}$ "density matrices"

$\mathcal{S}^N$, $\mathcal{H}^N$ block-column vectors with matrix-entries

# Notation

$\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \mathbf{tr}(\boldsymbol{X}^* \boldsymbol{Y})$, $\boldsymbol{X}, \boldsymbol{Y} \in \boldsymbol{\mathcal{H}}$ (or $\boldsymbol{\mathcal{S}}$)

$\langle \boldsymbol{X}, \boldsymbol{Y} \rangle = \sum_{k=1}^{N} \mathbf{tr}(\boldsymbol{X}_k^* \boldsymbol{Y}_k)$ for $\boldsymbol{X}, \boldsymbol{Y} \in \boldsymbol{\mathcal{H}}^N$ ($\boldsymbol{\mathcal{S}}^N$)

For $\boldsymbol{X} \in \boldsymbol{\mathcal{H}}^N$ (or $\boldsymbol{\mathcal{S}}^N$), $\boldsymbol{Y} \in \boldsymbol{\mathcal{H}}$ (or $\boldsymbol{\mathcal{S}}$),

$$\boldsymbol{X}\boldsymbol{Y} = \begin{bmatrix} \boldsymbol{X}_1 \\ \vdots \\ \boldsymbol{X}_N \end{bmatrix} \boldsymbol{Y} := \begin{bmatrix} \boldsymbol{X}_1 \boldsymbol{Y} \\ \vdots \\ \boldsymbol{X}_N \boldsymbol{Y} \end{bmatrix},$$

and

$$\boldsymbol{Y}\boldsymbol{X} = \boldsymbol{Y} \begin{bmatrix} \boldsymbol{X}_1 \\ \vdots \\ \boldsymbol{X}_N \end{bmatrix} := \begin{bmatrix} \boldsymbol{Y} \boldsymbol{X}_1 \\ \vdots \\ \boldsymbol{Y} \boldsymbol{X}_N \end{bmatrix}.$$

# Some calculus

Note for functions:

$f(x) \; : \; g(x) \mapsto f(x)g(x)$

$\partial_x \; : \; g(x) \mapsto \partial_x g(x)$

$[\partial_x, f(x)] \; : \; g(x) \mapsto \partial_x f(x)g(x) - f(x)\partial_x g(x) = (\partial_x f(x))g(x)$

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For matrices:

$\partial_{L_i} X = [L_i, X] = [L_i X - X L_i]$

define the *gradient operator* for $L \in \mathcal{H}^N$

$$\nabla_L : \mathcal{H} \to \mathcal{S}^N, \quad X \mapsto \begin{bmatrix} L_1 X - X L_1 \\ \vdots \\ L_N X - X L_N \end{bmatrix}$$

# Some calculus

$\boldsymbol{\nabla}_{\boldsymbol{L}}$ is a derivation

$$\boldsymbol{\nabla}_{\boldsymbol{L}}(\boldsymbol{X}\boldsymbol{Y}+\boldsymbol{Y}\boldsymbol{X}) = (\boldsymbol{\nabla}_{\boldsymbol{L}}\boldsymbol{X})\boldsymbol{Y}+\boldsymbol{X}(\boldsymbol{\nabla}_{\boldsymbol{L}}\boldsymbol{Y}) \\ +(\boldsymbol{\nabla}_{\boldsymbol{L}}\boldsymbol{Y})\boldsymbol{X}+\boldsymbol{Y}(\boldsymbol{\nabla}_{\boldsymbol{L}}\boldsymbol{X}), \quad \forall \boldsymbol{X},\boldsymbol{Y}\in\boldsymbol{\mathcal{H}}.$$

dual is an analogue of the (negative) *divergence operator*:

$$\boldsymbol{\nabla}_{\boldsymbol{L}}^{*} : \boldsymbol{\mathcal{S}}^{\boldsymbol{N}} \to \boldsymbol{\mathcal{H}},\ \boldsymbol{Y} = \begin{bmatrix} \boldsymbol{Y}_1 \\ \vdots \\ \boldsymbol{Y}_{\boldsymbol{N}} \end{bmatrix} \mapsto \sum_{\boldsymbol{k}}^{\boldsymbol{N}} \boldsymbol{L}_{\boldsymbol{k}}\boldsymbol{Y}_{\boldsymbol{k}} - \boldsymbol{Y}_{\boldsymbol{k}}\boldsymbol{L}_{\boldsymbol{k}}.$$

$$\langle \boldsymbol{\nabla}_{\boldsymbol{L}}\boldsymbol{X}, \boldsymbol{Y}\rangle = \langle \boldsymbol{X}, \boldsymbol{\nabla}_{\boldsymbol{L}}^{*}\boldsymbol{Y}\rangle$$

# Lindblad term

*Laplacian*:

$$\Delta_L X := -\nabla_L^* \nabla_L X = \sum_{k=1}^{N} (2L_k X L_k - X L_k L_k - L_k L_k X),\ X \in \mathcal{H},$$

Lindblad's equation:

$$\dot{\rho} + [iH, \rho] = \sum_{k=1}^{N} (L_k \rho L_k - \frac{1}{2}\rho L_k L_k - \frac{1}{2} L_k L_k \rho),$$

becomes

$$\dot{\rho} + \nabla_{iH}\,\rho = \frac{1}{2}\Delta_L \rho.$$

# Continuity equation

$$\dot{\rho} = \nabla_L^* M_\rho(v),$$

with $M_\rho(v)$ a *"multiplication"* between $\rho$ and $v$

momentum field "$\rho v$" $= M_\rho(v) \in \mathcal{S}^N$.

choices of non-commutative multiplication:

i) $\frac{1}{2}(\rho v + v\rho)$ ("anti-commutator")

ii) $\int_0^1 \rho^s v \rho^{1-s} ds$ (Kubo-Mori)

iii) $\rho^{1/2} v \rho^{1/2}$

# Case i) “anti-commutator”

Problem i):

$$
\begin{aligned}
W_{2,a}(\rho_0,\rho_1)^2 &:= \min_{\rho\in\mathcal{D}_+, v\in\mathcal{S}^N} \int_0^1 \mathrm{tr}(\rho v^* v)\,dt, \\
\dot{\rho} &= \frac{1}{2}\nabla_L^*(\rho v + v\rho), \\
\rho(0) &= \rho_0, \quad \rho(1) = \rho_1,
\end{aligned}
$$

Note: $v^* v = \sum_{k=1}^N v_k^* v_k$ and $v \in \mathcal{S}^N$.

# Duality

$\boldsymbol{\lambda}(\cdot) \in \boldsymbol{\mathcal{H}}$ Lagrangian multiplier

$$\boldsymbol{\mathcal{L}(\rho, v, \lambda) = \int_0^1 \left\{ \frac{1}{2} \mathrm{tr}(\rho v^* v) - \mathrm{tr}(\lambda(\dot{\rho} - \frac{1}{2} \nabla_L^* (\rho v + v \rho))) \right\} dt}$$

Point-wise minimization $\Rightarrow$

$$\boldsymbol{v_{opt}(t) = -\nabla_L \lambda(t).}$$

# Duality

If $\boldsymbol{\lambda}(\cdot) \in \mathcal{H}$:

$$\dot{\boldsymbol{\lambda}} = \frac{1}{2}(\nabla_L \boldsymbol{\lambda})^*(\nabla_L \boldsymbol{\lambda}) = \frac{1}{2}\sum_{k=1}^{N}(\nabla_L \boldsymbol{\lambda})_k^*(\nabla_L \boldsymbol{\lambda})_k$$

and

$$\dot{\boldsymbol{\rho}} = -\frac{1}{2}\nabla_L^*(\boldsymbol{\rho}\nabla_L \boldsymbol{\lambda} + \nabla_L \boldsymbol{\lambda}\boldsymbol{\rho})$$

matches the marginals $\boldsymbol{\rho}(0) = \boldsymbol{\rho}_0, \boldsymbol{\rho}(1) = \boldsymbol{\rho}_1$,

then $(\boldsymbol{\rho}, \boldsymbol{v})$ with $\boldsymbol{v} = -\nabla_L \boldsymbol{\lambda}$ solves Problem i)

# Riemannian structure

$$\boldsymbol{\delta_j \in \mathbf{TangentSpace}_\rho = \{\delta \in \mathcal{H} \mid \mathrm{tr}(\delta) = 0\},}\ \text{for } \boldsymbol{j = 1, 2}$$

"Poisson" equation: $\boldsymbol{\delta}$'s $\Leftrightarrow$ $\boldsymbol{\lambda}$'s

$$\boldsymbol{\delta_j = -\frac{1}{2}\nabla_L^*(\rho\nabla_L\lambda_j + \nabla_L\lambda_j\rho)}$$

and

$$\boldsymbol{\langle\delta_1, \delta_2\rangle_\rho = \frac{1}{2}\mathrm{tr}(\rho\nabla\lambda_1^*\nabla\lambda_2 + \rho\nabla\lambda_2^*\nabla\lambda_1)}$$

Note: given $\boldsymbol{\delta}$, then $-\boldsymbol{\nabla_L\lambda}$ is the unique minimizer of $\mathbf{tr}(\boldsymbol{\rho v^* v})$ over $\boldsymbol{v} \in \boldsymbol{\mathcal{S}}^{\boldsymbol{N}}$ satisfying

$$\boldsymbol{\delta = \frac{1}{2}\nabla_L^*(\rho v + v\rho).}$$

# Riemannian metric

$W_{2,a}(\cdot,\cdot)$ is a metric on $\mathcal{D}_+$

$$W_{2,a}(\rho_0,\rho_1) = \min_{\rho} \int_0^1 \sqrt{\langle \dot{\rho}(t), \dot{\rho}(t) \rangle_{\rho(t)}} dt,$$

over piecewise smooth path on $\mathcal{D}_+$

# Computation – convex problem

momentum field $u = \rho v$, i.e. $u_i = \rho v_i$

$$\mathrm{tr}(\rho v^* v) = \sum_{k=1}^{N} \mathrm{tr}(\rho v_k^* v_k) = \mathrm{tr}(u^* \rho^{-1} u),$$

define $u_* := [u_1, \ldots, u_N]^*$, then

$$\begin{aligned} W_{2,a}(\rho_0, \rho_1)^2 = \quad & \min_{\rho, u} \int_0^1 \mathrm{tr}(u^* \rho^{-1} u) dt, \\ & \dot{\rho} = \frac{1}{2} \nabla_L^* (u - u_*), \\ & \rho(0) = \rho_0, \quad \rho(1) = \rho_1 \end{aligned}$$

Note: optimal $u$ automatically satisfies $u = \rho v$ for some $v \in \mathcal{S}^N$

no need for a constraint

# Matrix transport with added spatial component

$$\mathcal{D} = \{\rho(\cdot) \mid \rho(x) \in \mathcal{H}_+ \text{ such that } \int_{\mathbb{R}^m} \mathrm{tr}(\rho(x))dx = 1\}.$$

## Continuity equation: $w \in \mathcal{H}$ along space dimension

$$\frac{\partial \rho}{\partial t} + \frac{1}{2}\nabla_x \cdot (\rho w + w\rho) - \frac{1}{2}\nabla_L^*(\rho v + v\rho) = 0.$$

## Metric:

$$\begin{aligned} W_{2,a}(\rho_0,\rho_1)^2 := \min \int_0^1 \int_{\mathbb{R}^m} &\{\mathrm{tr}(\rho w^* w) + \gamma\, \mathrm{tr}(\rho v^* v)\}\, dxdt, \\ &\rho \in \mathcal{D}_+, w \in \mathcal{H}^m, v \in \mathcal{S}^N \\ &\frac{\partial \rho}{\partial t} + \frac{1}{2}\nabla_x \cdot (\rho w + w\rho) - \frac{1}{2}\nabla_L^*(\rho v + v\rho) = 0, \\ &\rho(0,\cdot) = \rho_0, \quad \rho(1,\cdot) = \rho_1 \end{aligned}$$

# Metric, computation, etc.

Same as before:

duality..

$$w_{\text{opt}}(t,x) = -\nabla_x \lambda(t,x), \; v_{\text{opt}} = -\frac{1}{\gamma}\nabla_L \lambda(t,x)$$

$\delta_j \xrightarrow[\text{Poisson}]{} \lambda_j$'s

and then $\langle \delta_1, \delta_2 \rangle = \int$ "symmetrized kinetic energy" $dx$

metric computed via convex optimization, with $q = \rho w$, $u = \rho v$:

$$\min_{\rho,q,u} \int_0^1 \int_{\mathbb{R}^m} \left\{ \text{tr}(q^* \rho^{-1} q) + \gamma\, \text{tr}(u^* \rho^{-1} u) \right\} dx dt$$

$$\frac{\partial \rho}{\partial t} + \frac{1}{2}\nabla_x \cdot (q + q_*) - \frac{1}{2}\nabla_L^*(u - u_*) = 0,$$

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

# Gradient flow of Entropy

$$S(\rho) = -\operatorname{tr}(\rho \log \rho).$$

then

$$\begin{aligned} \frac{dS(\rho(t))}{dt} &= \cdots \\ &= -\frac{1}{2}\operatorname{tr}(\rho v^* \nabla_L \log \rho + \rho(\nabla_L \log \rho)^* v), \end{aligned}$$

$\Rightarrow$ steepest ascent

$$v = -\nabla_L \log \rho$$

$\Rightarrow$ **gradient flow**

$$\dot{\rho} = -\frac{1}{2}\nabla_L^* \{\rho, \nabla_L \log \rho\}$$

Note: this is nonlinear, different from Lindblad

Note: similar with space component..

# Case ii) “logarithmic”

Problem ii):

$$\boldsymbol{W_{2,b}(\rho_0,\rho_1)^2 := \min_{\rho\in\mathcal{D}_+, v\in\mathcal{S}^N} \int_0^1 \int_0^1 \mathrm{tr}(v^*\rho^s v\rho^{1-s})\,ds\,dt}$$

$$\boldsymbol{\dot\rho = \nabla_L^* \int_0^1 \rho^s v \rho^{1-s} ds,}$$

$$\boldsymbol{\rho(0) = \rho_0, \quad \rho(1) = \rho_1.}$$

Note: computations?

# duality

If $\boldsymbol{\lambda}(\cdot) \in \boldsymbol{\mathcal{H}}$, $\boldsymbol{\rho}$ satisfy

$$\dot{\boldsymbol{\lambda}} = \int_0^1\int_0^1\int_0^\alpha \left\{ \frac{\boldsymbol{\rho}^{\alpha-\beta}}{(1-s)\boldsymbol{I}+s\boldsymbol{\rho}} (\nabla_L \boldsymbol{\lambda})^* \boldsymbol{\rho}^{1-\alpha} \nabla_L \boldsymbol{\lambda} \frac{\boldsymbol{\rho}^{\beta}}{(1-s)\boldsymbol{I}+s\boldsymbol{\rho}} \right\} d\beta d\alpha ds$$

$$\dot{\boldsymbol{\rho}} + \nabla_L^* \int_0^1 \boldsymbol{\rho}^s \nabla_L(\boldsymbol{\lambda}))\boldsymbol{\rho}^{1-s} ds = 0,$$

$$\boldsymbol{\rho}(0) = \boldsymbol{\rho}_0, \quad \boldsymbol{\rho}(1) = \boldsymbol{\rho}_1.$$

then $(\boldsymbol{\rho}, -\nabla_L(\boldsymbol{\lambda}))$ is optimal.

# Gradient flow of Entropy

$$\frac{dS(\rho(t))}{dt} = \dots$$
$$= -\operatorname{tr}((\nabla_L \log\rho)^* \int_0^1 \rho^s v \rho^{1-s} ds),$$

$\Rightarrow$ greatest ascent direction $v = -\nabla_L \log\rho$.

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non-commutative analog of: $\partial_x \rho = \rho\, \partial_x(\log\rho)$):

$$\nabla_L \rho = \int_0^1 \rho^s (\nabla_L \log\rho) \rho^{1-s} ds$$

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**Gradient flow:**

$$\dot{\rho} = -\nabla_L^* \int_0^1 \rho^s (\nabla_L \log\rho)\rho^{1-s} ds = -\nabla_L^* \nabla_L \rho = \Delta_L \rho,$$

Linear heat equation (now Lindblad) just as in the scalar case!

# Recap

With $M_\rho(v) = \rho v + v\rho$:

metric computable via convex optimization

gradient flow of entropy: nonlinear

With $M_\rho(v) = \int_0^1 \rho^s v \rho^{1-s} ds$:

metric computability questionable

gradient flow of entropy: linear, Lindblad

# Strong duality & conservation of Hamiltonian

Y. Chen, Wilfrid Gangbo, TTG & A. Tannenbaum

“On the Matrix Monge-Kantorovich Problem, arXiv 2017

**Strong duality:** define $F(\rho, m) := \frac{1}{2}\langle m, m\rho^{-1}\rangle$

Let $\rho_0, \rho_1 \in \mathcal{D}_+$. Then

$$\min_{(\rho,m)\in\mathcal{A}}\Big\{\int_0^1 F(\rho,m)dt \;\Big|\; \rho(0)=\rho_0,\ \rho(1)=\rho_1, \quad \text{and} \quad \dot{\rho} = \frac{1}{2}\nabla_L^*(m - m_*)\Big\}$$

$$= \sup_{\lambda\in\mathcal{B}}\Big\{\langle\lambda(1);\rho_1\rangle - \langle\lambda(0);\rho_0\rangle \;\Big|\; \dot{\lambda} + \frac{1}{2}(\nabla_L\lambda)^*(\nabla_L\lambda) \le 0 \quad \text{a.e. on} \quad (0,1)\Big\}.$$

$\mathcal{A} := \{\rho \in L^2(0,1;\mathcal{H}) \mid \operatorname{tr}(\rho) \equiv 1\} \times L^2(0,1;\mathbb{C}^{nN\times n})$

$\mathcal{B} := W^{1,2}(0,1;\mathcal{H})$

**Conservation of the Hamiltonian**:

Let $\rho_0, \rho_1 \in \mathcal{D}_+$ and $(\rho, m)$ a minimizer as before. Then:

(i) $$F(\rho(t), m(t)) \equiv F(\rho(0), m(0)).$$

(ii) If $0 \leq s \leq t \leq 1$ then

$$W_2(\rho(s), \rho(t)) = (t-s)\sqrt{2F(\rho(t), m(t))} = (t-s)W_2(\rho_0, \rho_1).$$

(iii) If we further assume that $\lambda \in W^{1,1}(0,1;\mathcal{H})$ is a maximizer of the dual, then

$$\langle \lambda(t); \rho(t) \rangle = \langle \lambda(0); \rho_0 \rangle + \frac{W_2(\rho_0, \rho(t))^2}{2t}, \quad t \in (0,1].$$

# unbalanced transport

J.-D. Benamou and Y. Brenier
"A computational fluid mechanics solution .." $L^2$ and Wasserstein

L. Chizat, B. Schmitzer, G. Peyré, and F.-X. Vialard
"An interpolating ... optimal transport and Fisher-Rao"

S. Kondratyev, L. Monsaingeon, and D. Vorotnikov
"A new optimal trasnport distance...," OMT and Fisher-Rao

M. Liero, A. Mielke, Giuseppe Savaré

"Optimal entropy-transport problems and a new Hellinger-Kantorovich distance.."

# unbalanced: $\mathbf{trace}\,\rho_0 \neq \mathbf{trace}\,\rho_1$

arXiv: Y. Chen, TTG & A. Tannenbaum

"Interpolation of Matrix-Valued Measures: The Unbalanced Case

Interpolation between Wasserstein and Bures:

$$W_{2,FR}(\rho_0,\rho_1)^2 := \inf_{\rho\in\mathcal{H}_{++}, v\in\mathcal{S}^N, r\in\mathcal{H}} \int_0^1 \{\mathrm{tr}(\rho v^* v) + \alpha\,\mathrm{tr}(\rho r^2)\} dt$$
$$\dot\rho = \frac{1}{2}\nabla_L^*(\rho v + v\rho) + \frac{1}{2}(\rho r + r\rho),$$
$$\rho(0) = \rho_0, \quad \rho(1) = \rho_1.$$

Interpolation between Wasserstein and Frobenius:

$$W_{2,F}(\rho_0,\rho_1)^2 := \inf_{\rho\in\mathcal{H}_{++}, v\in\mathcal{S}^N, s\in\mathcal{H}} \int_0^1 \{\mathrm{tr}(\rho v^* v) + \alpha\,\mathrm{tr}(s^2)\} dt$$
$$\dot\rho = \frac{1}{2}\nabla_L^*(\rho v + v\rho) + s,$$
$$\rho(0) = \rho_0, \quad \rho(1) = \rho_1.$$

- can be turned into convex problems as usual...

# transport of vector-valued distributions

$\boldsymbol{\rho} = [\boldsymbol{\rho_1}, \boldsymbol{\rho_2}, \cdots, \boldsymbol{\rho_\ell}]^{\boldsymbol{T}}$, on $\mathbb{R}_+^{\boldsymbol{N}}$

$$\sum_{i=1}^{\ell} \int_{\mathbb{R}^N} \rho_i(x)\,dx = 1,$$

*continuity equation*:

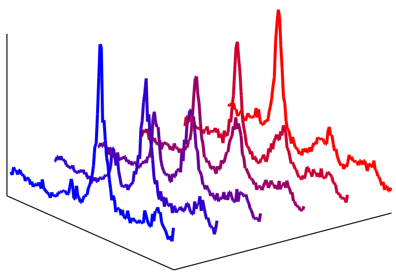
$$\frac{\partial \rho_i}{\partial t} + \nabla_x \cdot (\underbrace{\rho_i v_i}_{u_i}) - \sum_{j \neq i} (\underbrace{\rho_j w_{ji}}_{p_{ji}} - \rho_i w_{ij}) = 0, \quad \forall i = 1, \ldots, \ell.$$

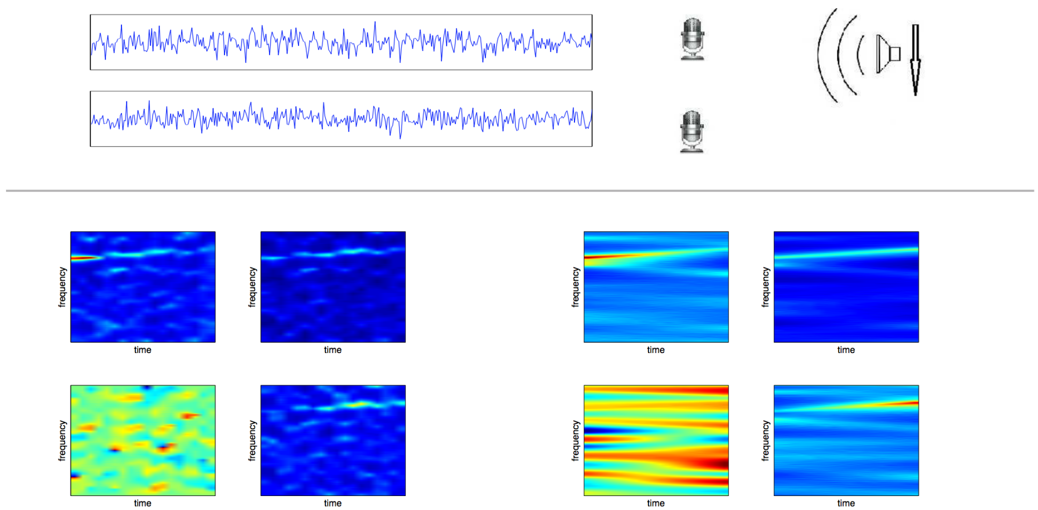
$$W_2(\mu,\nu)^2 := \inf_{\rho,v,w} \int_0^1 \int_{\mathbb{R}^N} \left\{ \sum_{i=1}^{\ell} \rho_i(t,x) \|v_i(t,x)\|^2 + \gamma \sum_{i,j=1}^{\ell} \rho_i w_{ij}^2(t,x) \right\} dx\,dt$$

– flows and metrics

for matrix and vector-valued distributions

for problems in signal analysis






thank you for your attention