A Spectral-Grassmann Wasserstein metric for operator representations of dynamical systems

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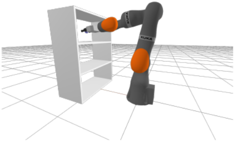
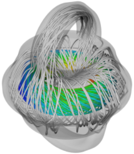
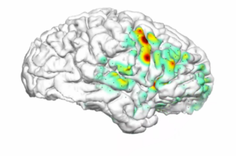
Dynamical system & machine learning



Robotic



Fluid dynamic



Brain dynamic

Dynamical systems

- Dynamical systems are backbone models of temporally evolving phenomena.
- Continuous time: $\frac{dx(t)}{dt} = g(t, x(t))$
- Discrete time: $x_{t+1} = g(t, x_t)$

Machine learning for dynamical systems

- Classical approach: ODE/PDE/SDE design + parameter fittting
- Data-driven approach: learn dynamics from data (with physics-informed constraints)

Learning dynamical systems with transfer operators

Definition: Transfer Operator

Let us assume:

- A stochastic process: $(X_t)_{t \geq 0} \in \mathcal{X}$
- A real-valued functional space: $\mathcal{F} \subseteq \mathbb{R}^{\mathcal{X}}$

Under some assumptions for $t \geq 0$, their exists a linear *transfer operator*, also known as *Koopman operator*, $A_t \colon \mathcal{F} \to \mathcal{F}$ that evolves an observable $f : \mathcal{X} \to \mathbb{R}$ for time t via the conditional expectation :

$$[A_t(f)](x) := E[f(X_t) \,|X_0 = x], \; x \in \mathcal{X}, f \in \mathcal{F}. \tag{1}$$

Remarks

- Even if the dynamical system is non-linear, the transfert operator is linear.
- Time-homogeneous systems : $A_{t+s} = A_t A_s$
- Continuous time: $A_t = \exp(tL)$ with L the infinitesimal generator of the semigroup $(A_t)_{t \geq 0}$.
- Discrete time: $A = A_1 = L$ is enough to describe the dynamics with $A_t = A_1^t$.

Spectral decomposition
Assuming that $\mathcal{F}$ is a separable Hilbert space (typically $L^2_\pi(\mathcal{X})$ with π the system's invariante measure) and L is a non defective operator with purely discrete spectrum. Then L can be written as:

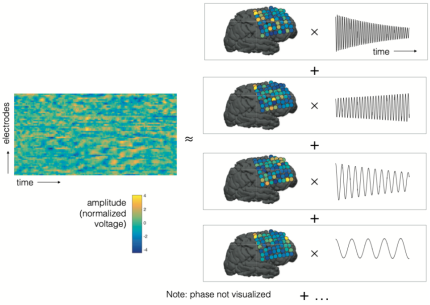
$$L = \sum_{j=1}^{\infty} \lambda_j g_j \otimes f_i, \text{ with } Lf_j{=}\lambda_j f_j,\ L^* g_j{=}\overline{\lambda_j} g_j \text{ , and } \langle f_j, g_j\rangle_{\mathcal{F}}{=}\delta_{i,j}$$

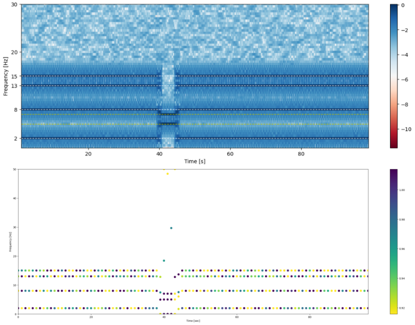
Properties :

- Fast computation : $A_t = \exp(tL) = \sum_{j=1}^{\infty} \exp(t\lambda_j) g_j \otimes f_i$
- Can be used to model evolution of densities of probability distributions.

Matrix view for operators

$$L = \underbrace{\begin{pmatrix} | & & | \\ f_1 & \cdots & f_r \\ | & & | \end{pmatrix}}_{F} \underbrace{\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_r \end{pmatrix}}_{\Lambda} \underbrace{\begin{pmatrix} - & g_1 & - \\ & \vdots & \\ - & g_r & - \end{pmatrix}}_{H^*} \quad \text{with} \quad H^* F = I_r$$





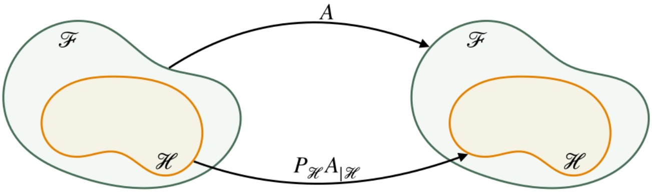
Spectral Decomposition

The spectral decomposition of $A_t = \exp(tL)$ decouples the evolution of any arbitrary observable $f \in \mathcal{F}$ as:

$$[A_t f](x) = E[f(X_t)|X_0 = x] = \sum_{j\in\mathbb{N}} e^{\lambda_j t}\langle f_j, g_j\rangle_{\mathcal{F}} f_j(x) = \sum_{j\in\mathbb{N}} e^{\tau_j t} e^{i2\pi\omega_j t} m_j^f(x),$$

into temporal and static components.

- Temporal: $e^{\tau_j t}$ (decay/growth) and $e^{i2\pi\omega_j t}$ (oscillation)
- Static: $m_j^f(x) = \langle f_j, g_j\rangle_{\mathcal{F}} f_j(x)$



Leraning operators from data

- Only trajectories of dynamical systems are observed. Neither the operator A nor its domain F are known.
- Learn the operator L from data in a RKHS $\mathcal{H} \subseteq \mathcal{F}$ with kernel $k(x, y) = \langle \phi(x), \phi(y) \rangle$ and estimate a projected operator.
- Given data $\{x_i, y_i\}_{i=1}^N$ (typically a trajectory with $y_i = x_{i+1}$) estimate $\hat{L}$ minimizing the empirical risk:

$$\min_{G \in HS(\mathcal{X})} \frac{1}{N} \sum_{i=1}^{N} \|\phi(y_i) - G\phi(x_i)\|_{\mathcal{H}}^2$$

Transfer operators in practice

Classical approaches

- Dynamic Mode Decomposition (DMD) [Kutz et al., 2016, Brunton et al., 2022] (Linear kernel but only for $f = Id$).
- Koopman operators with kernel methods [Williams et al., 2014, Kawahara, 2016].
- Reduced rank operator estimation [Kostic et al., 2022].
- Neural network approaches [Lusch et al., 2018, Kostic et al., 2024].

Open questions

- How to compare transfer operators ?
- Existing approaches:
  - Hilbert-Schmidt and operator norms are too conservative.
  - Martin distance [Martin, 2002]: pseudo-metric on ARMA models
  - Binet-Cauchy kernel [Chaudhry and Vidal, 2013]: Martin distance extension to LDS
  - Optimal Transport on spectrum (SOT)[Redman et al., 2024].
  - Optimal transport on eigenspaces (GOT) [Antonini and Cavalletti, 2021].
- $\rightarrow$ Propose a novel geometry for transfer operators based on optimal transport.

Spectral-Grassmann Wasserstein Metric (SGOT)

SGOT intuition & assumptions

Assumptions

1. **Time homogeneous Markovian dynamical systems** $\{L_k\}_{k\in[N]}$ (stationary).
2. **Low rank operators**: For all k, L_k has rank $r \ll N$.
3. **Common functional space** $\mathcal{H}$ for all operators. There exists an RKHS $\mathcal{H}$ such that for any operator, the estimation of its r-restriction, $Tk = exp(L_{k|r})$, is well defined.

Low rank spectral decomposition

$$L = \sum_{i\in[\ell]} \sum_{j\in[m_i]} \lambda_i g_{i,j} \otimes f_{i,j} = \sum_i \lambda_i P_i, \quad \langle f_{i,j}, g_{i',j'} \rangle_{\mathcal{H}} = \delta_{i,i'}\delta_{j,j'}, \quad \sum_i m_i = r$$

The representatin above is unique up to :

- Permutation of the indexes of the decomposition i.
- Change of basis of each spectral projectors P_i (Grassmann manifold).

$\rightarrow$ We need a metric invariant to these transformations : OT with proper geometry.

Low rank spectral decomposition

$$L = \sum_{i \in [\ell]} \sum_{j \in [m_i]} \lambda_i g_{i,j} \otimes f_{i,j} = \sum_i \lambda_i P_i, \quad \langle f_{i,j}, g_{i',j'} \rangle_{\mathcal{H}} = \delta_{i,i'} \delta_{j,j'}, \quad \sum_i m_i = r$$

- m_i is the multiplicity of eigenvalue λ_i.
- $P_i = \sum_{j \in [m_i]} g_{i,j} \otimes f_{i,j}$ is the spectral projector associated to λ_i.
- $\mathcal{V}_i = \text{span}\{g_{i,j} \otimes f_{i,j}\}_{j \in [m_i]}$ is the subspace of $\mathcal{H}$ associated to λ_i.

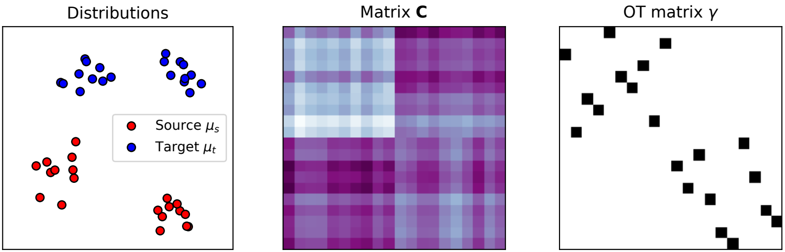
Property : distributional embedding

The operator L can be represented as a probability distribution over the product space of eigenvalues and projectors:

$$\mu(L) = \sum_{i \in [\ell]} \frac{m_i}{r} \delta_{(\lambda_i, \mathcal{V}_i)}$$

The embedding above is injective. For fixed rank r those distributions can be compared with discrete Optimal Transport

Optimal transport with discrete distributions



OT Linear Program and Wasserstein distance

When $\mu_s = \sum_{i=1}^{n} a_i \delta_{\mathbf{x}_i^s}$ and $\mu_t = \sum_{i=1}^{n} b_i \delta_{\mathbf{x}_i^t}$

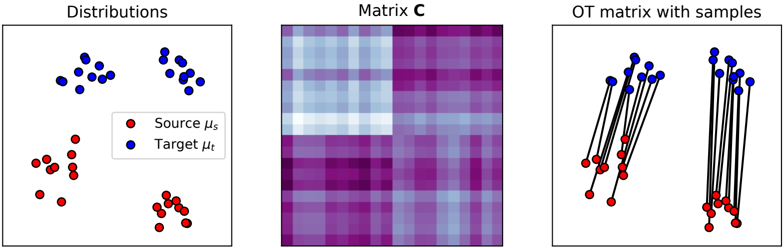
$$W_{d,p}^p(\mu_s, \mu_t) = \min_{\mathbf{T} \in \Pi(\mu_s, \mu_t)} \left\{ \langle \mathbf{T}, \mathbf{D} \rangle_F = \sum_{i,j} T_{i,j} c_{i,j}^p \right\}$$

where $\mathbf{D}$ is a distance matrix with $d_{i,j} = d(\mathbf{x}_i^s, \mathbf{x}_j^t)$ and the marginals constraints are

$$\Pi(\mu_s, \mu_t) = \left\{ \mathbf{T} \in (\mathbb{R}^+)^{n_s \times n_t} | \, \mathbf{T}\mathbf{1}_{n_t} = \mathbf{a}, \mathbf{T}^T \mathbf{1}_{n_s} = \mathbf{b} \right\}$$

Linear program with $n_s n_t$ variables and $n_s + n_t$ constraints, can be solved with complexity $O(r^3 \log r)$ if $n_s = n_t = r$.

Optimal transport with discrete distributions



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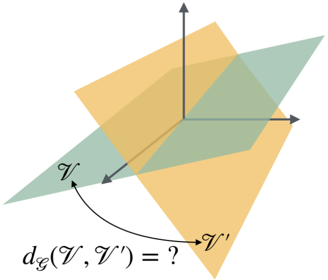


Proposition : Extension to infinite dimension space

Let $\mathcal{H}$ be a separable Hilbert space, and $\mathcal{G}_r(\mathcal{H})$ the set of vector subspaces of with dimension at most r. With the application:

$$d_{\mathcal{G}}(\mathcal{V}, \mathcal{V}') = \|P_{\mathcal{V}} - P_{\mathcal{V}'}\|_{\mathcal{H}}, \quad \forall \mathcal{V}, \mathcal{V}' \in \mathcal{G}_r(\mathcal{H})^2$$

where $P_{\mathcal{V}}$ is the orthogonal projector onto $\mathcal{V}$, then $(\mathcal{G}_r(\mathcal{H}), d_{\mathcal{G}})$ is a metric space.

Example for 1D subspaces:

$d_{\mathcal{G}}(\mathcal{V}, \mathcal{V}') = \sqrt{2 - 2\langle f, f' \rangle \langle g, g' \rangle}$ with f, f', g, g' normalized.

SGOT definition

Spectral-Grassmann Optimal Transport (SGOT)

Let H be a separable $\mathbb{C}$-Hilbert space and $\mathcal{S}_r(\mathcal{H})$ the set of non-defective operator on $\mathcal{H}$ with rank at most r. For $p \geq 1$ and $\eta \in [0,1]$, we define the Spectral-Grassmann Wasserstein metric distance between two operators $L, L' \in \mathcal{S}_r(\mathcal{H})$ as:

$$d^p_{SGOT,p}(L, L') = W^p_{c_\eta,p}(\mu(L'), \mu(L'))$$

where the cost matrix is defined as:

$$c_\eta((\lambda, \mathcal{V}), (\lambda', \mathcal{V}')) = \eta|\lambda^s_i - \lambda^t_j| + (1-\eta)d_{\mathcal{G}}(\mathcal{V}, \mathcal{V}')$$

Then the space $(\mathcal{S}_r(\mathcal{H}), d_{SGOT,p})$ is a metric space.

Computation

- Pre-compute the cost matrix $\mathbf{C}$ with complexity $O(n^2r^2)$.
- Solve the OT problem with complexity $O(r^3 \log r)$ with network simplex.
- Overall complexity: $O(n^2r^2 + r^3 log(r))$.

Existing bounds for operator estimation

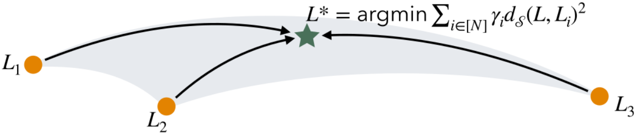
Under kernel universality assumption, estimation of Koopman operators come with spectral estimation guarantees [Kostic et al., 2023], specifically for the Reduced Rank Regression (RRR) method [Kostic et al., 2022].

Theorem (simplified)

Suppose two dynamical systems with low rank operator projection $L_1, L_2 \in \mathcal{S}_r(\mathcal{H})$ and their estimations $\hat{L}_1, \hat{L}_2 \in \mathcal{S}_r(\mathcal{H})$ from n samples with the RRR method [Kostic et al., 2022]. Suppose $\alpha \in (1, 2)$, and $\beta \in [0, 1]$ bounding the empirical covariance. In the i.i.d setting, for any $\delta \in (0, 1)$, with probability $1 - \delta$ it holds:

$$|d_{SGOT,p}(\hat{L}_1, \hat{L}_2) - d_{SGOT,p}(L_1, L_2)| \lesssim n^{-\frac{\alpha-1}{2(\alpha+\beta)}} \ln(2\delta^{-1})$$

Proof sketch: Use convergence of individual spectral elements [Kostic et al., 2023] and use the identity OT plan for upper bound.



SGOT Frechet mean

$$\underset{L\in\mathcal{S}_r(\mathcal{H})}{\text{argmin}} \sum_{k\in[N]} \gamma_i d_{SGOT}(L, L_k)^2, \tag{2}$$

where $\gamma \in \Sigma_N$ is a weight vector.

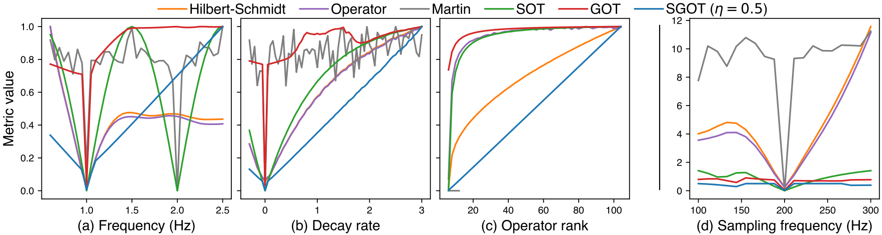
Numerical optimization of SGOT barycenter
We consider in the kernel case the operator $L_{\boldsymbol{\theta}}$ representation parametrized by $\boldsymbol{\theta} \triangleq (\boldsymbol{\lambda}, \boldsymbol{\alpha}, \boldsymbol{\beta}, \mathbf{x})$:

$$L_{\boldsymbol{\theta}} : h \in \mathcal{H} \mapsto \sum_{i\in[r]} \lambda_i \langle \kappa_{\mathbf{x}} \boldsymbol{\alpha}_i, h\rangle_{\mathcal{H}} \kappa_{\mathbf{x}} \boldsymbol{\beta}_i \in \mathcal{H}$$

The barycenter is optimized by optimizing:

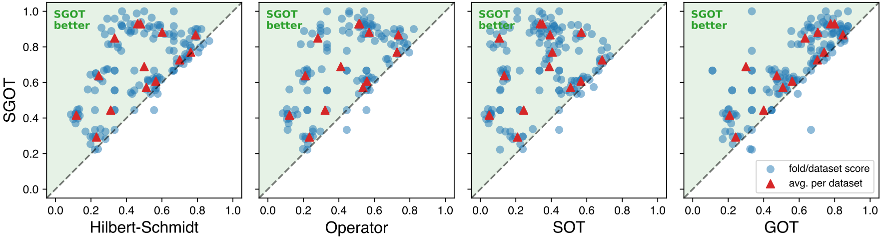
$$\underset{\boldsymbol{\theta},\mathbf{P}}{\text{argmin}} \sum_{i\in[N]} \gamma_i \langle \mathbf{C}_i(\boldsymbol{\theta}), \mathbf{P}_i\rangle_F \text{ s.t. } \begin{cases} \boldsymbol{\alpha}^* \mathbf{K} \boldsymbol{\beta} = \mathbf{I} & \mathbf{K} = \{\kappa(x_i, x_j)\}_{(i,j)\in[n]^2} \\ \boldsymbol{\beta}_j^* \mathbf{K} \boldsymbol{\beta}_j = 1, \ \forall j \in [r] & \mathbf{P}_i \in \Pi(\mu(L_{\boldsymbol{\theta}}), \mu(L_i)), \ \forall i \end{cases}$$

Numerical experiments



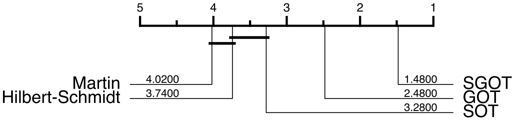
Numerical setup

- Compare SGOT with operator, Hislbert-Schmidt Martin, SOT and GOT distances.
- Simple 1D oscillatory dynamical systems with varying frequency, damping, rank and sampling frequency.
- SGOT has a unique minimum at the true parameters and capture well the variations of the systems.
- SGOT is robust (invariant) to sampling frequency changes.



Numerical setup

- 14 multivariate time series datasets from the UEA database [Ruiz et al., 2021].
- Each time series is modeled as a dynamical system (linear, kernel and MLP) and its transfer operator is estimated with RRR [Kostic et al., 2022].
- 1-NN classification with SGOT, GOT, SOT, Martin and Hilbert-Schmidt.
- SGOT outperforms other operator distances on most datasets.
- SGOT computation time is comparable to best existing methods and much faster than Hilbert-Schmidt and Operator norms.



Hilbert-Schmidt	Operator	Martin	SOT	GOT	SGOT
4.96ms	13.04ms	0.02ms	0.03ms	0.14ms	0.12ms

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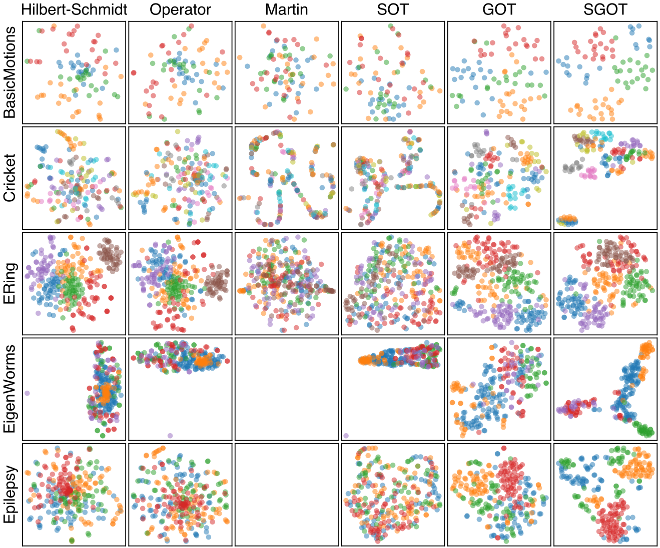
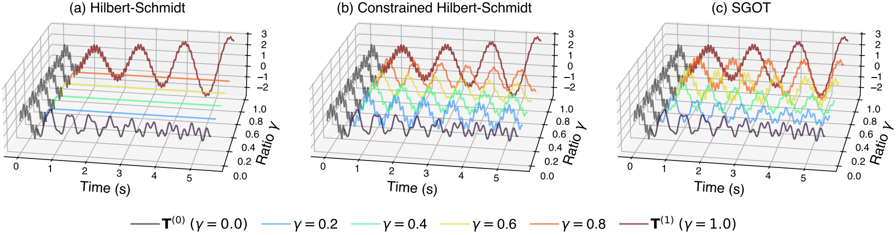
TSNE Embeddings of time series



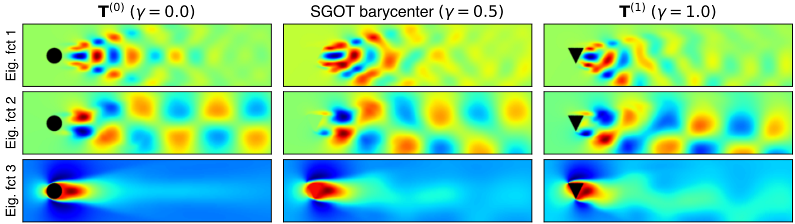
TNSE embeddings of time series using SGOT and other metrics.

Interpolation for 1D system



Numerical setup

- Consider two 1D oscillatory dynamical systems with different frequencies and dampings.
- Estimate their transfer operators and compute their SGOT, HS and constrained (low rank on manifold) HS barycenters for varying weights.
- Simulate the barycenter dynamical system, starting form the same initialization.
- SGOT barycenters interpolate well between the two systems while HS barycenters fail to capture the change in dynamics.

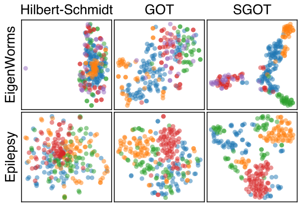


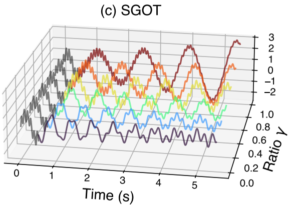
Numerical setup

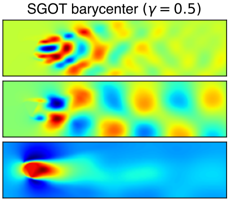
- Consider two fluid dynamics simulations with different shapes: circular with symmetry and triangular without symmetry.
- Estimate their transfer operators and compute their SGOT barycenter.
- Recovered eigen functions and dynamics interpolate well between the two systems.

Conclusion

Conclusion







Contributions

- A novel geometry for transfer operators based on optimal transport on the joint spectral and Grassmann manifolds.
- Statistical guarantees for the SGOT metric estimation from data.
- Numerical experiments showing the interest of SGOT for time series classification and barycenter computation.

Future works

- Comparison of baryenter with physics-based interpolation methods.
- Application on simulated nuclear fusion data (Tokam2D simulator).

Thank you

Doc : https://pythonot.github.io/

Code : https://github.com/PythonOT/POT

- OT LP solver, Sinkhorn (stabilized, GPU)
- Sliced OT, OT on sphere, Gaussian and Gaussian Mixture OT.
- Gromov-Wasserstein, Unbalanced.
- Barycenters, Wasserstein unmixing.
- Differentiable solvers for Numpy/Pytorch/tensorflow/Cupy

Course on OT for ML:
https://tinyurl.com/otml-course

Papers available on my website:
https://remi.flamary.com/

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