## Sequential transport for density estimation and its applications

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## Joint work with Olivier Zahm<sup>1</sup>, Tiangang Cui<sup>3</sup>, and Martin Schreiber<sup>1,2</sup>

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#### The task of density estimation

There are generally two distinct tasks of density estimation:

#### From a model

From data

Access to unnormalized density:

 $\pi(\mathbf{x}) \propto \mathcal{L}(\mathbf{x}) \pi_0(\mathbf{x})$ 

Access to data:

$$x^{(i)} \sim \pi$$

#### Goal

Sample from estimated distribution and/or evaluate its density

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Building a transport map  $\mathcal{T}$  from  $\rho_{\text{ref}}$  to  $\pi$ , so that  $\mathcal{T}_{\sharp} \rho_{\text{ref}} = \pi$  enables to efficiently sample from  $\pi$ .

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# Measure transport $\rho_{ref}$ $\tau$ $\tau$

Building a transport map  $\mathcal{T}$  from  $\rho_{\text{ref}}$  to  $\pi$ , so that  $\mathcal{T}_{\sharp} \rho_{\text{ref}} = \pi$  enables to efficiently sample from  $\pi$ .

$$\begin{array}{ll} \text{Pushforward of density:} & \mathcal{T}_{\sharp} \, \rho_{\mathsf{ref}} := \rho(\mathcal{T}^{-1}(\textbf{\textit{x}})) \, \mathsf{det} \, \nabla \mathcal{T}^{-1}(\textbf{\textit{x}}) = \tilde{\pi} \\ \text{Pushforward of samples:} & \mathcal{T}(\textbf{\textit{z}}) \sim \tilde{\pi} \quad \mathsf{with} \ \textbf{\textit{z}} \sim \rho_{\mathsf{ref}} \, . \end{array}$$

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#### Sequential measure transport



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#### Sequential measure transport



 $\begin{array}{c} \text{sequential estimation} \ + \ & \begin{array}{c} \text{Measure} \\ \text{transport} \end{array} = \ & \begin{array}{c} \text{sequential Measure} \\ \text{transport} (\textbf{SMT}) \end{array}$ 

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Sequential measure transport and SoS

April 22, 2025

## Sequential measure transport



Examples of combination of these two methods:

- Denoising diffusion
- Normalizing flow based as Grenioux et al. 2023; Rezende and Mohamed 2016
- Others like Cui et al. 2024; Marzouk et al. 2016

- 1 Proposed sequential measure transport (SMT) method
- 2 Design of Bridging densities and convergence analysis
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- 4 Application in Optimal Transport
- 5 Summary & future work

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#### Outline

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2 Design of Bridging densities and convergence analysis

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4 Application in Optimal Transport

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VDE Variation density estimation of  $\pi^{(1)}$ 

$$ilde{f}^{(1)} = \mathop{\arg\min}\limits_{ ilde{f} \in \mathcal{M}} \frac{\mathrm{D}_{lpha}\left(\pi^{(1)} || ilde{f}
ight)}{1}$$

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VDE Variation density estimation of  $\pi^{(1)}$ 

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SoS-densities for  $\mathcal{M}$ 

$$egin{aligned} f_A(oldsymbol{x}) &= \sum ig( \Phi(oldsymbol{x})^{ op} oldsymbol{a}_i ig)^2 \ &= \Phi(oldsymbol{x})^{ op} A \Phi(oldsymbol{x}) \quad A \succeq 0 \end{aligned}$$



VDE Variation density estimation of  $\pi^{(1)}$ 

$$\widetilde{f}^{(1)} = \operatorname*{arg\,min}_{\widetilde{f} \in \mathcal{M}} \mathbb{D}_{\alpha} \left( \pi^{(1)} || \widetilde{f} \right)$$

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 $\alpha$ -divergences  $D_{\alpha}$ 

- Includes: (reversed) KL-divergence,  $\chi^2$  divergence, ...
- Extension to unnormalized densities

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KR Build the Knothe-Rosenblatt map  $Q_1$  from  $\tilde{\pi}^{(1)}$ 

**1** Normalize  $\tilde{f}^{(1)}$  to get  $\tilde{\pi}^{(1)}$ 

With  $\Phi(\mathbf{x})$  orthonormal in  $L^2_{\mu}$ ,

$$\pi_A(\mathbf{x}) = rac{\Phi(\mathbf{x})A\Phi(\mathbf{x})}{\mathrm{tr}A}\mu(\mathbf{x}).$$

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- **1** Normalize  $\tilde{f}^{(1)}$  to get  $\tilde{\pi}^{(1)}$
- **2** Build marginals  $\pi(\mathbf{x}_{1:k})$  and CDFs of marginals

$$\Pi(\boldsymbol{x}_k|\boldsymbol{x}_{1:k-1}) = \frac{\Pi(\boldsymbol{x}_{1:k-1},\boldsymbol{x}_k)}{\pi(\boldsymbol{x}_{1:k-1})}$$

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- **2** Build marginals  $\pi(\mathbf{x}_{1:k})$  and CDFs of marginals
- **3** Map  $\overline{\mathcal{Q}}$  from uniform distribution to  $\tilde{\pi}^{(1)}$

$$\overline{\mathcal{Q}}(\xi_1,\ldots,\xi_d) = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} = \begin{pmatrix} \Pi^{-1}(\xi_1) & & \\ \Pi^{-1}(\xi_2|x_1) & \\ \vdots \\ \Pi^{-1}(\xi_d|x_1,\ldots,x_{d-1}) \end{pmatrix}$$



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- **3** Map  $\overline{\mathcal{Q}}$  from uniform distribution to  $\tilde{\pi}^{(1)}$
- 4 Map  ${\cal Q}$  from  $ho_{\rm ref}$  to  ${ ilde \pi}^{(1)}$

$$\mathcal{R}_{\sharp} \rho_{\mathsf{ref}} = U \quad \Rightarrow \quad (\mathcal{R} \circ \overline{\mathcal{Q}})_{\sharp} \rho_{\mathsf{ref}} = \tilde{\pi}^{(1)}$$

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|PB| Use  $T_1 = Q_1$  to simplify  $\pi^{(2)}$  using a *pullback* (idea originally from Cui and Dolgov 2021)

 $\tau^{(2)} = \mathcal{T}_1^{\sharp} \pi^{(2)}$ 

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VDE on density  $\tau^{(2)}$  to get  $\tilde{\tau}^{(2)}$ 

$$\tilde{\tau}^{(2)} = \operatorname*{arg\,min}_{\tilde{\pi} \in \mathcal{M}} \mathrm{D}_{\alpha} \left( \mathcal{T}_{1}^{\sharp} \pi^{(2)} || \tilde{\tau} \right)$$

KR map  $Q_2$  from  $\tilde{\tau}^{(2)}$ 

$$\Rightarrow \tilde{\pi}^{(2)} = (\mathcal{T}_1)_{\sharp} \tilde{\tau}^{(2)}$$
$$= \underbrace{(\mathcal{T}_1 \circ \mathcal{Q}_2)_{\sharp}}_{\mathcal{T}_2} \rho_{\text{ref}}$$

Sequential measure transport and SoS

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#### **Algorithm** SMT with KR maps

1:  $\mathcal{T}_0 = \mathrm{id}$ 

2: for 
$$\ell = 1$$
 to  $L$  do

3: 
$$PB \tau^{(\ell)} = \mathcal{T}_{\ell-1}^{\sharp} \pi^{(\ell)}$$

4: VDE to estimate 
$$au^{(\ell)}$$
 by  $ilde{ au}^{(\ell)}$ 

KR map  $\mathcal{Q}_{\ell}$  from  $\tilde{\tau}^{(\ell)}$ 5:

6: 
$$\mathcal{T}_\ell = \mathcal{T}_{\ell-1} \circ \mathcal{Q}_\ell$$



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7: end for

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tempering and diffusion among most popular bridging densities

Tempering

$$\pi^{(\ell)}(\mathbf{x}) = \rho_{\mathsf{ref}}(\mathbf{x})^{1-\beta_{\ell}}\pi(\mathbf{x})^{\beta_{\ell}}$$

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tempering and diffusion among most popular bridging densities

Diffusion

$$X_{t_{\ell}}^{(i)} = \exp(-t_{\ell})X^{(i)} + \sqrt{1 - \exp(-2t_{\ell})}Z^{(i)}$$
  $X^{(i)}$ 

$$X^{(i)} \sim \pi, Z^{(i)} \sim \mathcal{N}(0, I)$$

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tempering and diffusion among most popular bridging densities
 How to choose hyperparamters, β<sub>1</sub>, β<sub>2</sub>, ... and t<sub>1</sub>, t<sub>2</sub>, ...?

 $\Rightarrow$  Scheduling problem (Kingma et al. 2023)

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Let  $\eta$  be so that

$$\mathsf{D}_{lpha}(\pi^{(\ell+1)}||\pi^{(\ell)}) \leq \eta$$
 for all  $\ell = 1, \dots, L$ .

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Let  $\eta$  be so that

$$\mathsf{D}_{\alpha}(\pi^{(\ell+1)}||\pi^{(\ell)}) \leq \eta$$
 for all  $\ell = 1, \dots, L$ .

Sequences of  $\beta_\ell$  and  $t_\ell$  exists which satisfy  $\eta = \mathcal{O}(1/L^2)$ 

## Bridging densities – scheduling

Let  $\omega$  be

$$\mathsf{D}_{\alpha}\left(\pi^{(\ell)}||\tilde{\pi}^{(\ell)}\right) \leq \omega \, \mathsf{D}_{\alpha}\left(\pi^{(\ell)}||\tilde{\pi}^{(\ell-1)}\right) \qquad \text{for all } \ell = 1,\ldots,L.$$

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## Bridging densities - scheduling

Let  $\omega$  be

$$\mathsf{D}_{\alpha}\left(\pi^{(\ell)}||\tilde{\pi}^{(\ell)}\right) \leq \omega \, \mathsf{D}_{\alpha}\left(\pi^{(\ell)}||\tilde{\pi}^{(\ell-1)}\right) \qquad \text{for all } \ell = 1, \dots, L.$$

Proposition (informal, Zanger et al. 2024)

If  $\omega < 1$ , then the estimation of  $\pi^{(L)}$  is bounded with

$$\mathsf{D}_{\alpha}\left(\pi^{(L)}||\widetilde{\pi}^{(L)}
ight) \leq rac{\omega(1+\epsilon)}{1-\omega}\eta$$

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## Bridging densities - scheduling

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Proposition (informal, Zanger et al. 2024)

If  $\omega < 1$ , then the estimation of  $\pi^{(L)}$  is bounded with

$$\mathsf{D}_{\alpha}\left(\pi^{(L)}||\widetilde{\pi}^{(L)}\right) \leq \frac{\omega(1+\epsilon)}{1-\omega}\eta_{\epsilon}$$

- **Our strategy:** Equidistant changes to minimize *η*.
- Different approach: Best for the given approximation tool to minimize ω, see Marzouk et al. 2024.

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#### Outline

1 Proposed sequential measure transport (SMT) method

2 Design of Bridging densities and convergence analysis

#### 3 Numerical examples

4 Application in Optimal Transport

5 Summary & future work

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### Numerical example - SIR model

Model from epidemiology:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}S = -\beta IS \\ \frac{\mathrm{d}}{\mathrm{d}t}I = \beta SI - \gamma I \\ \frac{\mathrm{d}}{\mathrm{d}t}R = \gamma I \end{cases}$$

Given observations of I, determine  $\beta$  and  $\gamma$  with  $\pi_{\text{prior}} = U([0, 2])^2$ .

$$\mathcal{L}(oldsymbol{y}|oldsymbol{x}) \propto \exp\left(-rac{1}{2\sigma^2}\sum_i(I_{t_i}-y_i)^2
ight)$$



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- Legendre polynomials of  $\deg(\Phi) \leq 6$
- 1000 density evaluations for each VDE



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#### Learning from datasets - Conditional density estimation

- 10 runs with different split of training/validation data
- Comparison with Baptista et al. 2023
- SoS polynomials of dimension 8, degree  $\leq$  3, use of random lazy maps

Table: Comparison of negative log likelihood function for different UCI datasets and conditional density estimation methods.

Dataset	(d, N)	SoS (1 sample)	SoS (4 samples)	ATM	# seq.
Boston	(12, 506)	$2.8\pm0.2$	$2.5 \pm 0.2$	$2.6 \pm 0.2$	$27.4\pm4.2$
Concrete	(9, 1030)	$3.4\pm0.3$	$3.1\pm0.1$	$3.1\pm0.1$	$44.0\pm4.8$
Energy	(10, 768)	$2.2\pm0.2$	$1.7 \pm 0.2$	$1.5 \pm 0.1$	$34.8\pm6.1$
Yacht	(7,308)	$3.4\pm1.1$	$2.0\pm0.6$	$0.5 \pm 0.2$	$40.8\pm12.7$

## Calibration of Ocean-Surface parametrization

Joint work with Manolis Perrot and Florian Lemarié (Perrot et al. 2025).



 $\Rightarrow \text{ Parametrization of the ocean surface using 9 free parameters which need to be calibrated.}$ 

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## Calibration of Ocean-Surface parametrization

- 2 reference trajectories
- Calibration using the temperature at different depths
- 5 bridging densities
- 5000 density evaluations per estimation
- Polynomials with  $deg(\Phi) \leq 3$  and Putinar's Positivstellensatz



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### Calibration of Ocean-Surface parametrization

#### Prior:



#### **Posterior:**



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#### Outline

1 Proposed sequential measure transport (SMT) method

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### Regularized Optimal Transport

Shortest path between p and q with cost c. Kantorovich formulation:

$$\pi^* = \underset{\pi \in \Pi(p,q)}{\arg\min} \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) \mathrm{d}\pi(\mathbf{x}, \mathbf{y}) + \epsilon \cdot \mathrm{D}_{\varphi}\left(\pi || \pi_{\mathsf{ref}}\right)$$



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## Regularized Optimal Transport

Shortest path between p and q with cost c. Kantorovich formulation:

$$\pi^* = \arg\min_{\pi \in \Pi(\rho,q)} \int_{\mathcal{X} \times \mathcal{Y}} c(\mathbf{x}, \mathbf{y}) d\pi(\mathbf{x}, \mathbf{y}) + \epsilon \cdot D_{\varphi}(\pi || \pi_{\text{ref}})$$

#### Our idea:

Model the transport plan  $\pi$  using sequential measure transport:

$$\pi^{(\ell)} = (\mathcal{T}_{\ell-1})_{\sharp} \tau^{(\ell)} = (\mathcal{T}_{\ell})_{\sharp} \rho_{\mathsf{ref}}$$

with  $\pi^{(\ell)}$  solution to regularized OT with  $\epsilon_{\ell}$ .

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#### Regularized Optimal Transport

Shortest path between p and q with cost c. Kantorovich formulation:

$$\tau^{(\ell)} = \argmin_{(\mathcal{T}_{\ell-1})_{\sharp} \tau \in \Pi(p,q)} \int_{\mathcal{X} \times \mathcal{Y}} c \circ \mathcal{T}_{\ell-1}(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\tau(\boldsymbol{x}, \boldsymbol{y}) + \epsilon_{\ell} \cdot \mathrm{D}_{\varphi}\left(\tau || \mathcal{T}_{\ell-1}^{\sharp} \pi_{\mathsf{ref}}\right)$$



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## Regularized Optimal transport

Shortest path between p and q with cost c. Kantorovich formulation:

$$\pi^{(\ell)} = \operatorname*{arg\,min}_{\pi \in \Pi(\rho,q)} \int_{\mathcal{X} \times \mathcal{Y}} c(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\pi(\boldsymbol{x}, \boldsymbol{y}) + \epsilon_{\ell} \cdot \mathrm{D}_{\varphi}\left(\pi || \pi_{\mathsf{ref}}\right)$$

#### **Dual formulation:**

$$egin{argmax}{l} rgmax \int_{\mathcal{X}} u(m{x}) \mathrm{d} p(m{x}) + \int_{\mathcal{Y}} v(m{y}) \mathrm{d} q(m{y}) \ & - \epsilon_\ell \cdot \int_{\mathcal{X} imes \mathcal{Y}} arphi^\dagger \left( rac{u(m{x}) + v(m{y}) - c(m{x},m{y})}{\epsilon_\ell} 
ight) \mathrm{d} \pi_{\mathrm{ref}}. \end{array}$$

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### Regularized Optimal transport

Shortest path between p and q with cost c. Kantorovich formulation:

$$\pi^{(\ell)} = \arg\min_{\pi \in \Pi(\rho,q)} \int_{\mathcal{X} \times \mathcal{Y}} c(\boldsymbol{x}, \boldsymbol{y}) d\pi(\boldsymbol{x}, \boldsymbol{y}) + \epsilon_{\ell} \cdot \mathbf{D}_{\varphi} \left( \pi || \pi_{\mathsf{ref}} \right)$$

#### **Dual formulation:**

$$\underset{u,v}{\operatorname{arg\,max}} \int_{\mathcal{X}} u(\boldsymbol{x}) \mathrm{d} \boldsymbol{\rho}(\boldsymbol{x}) + \int_{\mathcal{Y}} v(\boldsymbol{y}) \mathrm{d} \boldsymbol{q}(\boldsymbol{y}) \\ - \epsilon_{\ell} \cdot \int_{\mathcal{X} \times \mathcal{Y}} \varphi^{\dagger} \left( \frac{u(\boldsymbol{x}) + v(\boldsymbol{y}) - c(\boldsymbol{x}, \boldsymbol{y})}{\epsilon_{\ell}} \right) \frac{\pi_{\mathrm{ref}}}{(\mathcal{T}_{\ell-1})_{\sharp} \rho} \cdot \mathrm{d}(\mathcal{T}_{\ell-1})_{\sharp} \rho.$$

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### Regularized Optimal transport

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**Application of this idea in Sinkhorn algorithm:** Schmitzer 2019 and Li et al. 2023

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#### Outline

- 1 Proposed sequential measure transport (SMT) method
- **2** Design of Bridging densities and convergence analysis
- 3 Numerical examples
- 4 Application in Optimal Transport
- 5 Summary & future work

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## Summary & Future work

We presented the framework of **Sequential measure transport** which includes state-of-the art density estimation methods.

- KR maps with SoS densities
- Problem of scheduling
- Unified convergence analysis for  $\alpha$ -divergences

Challenges and open problems:

- Amount of density evaluations: In Westermann and Zech 2023 and Cui et al. 2023b sampling is clear (least squares problem). Combination of SoS with α-divergences less clear → cross-validation.
- Curse of dimensionality: Scaling to high dimension requires adaptivity.

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Generic implementation of sequential measure transport mechanism and SoS maps

Many thanks to my supervisors, collaborators, and for helpful discussions with Ricardo Baptista.

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#### References I

Baptista, Ricardo, Youssef Marzouk, and Olivier Zahm (2023). "On the representation and learning of monotone triangular transport maps". In: Foundations of Computational Mathematics, pp. 1–46. Cui, Tiangang and Sergey Dolgov (Sept. 2021). "Deep composition of tensor-trains using squared inverse Rosenblatt transports". en. In: Foundations of Computational Mathematics. arXiv:2007.06968 [cs. math, stat]. ISSN: 1615-3375, 1615-3383. DOI: 10.1007/s10208-021-09537-5. URL: http://arxiv.org/abs/2007.06968 (visited on 07/19/2022). Cui, Tiangang, Sergey Dolgov, and Robert Scheichl (2024). "Deep Importance Sampling Using Tensor Trains with Application to a Priori and a Posteriori Rare Events". In: SIAM Journal on Scientific *Computing* 46.1, pp. C1–C29.

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#### References II

Cui, Tiangang, Sergey Dolgov, and Olivier Zahm (2023a). "Scalable conditional deep inverse Rosenblatt transports using tensor trains and gradient-based dimension reduction". In: Journal of Computational Physics 485, p. 112103. ISSN: 0021-9991. DOI: https://doi.org/10.1016/j.jcp.2023.112103. URL: https://www.sciencedirect.com/science/article/pii/S0021999123001985.

- (Mar. 2023b). Self-reinforced polynomial approximation methods for concentrated probability densities. en. arXiv:2303.02554 [cs, math, stat]. URL: http://arxiv.org/abs/2303.02554 (visited on 03/20/2023).
- Grenioux, Louis, Alain Durmus, Éric Moulines, and Marylou Gabrié (2023). "On Sampling with Approximate Transport Maps". In: *arXiv* preprint arXiv:2302.04763.

#### References III

- Kingma, Diederik P., Tim Salimans, Ben Poole, and Jonathan Ho (2023). Variational Diffusion Models. arXiv: 2107.00630 [cs.LG]. URL: https://arxiv.org/abs/2107.00630.
- Li, Mengyu, Jun Yu, Tao Li, and Cheng Meng (2023). "Importance Sparsification for Sinkhorn Algorithm". en. In: *Journal of Machine Learning Research* 24, pp. 1–44.
- Marzouk, Youssef, Tarek Moselhy, Matthew Parno, and Alessio Spantini (2016). "An introduction to sampling via measure transport". en. In: arXiv:1602.05023 [math, stat], pp. 1–41. DOI: 10.1007/978-3-319-11259-6\_23-1. URL:

http://arxiv.org/abs/1602.05023 (visited on 07/20/2022).

 Marzouk, Youssef, Zhi Ren, Sven Wang, and Jakob Zech (2024).
 "Distribution Learning via Neural Differential Equations: A Nonparametric Statistical Perspective". en. In: *Journal of Machine Learning Research*.

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#### References IV

Perrot, M., F. Lemarié, and T. Dubos (Jan. 2025). "Energetically Consistent Eddy-Diffusivity Mass-Flux Convective Schemes: 1. Theory and Models". en. In: Journal of Advances in Modeling Earth Systems 17.1. e2024MS004273. ISSN: 1942-2466. 1942-2466. DOI: 10.1029/2024MS004273. URL: https://agupubs.onlinelibrary. wiley.com/doi/10.1029/2024MS004273 (visited on 04/21/2025). 📔 Rezende, Danilo Jimenez and Shakir Mohamed (June 2016). Variational Inference with Normalizing Flows. en. arXiv:1505.05770 [cs, stat]. URL: http://arxiv.org/abs/1505.05770 (visited on 06/13/2023). Schmitzer, Bernhard (Feb. 2019). Stabilized Sparse Scaling Algorithms for Entropy Regularized Transport Problems. en. arXiv:1610.06519 [math]. DOI: 10.48550/arXiv.1610.06519. URL: http://arxiv.org/abs/1610.06519 (visited on 03/20/2025).

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#### References V

- Westermann, Josephine and Jakob Zech (Nov. 2023). Measure transport via polynomial density surrogates. en. arXiv:2311.04172 [cs, math, stat]. URL: http://arxiv.org/abs/2311.04172 (visited on 12/01/2023).
- Zanger, Benjamin, Olivier Zahm, Tiangang Cui, and Martin Schreiber (Oct. 2024). Sequential transport maps using SoS density estimation and \$

*alpha\$-divergences.* en. arXiv:2402.17943 [stat]. URL: http://arxiv.org/abs/2402.17943 (visited on 11/17/2024).

#### Convergence analysis - general idea

General proof idea from Cui et al. 2023a

$$D\left(\pi^{(L)}||\widetilde{\pi}^{(L)}\right) \leq \omega D\left(\pi^{(L)}||\widetilde{\pi}^{(L-1)}\right)$$
$$\leq \omega D\left(\pi^{(L)}||\pi^{(L-1)}\right) + \omega D\left(\pi^{(L-1)}||\widetilde{\pi}^{(L-1)}\right)$$

recursion...

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$$\leq \omega D\left(\pi^{(L)}||\pi^{(L-1)}\right) + \omega D\left(\pi^{(L-1)}||\widetilde{\pi}^{(L-1)}\right)$$

recursion...

Problem: triangle inequality does not hold for  $\alpha$ -divergences!

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## Convergence analysis by geometric properties of $\alpha$ -divergences



#### Assumption

We assume that there exists an  $\epsilon \geq 0$  so that

$$\mathsf{D}_{\alpha}\left(\pi^{(\ell+1)}||f_{\mathrm{proj}}^{(\ell)}\right) \leq (1+\epsilon)\,\mathsf{D}_{\alpha}\left(\pi^{(\ell+1)}||\pi^{(\ell)}\right) \qquad \forall l \in [L].$$

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## Convergence analysis by geometric properties of $\alpha$ -divergences

Pythagorean theorem instead of the triangle inequality:

$$\begin{split} \mathsf{D}_{\alpha}\left(\pi^{(L)}||\widetilde{\pi}^{(L)}\right) &\leq \omega\,\mathsf{D}_{\alpha}\left(\pi^{(L)}||\widetilde{\pi}^{(L-1)}\right) \\ &= \omega\,\mathsf{D}_{\alpha}\left(\pi^{(L)}||f_{\mathrm{proj}}^{(L-1)}\right) + \omega\,\mathsf{D}_{\alpha}\left(f_{\mathrm{proj}}^{(L-1)}||\widetilde{\pi}^{(L-1)}\right) \\ &\leq \omega(1+\epsilon)\,\mathsf{D}_{\alpha}\left(\pi^{(L)}||\pi^{(L-1)}\right) + \omega\,\mathsf{D}_{\alpha}\left(f_{\mathrm{proj}}^{(L-1)}||\widetilde{\pi}^{(L-1)}\right) \\ &\leq \omega(1+\epsilon)\,\mathsf{D}_{\alpha}\left(\pi^{(L)}||\pi^{(L-1)}\right) + \omega\,\mathsf{D}_{\alpha}\left(\pi^{(L-1)}||\widetilde{\pi}^{(L-1)}\right) \end{split}$$

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#### Proposition

Furthermore, let  $D_{\alpha}(\pi^{(0)}||\tilde{\pi}^{(0)}) = 0$ , for example by  $\pi^{(0)} = \rho_{ref}$ . If  $\omega < 1$ , than the estimation of  $\pi^{(L)}$  is bounded with

$$\mathsf{D}_lpha\left(\pi^{(L)}||\widetilde{\pi}^{(L)}
ight)\leq rac{\omega(1+\epsilon)}{1-\omega}\eta(L).$$

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#### Entropic regularized optimal transport

The entropic regularized optimal transport problem between distributions p and q with cost c can be written as

$$\tilde{\pi} = \arg\min_{\tilde{\pi}} D_{\mathrm{KL}}(\pi || \xi_{\epsilon}) \qquad \text{s.t.} \quad \int_{\mathcal{X}} \pi(\mathbf{x}, \mathbf{y}) d\mathbf{x} = q(\mathbf{y})$$
$$\int_{\mathcal{Y}} \pi(\mathbf{x}, \mathbf{y}) d\mathbf{y} = p(\mathbf{x})$$
$$\epsilon = 10 \qquad \epsilon = 0.5 \qquad \epsilon = 0.03 \qquad \epsilon = 0.001$$

#### Entropic regularized optimal transport

The entropic regularized optimal transport problem between distributions p and q with cost c can be written as

$$egin{aligned} & ilde{\pi}^{(2)} = rgmin_{\pi} \mathsf{D}_{\mathrm{KL}}\left(\pi || \mathcal{T}_{1}^{\sharp} \xi_{\epsilon}
ight) \qquad ext{s.t.} \quad \int_{\mathcal{X}} (\mathcal{T}_{1})_{\sharp} \pi(oldsymbol{x},oldsymbol{y}) \mathrm{d}oldsymbol{x} = q(oldsymbol{y}) \ & \int_{\mathcal{Y}} (\mathcal{T}_{1})_{\sharp} \pi(oldsymbol{x},oldsymbol{y}) \mathrm{d}oldsymbol{y} = p(oldsymbol{x}) \end{aligned}$$



#### Entropic regularized optimal transport

The entropic regularized optimal transport problem between distributions p and q with cost c can be written as

$$\begin{split} \widetilde{\pi}^{(2)} &= \operatorname*{arg\,min}_{\pi} \mathsf{D}_{\mathrm{KL}}\left(\pi || \mathcal{T}_{1}^{\sharp} \xi_{\epsilon}
ight) \qquad ext{s.t.} \quad \int_{\mathcal{X}} (\mathcal{T}_{1})_{\sharp} \pi(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{x} = q(\mathbf{y}) \\ &\int_{\mathcal{V}} (\mathcal{T}_{1})_{\sharp} \pi(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} = p(\mathbf{x}) \end{split}$$