

Tree-based Diffusion Schrödinger Bridge with Applications to Wasserstein Barycenters

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Entropic Optimal Transport (EOT)

Ingredients

- | Probability distributions μ_0, μ_1
- | Cost function c
- | Entropic regularization ($\varepsilon > 0$)

Principle

- | Find a plan $\pi \in \Pi(\mu_0, \mu_1)$ that minimizes

$$\mathbb{E}_\pi [C(\mathbf{X}_0, \mathbf{X}_1)] - \varepsilon H(\pi)$$

When c is quadratic:

EOT (static) \iff Schrödinger Bridge (SB) problem (dynamic)

Algorithm: **Dis**use Schrödinger Bridge (DSB) (De Bortoli et al., 2021)

- | Iterates: *path measures*.
- | Sequence of **projections**.
- | Based upon **score-based methods** (Song et al., 2021).
- | Scalable with dimension.

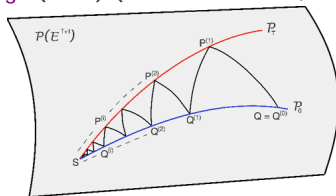


Figure 1: Iterations of DSB.

Extension to the multi-marginal setting

Tree-based setting: encodes a *probabilistic graphical model*.

- | **Nodes** → marginals.
 - **Leaves** are *fixed*.
- | **Edges** → dependence.

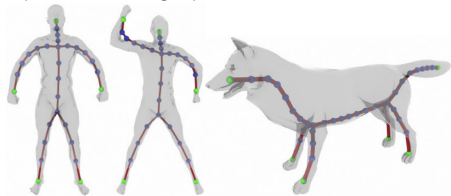


Figure 2: Trees from [Solomon et al. \(2015\)](#).

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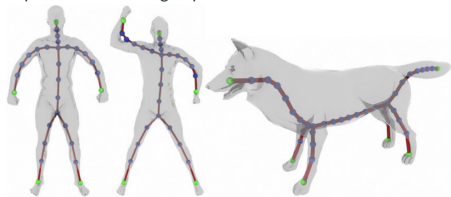


Figure 2: Trees from Solomon et al. (2015).

Case of interest: **Wasserstein-2 barycenter** (Agueh and Carlier, 2011)

⇒ Quadratic cost c & Star-shaped tree

Several **static** methods

- | In-sample (Cuturi and Doucet, 2014; Benamou et al., 2015)
- | Out-of-sample (*parametric*) (Fan et al., 2020; Li et al., 2020)

Questions

- | **Multi-marginal** SB ? (Haasler et al. (2021): discrete state-space)
- | **Dynamic** methodology ?

Our contribution: TreeDSB

- | Correspondence with SB problem \rightarrow Tree SB.
- | Iterative DSB-like procedure \rightarrow TreeDSB.

\implies Dynamically solve a tree-based formulation of EOT.

💡 TreeDSB updates only occur on paths between the leaves.

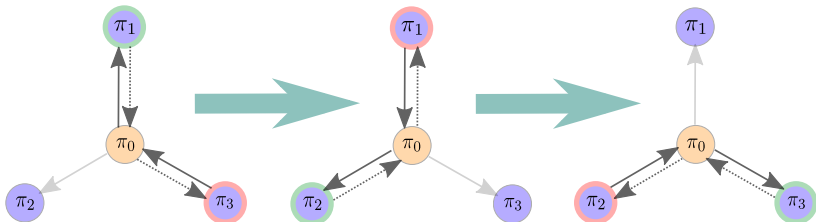


Figure 3: Illustration of a TreeDSB cycle over a star-shaped tree with 3 leaves.
After convergence

- | Fixed marginals are recovered.
- | The central node is the barycenter (for star-shaped trees).
 - Sampling: sample from a leaf and follow the edge.

Numerical experiments on MNIST dataset

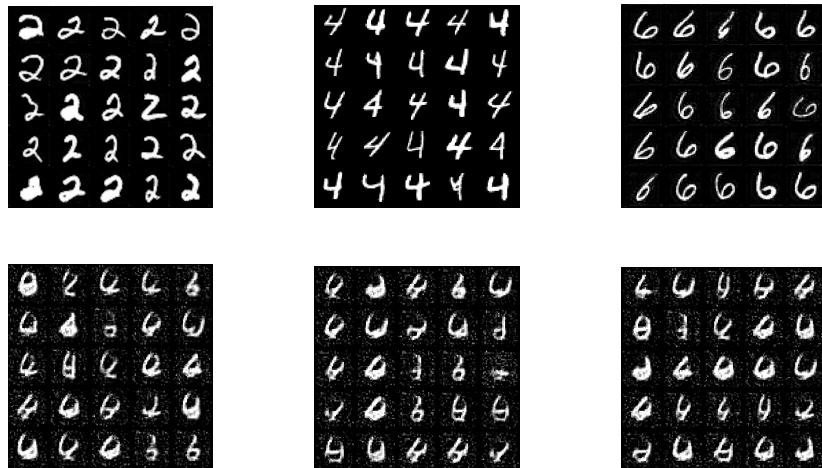


Figure 4: From left to right: estimated samples (*upper*) and estimated regularized Wasserstein barycenter samples (*bottom*) for MNIST digits 2,4 and 6.

- | Correspondence between **multi-marginal EOT** defined on general trees and **Schrödinger bridge** problems.
- | Algorithmic procedure to solve it: **TreeDSB**.
- | Application to **Wasserstein Barycenters**.
- | **Convergence** results & numerical experiments.

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Any questions ?

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- Martial Agueh and Guillaume Carlier. Barycenters in the Wasserstein space. *SIAM Journal on Mathematical Analysis*, 43(2):904–924, 2011.
- Jean-David Benamou, Guillaume Carlier, Marco Cuturi, Luca Nenna, and Gabriel Peyré. Iterative Bregman projections for regularized transportation problems. *SIAM Journal on Scientific Computing*, 37(2):A1111–A1138, 2015.
- Marco Cuturi and Arnaud Doucet. Fast computation of Wasserstein barycenters. In *International conference on machine learning*, pages 685–693. PMLR, 2014.
- Valentin De Bortoli, James Thornton, Jeremy Heng, and Arnaud Doucet. Diffusion Schrödinger bridge with applications to score-based generative modeling. *Advances in Neural Information Processing Systems*, 34:17695–17709, 2021.
- Jiaojiao Fan, Amirhossein Taghvaei, and Yongxin Chen. Scalable computations of Wasserstein barycenter via input convex neural networks. *arXiv preprint arXiv:2007.04462*, 2020.
- Isabel Haasler, Axel Ringh, Yongxin Chen, and Johan Karlsson. Multimarginal optimal transport with a tree-structured cost and the Schrödinger bridge problem. *SIAM Journal on Control and Optimization*, 59(4):2428–2453, 2021.
- Lingxiao Li, Aude Genevay, Mikhail Yurochkin, and Justin M Solomon. Continuous regularized Wasserstein barycenters. *Advances in Neural Information Processing Systems*, 33:17755–17765, 2020.
- Justin Solomon, Fernando De Goes, Gabriel Peyré, Marco Cuturi, Adrian Butscher, Andy Nguyen, Tao Du, and Leonidas Guibas. Convolutional Wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Transactions on Graphics (ToG)*, 34(4):1–11, 2015.
- Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. *International Conference on Learning Representations*, 2021.