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

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

When c is quadratic:

EOT (*static*) $\Longleftrightarrow$ Schrödinger Bridge (SB) problem (*dynamic*)

Algorithm: Diffusion 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.

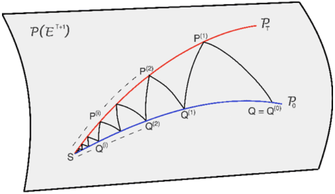

Figure 1: Iterations of DSB.

Extension to the multi-marginal setting

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

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

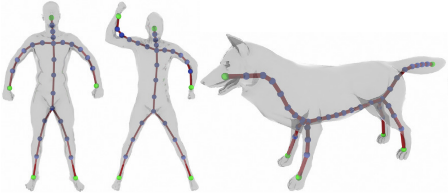

Figure 2: Trees from Solomon et al. (2015).

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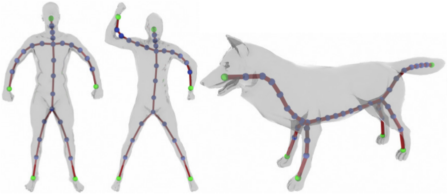

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Case of interest: Wasserstein-2 barycenter (Agueh and Carlier, 2011)
$\Longrightarrow$ Quadratic cost c & Star-shaped tree

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 → **Tree SB**.
- Iterative DSB-like procedure → **TreeDSB**.

$\Longrightarrow$ **Dynamically solve a tree-based formulation of EOT**.

💡 TreeDSB updates only occur on paths between the leaves.

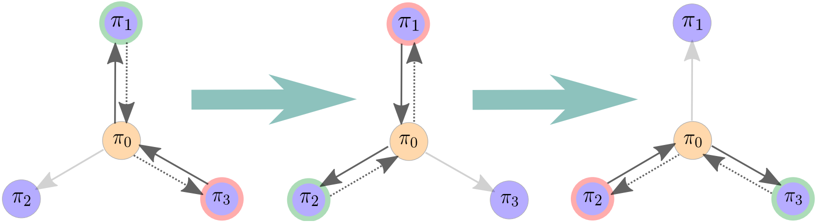

Figure 3: Illustration of a TreeDSB cycle over a star-shaped tree with 3 leaves.

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

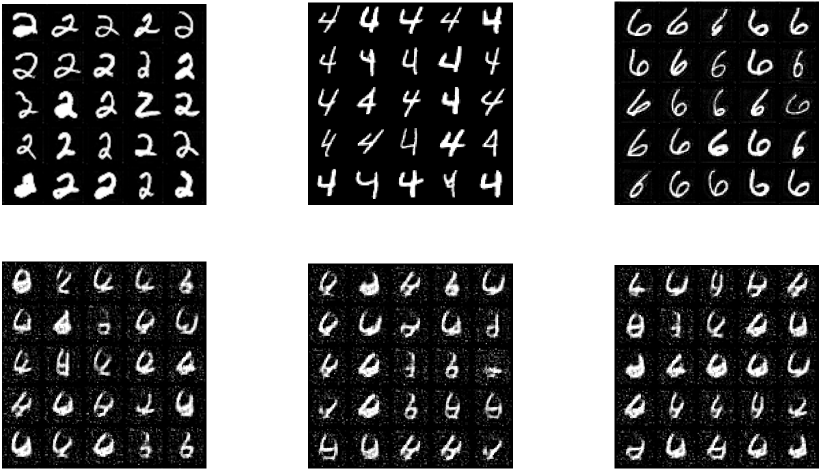

Figure 4: From left to right: estimated samples (*upper*) and estimated regularized Wasserstein barycenter samples (*bottom*) for MNIST digits 2,4 and 6.

- 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.