Progressive Entropic Optimal Transport

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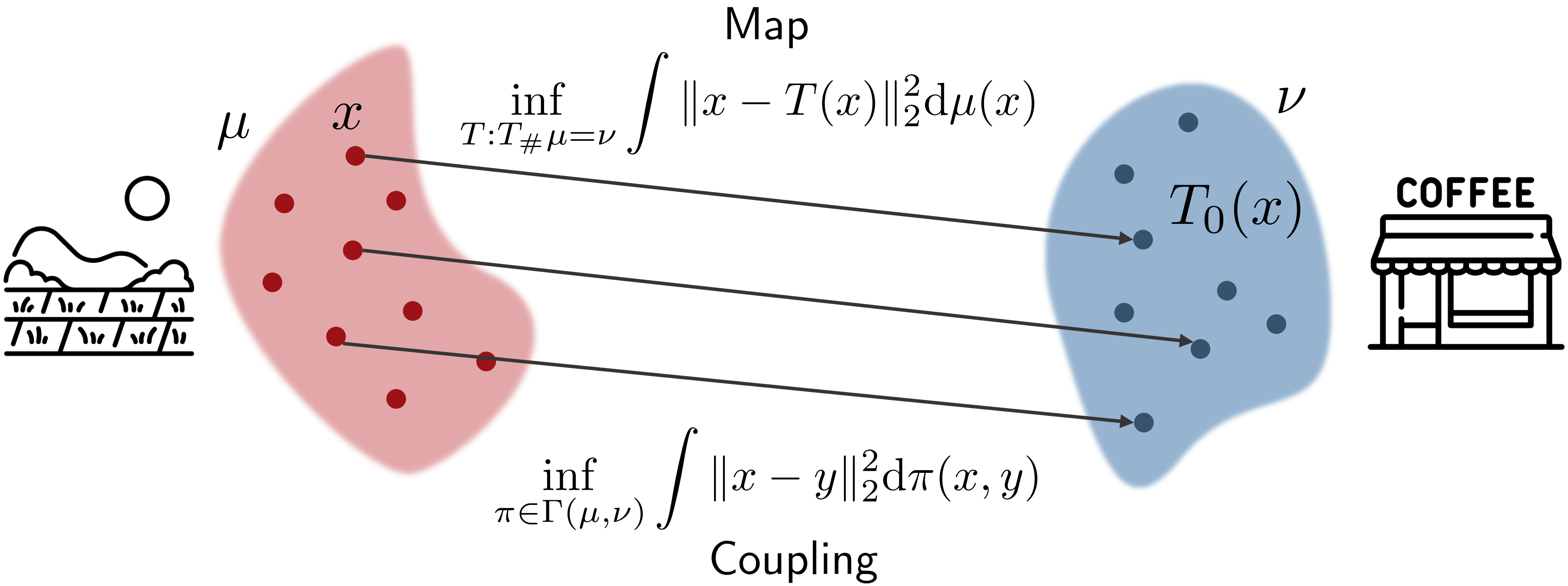
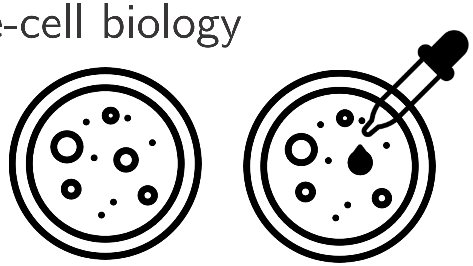
Optimal Transport

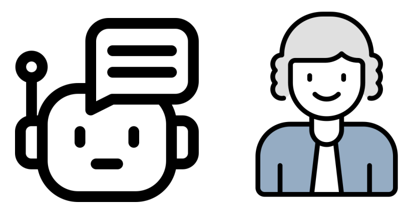


Single-cell biology



[1, 2]

RL/Alignment



[3, 4, 5, 6]

[Figures from flaticon.com]

How do you solve it?

In full generality, OT does not have a solution or is very tough to solve.

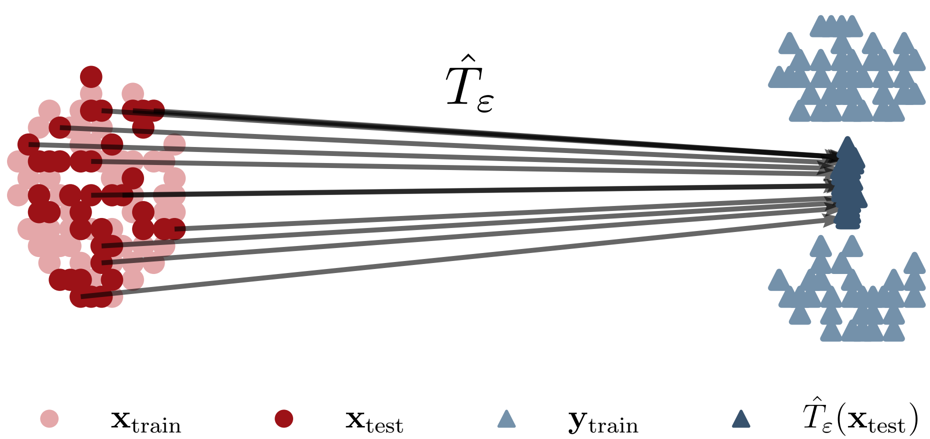
Entropic OT adds a regularization term to make things better:

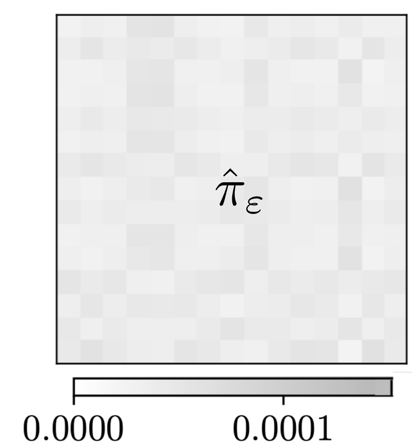
$$\inf_{\pi \in \Gamma(\nu,\mu)} \int \|x-y\|_2^2 \, \mathrm{d}\pi(x,y) + \varepsilon \, \mathrm{D}_{\mathrm{KL}} \left(\pi || \mu \otimes \nu\right)$$

Given $\hat{\mu}$, $\hat{\nu}$: Sinkhorn's algorithm can solve this and return $\hat{T}_\varepsilon$ and $\hat{\pi}_\varepsilon$

Small ε: the algorithm may not converge

Large ε:

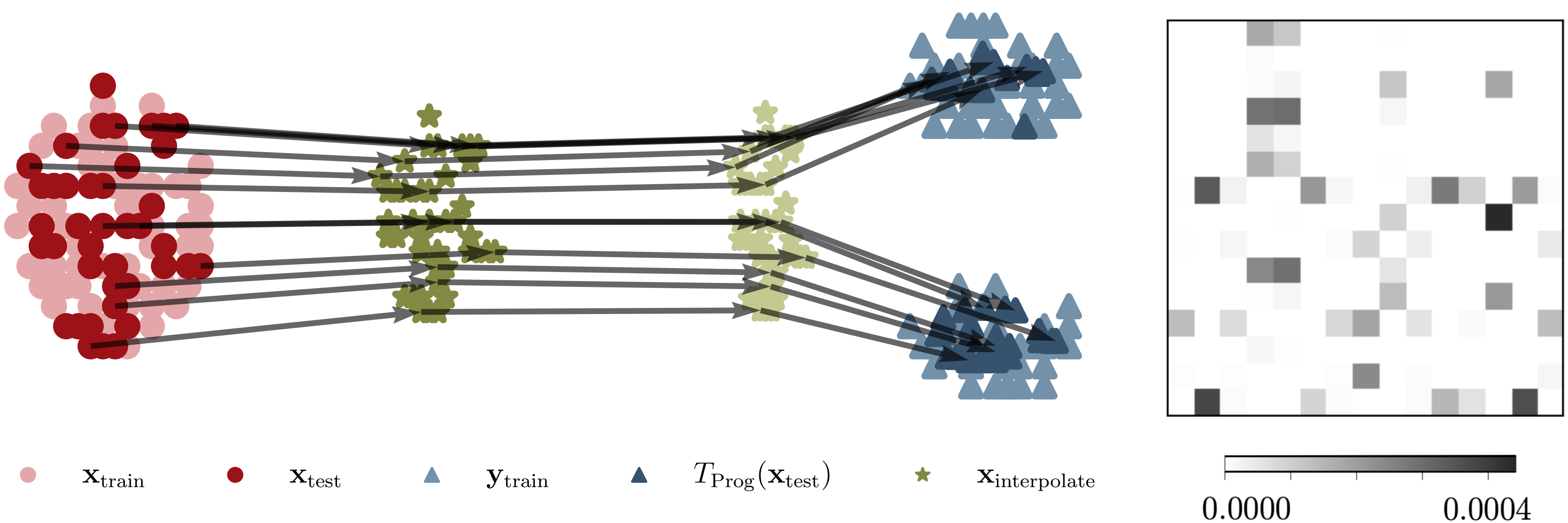




Our solution: ProgOT

Blend the static OT problem with the dynamic perspective.

Solve a series of EOT problems, with reduced sensitivity to ε



- Elevates issue of regularization parameter
- Convergences to the ground truth (statistical guarantee)
- Competitive performance, scalable, and computationally light

ProgOT algorithm

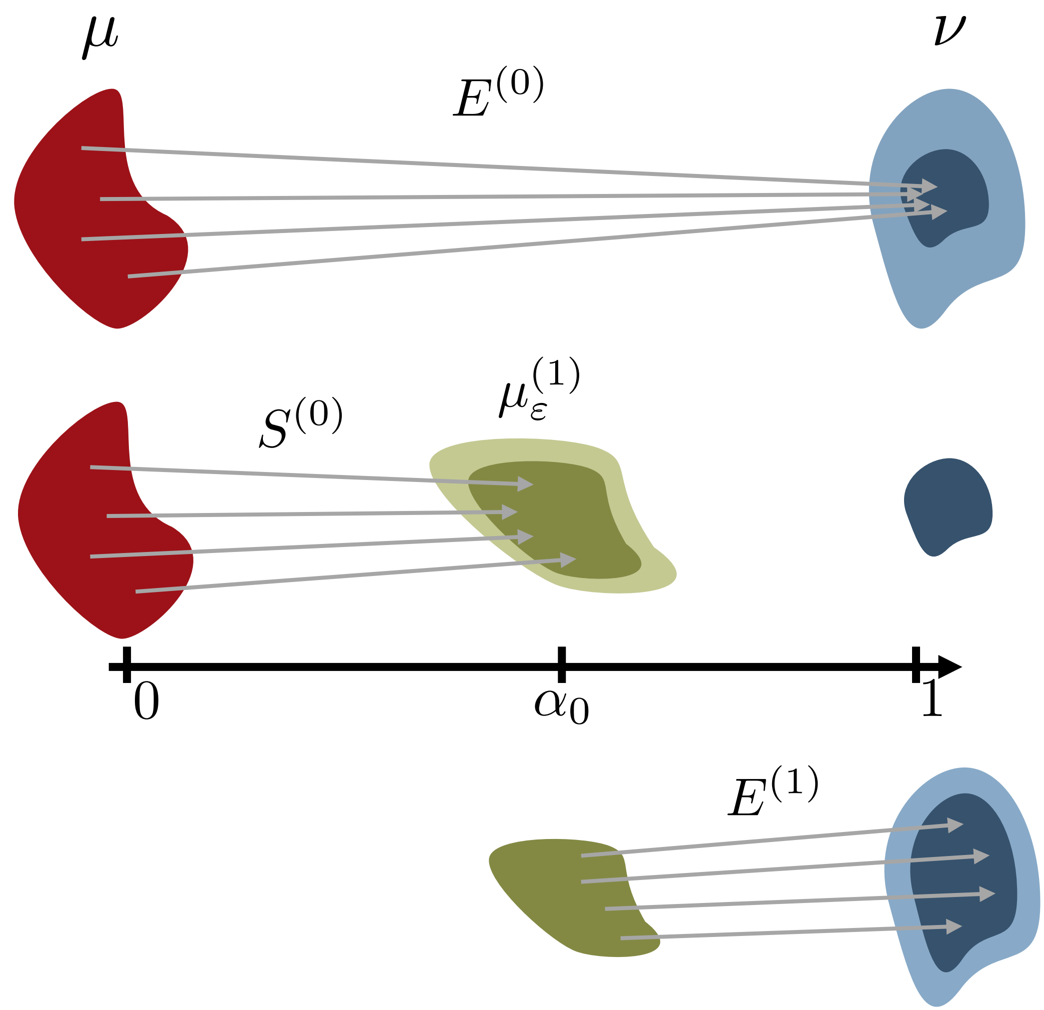
Solve Entropic OT with large ε_0

Linearly Interpolate

$$\mu_\varepsilon^{(1)} = \left[(1-\alpha_0)\mathrm{Id} + \alpha_0 E^{(0)}\right]_\# \mu$$

Reduce ε_1 and repeat

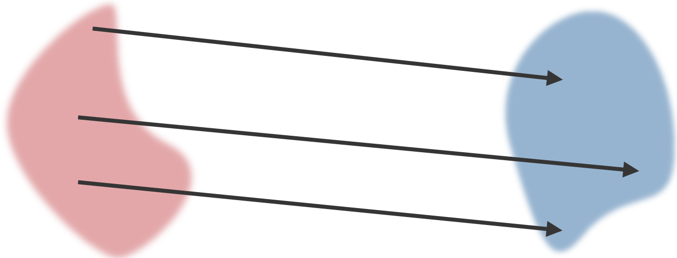
$$T_{\mathrm{Prog}}^{(1)} = E^{(1)} \circ S^{(0)}$$



We can repeat this K times to get $T_{\mathrm{Prog}}^{(K)}$

Theoretical guarantee

T_0: OT map between μ & ν



$T^{(K)}_{\mathrm{Prog}}$: ProgOT map between $\hat{\mu}_n$ & $\hat{\nu}_n$

Theorem (Non-Asymptotic Consistency)

Given n i.i.d. samples from μ and ν, for an appropriate choice of $(\varepsilon_k)_k$ and $(\alpha_k)_k$, the K-step progressive map $T^{(K)}_{Prog}$ satisfies

$$\mathbb{E}\left\| T^{(k)}_{Prog} - T_0 \right\|^2_{L^2(\mu)} \lesssim n^{\boxed{-\frac{1}{d}}},$$

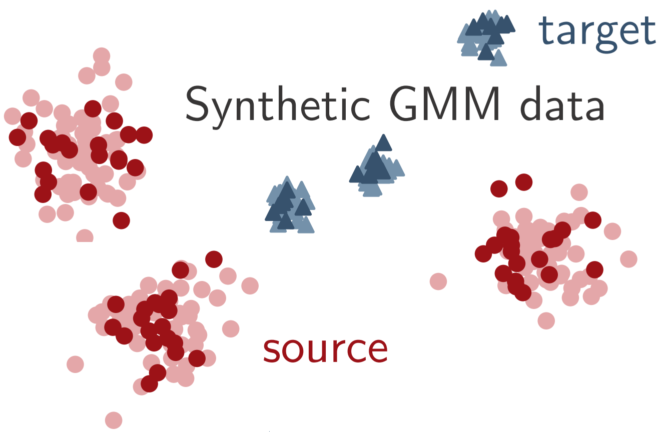
Independent of K!

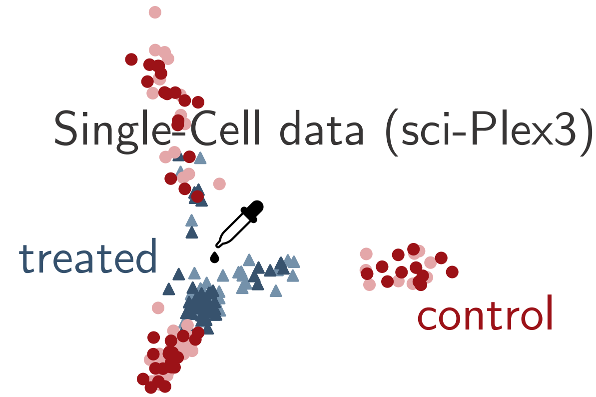
under regularity assumptions on μ, ν, and the true map T_0.

Proof idea: The intermediate steps of ProgOT are on the Wasserstein geodesic.

Map estimation

ProgOT outperforms other map estimators, including neural ones.





	$d = 128$	$d = 256$
ProgOT	**0.099**±0.009	**0.12**±0.01
EOT	0.12±0.01	0.16±0.02
Debiased EOT	0.11±0.01	0.128±0.002
Untuned EOT	0.250±0.023	0.276±0.006
Monge Gap	0.36±0.02	0.273±0.005
ICNN	0.177±0.023	0.117±0.005

Drug	Hesperadin			5-drug rank
d_{PCA}	16	64	256	
ProgOT	**3.7**±0.4	**10.1**±0.4	**23.1**±0.4	**1**
EOT	4.1±0.4	10.4±0.5	26±1.3	2
Debiased EOT	4.0±0.5	15.2±0.6	41±1.1	4
Monge Gap	3.7±0.5	11.0±0.5	36±1.1	3
ICNN	3.9±0.4	14.3±0.5	46±2	5

Ground truth is known: MSE between the maps over test points

SinkDiv between the predicted target and the test target point cloud

[more in the paper]

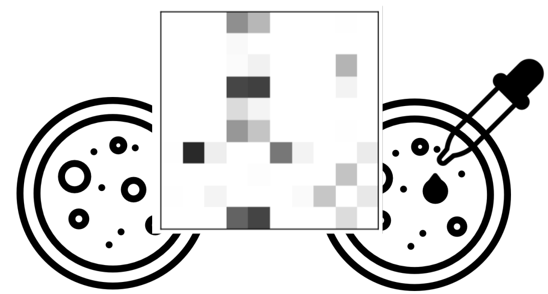
Coupling recovery

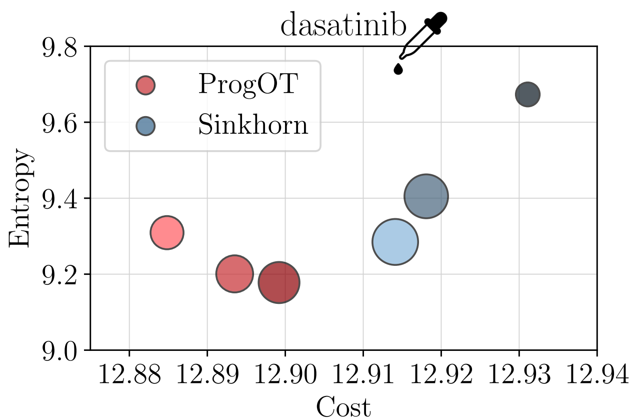
ProgOT attains lower OT cost and lower entropy, at a lower computational cost.

$$\text{Cost} = \sum_{i,j \in [n]} \hat{\pi}_{i,j} h(x_i - y_j)$$

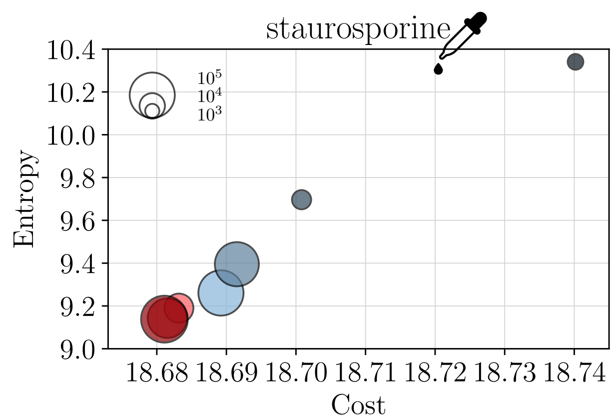
$$\text{Entropy} = \sum_{i,j \in [n]} -\hat{\pi}_{i,j} \log \hat{\pi}_{i,j}$$

Single-Cell data (4i)

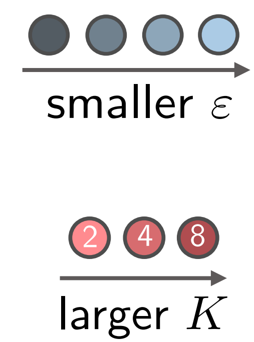




$$h(\cdot) = \frac{1}{2}\|\cdot\|_2^2$$



$$h(\cdot) = \frac{1}{1.5}\|\cdot\|_{1.5}^{1.5}$$



[more in the paper]

The bigger picture

ProgOT

- Light, off-the-shelf, competitive baseline
- Blending static and dynamic views of OT
- [paper], [JAX tutorial]

Follow-ups

- Scaling Limit
- Continuous time extension/implications

OT Applications

- Unbalanced OT
- The Schrödinger Bridge

Other Applications

- Drug purtubations
- Robust generation
- Preference Learning

Thank You

References

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