On amortizing convex conjugates for optimal transport

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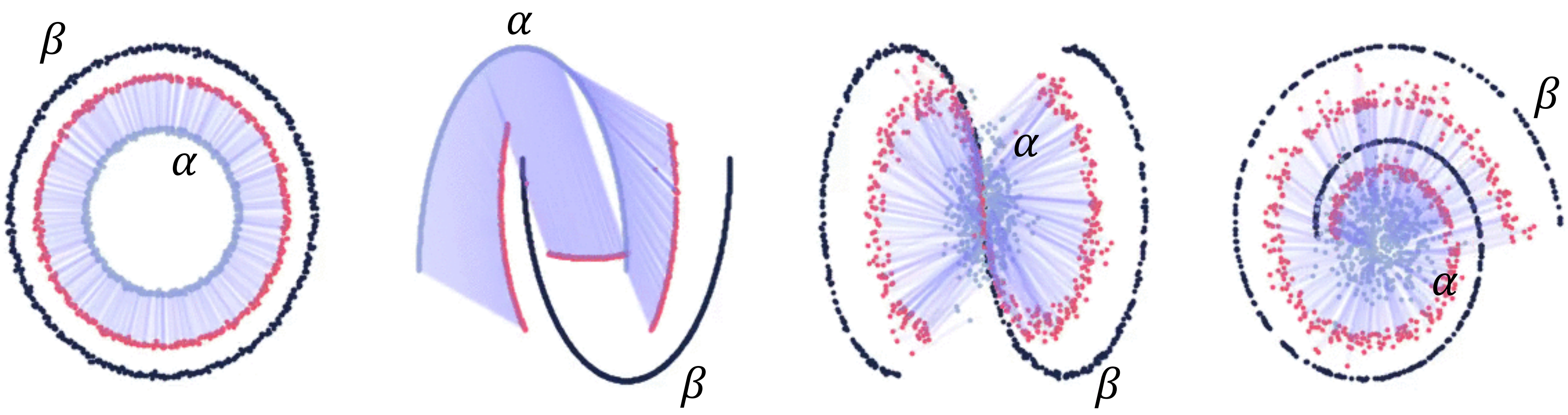
http://github.com/bamos/presentations
http://github.com/facebookresearch/w2ot

Optimal transport connects spaces

Monge (primal)

$$T^\star(\alpha,\beta) \in \underset{T\in\mathcal{C}(\alpha,\beta)}{\operatorname{argmin}} \mathbb{E}_{x\sim\alpha} \|x - T(x)\|_2^2$$

α, β are **measures**
$\mathcal{C}(\alpha,\beta)$ is the set of valid **coupling**
T is a **transport map** from α to β



Duality and continuous OT

Monge (primal)

$$T^\star(\alpha,\beta) \in \underset{T\in\mathcal{C}(\alpha,\beta)}{\operatorname{argmin}} \mathbb{E}_{x\sim\alpha}\|x - T(x)\|_2^2$$

$$\Updownarrow \quad T^\star = \nabla \hat{f}$$ (Brenier's Theorem)

Kantorovich (dual)

$$\hat{f} \in \underset{f\in\mathcal{L}^1(\alpha)}{\operatorname{argmax}} \; -\mathbb{E}_{x\sim\alpha}[f(x)] - \mathbb{E}_{y\sim\beta}[f^\star(y)]$$

$$f^\star(y) := -\inf_{x\in\mathcal{X}} J_f(x;y) \quad \text{with objective} \quad J_f(x;y) := f(x) - \langle x, y\rangle$$

Solving Kantorovich's dual with a neural net

$$\max_\theta \mathcal{V}(\theta) \quad \text{where} \quad \mathcal{V}(\theta) := -\mathop{\mathbb{E}}_{x\sim\alpha}[f_\theta(x)] - \mathop{\mathbb{E}}_{y\sim\beta}[f_\theta^\star(y)]$$

2-wasserstein approximation via restricted convex potentials. Taghvaei and Jalali, 2019.
Three-Player Wasserstein GAN via Amortised Duality. Nhan Dam et al., IJCAI 2019.
Optimal transport mapping via input convex neural networks. Makkuva et al., ICML 2020.
Wasserstein-2 generative networks. Korotin et al., ICLR 2020.

Focus: computing the conjugate

$$\max_\theta \mathcal{V}(\theta) \quad \text{where} \quad \mathcal{V}(\theta) := -\mathop{\mathbb{E}}_{x\sim\alpha}[f_\theta(x)] - \boxed{\mathop{\mathbb{E}}_{y\sim\beta}[f_\theta^\star(y)]}$$

$$\overbrace{f^\star(y) := -\inf_{x\in\mathcal{X}} J_f(x;y) \quad \text{with objective} \quad J_f(x;y) := f(x) - \langle x, y\rangle}$$

Amortization: Approximate the arginf with (another) neural network

2-wasserstein approximation via restricted convex potentials. Taghvaei and Jalali, 2019.
Three-Player Wasserstein GAN via Amortised Duality. Nhan Dam et al., IJCAI 2019.
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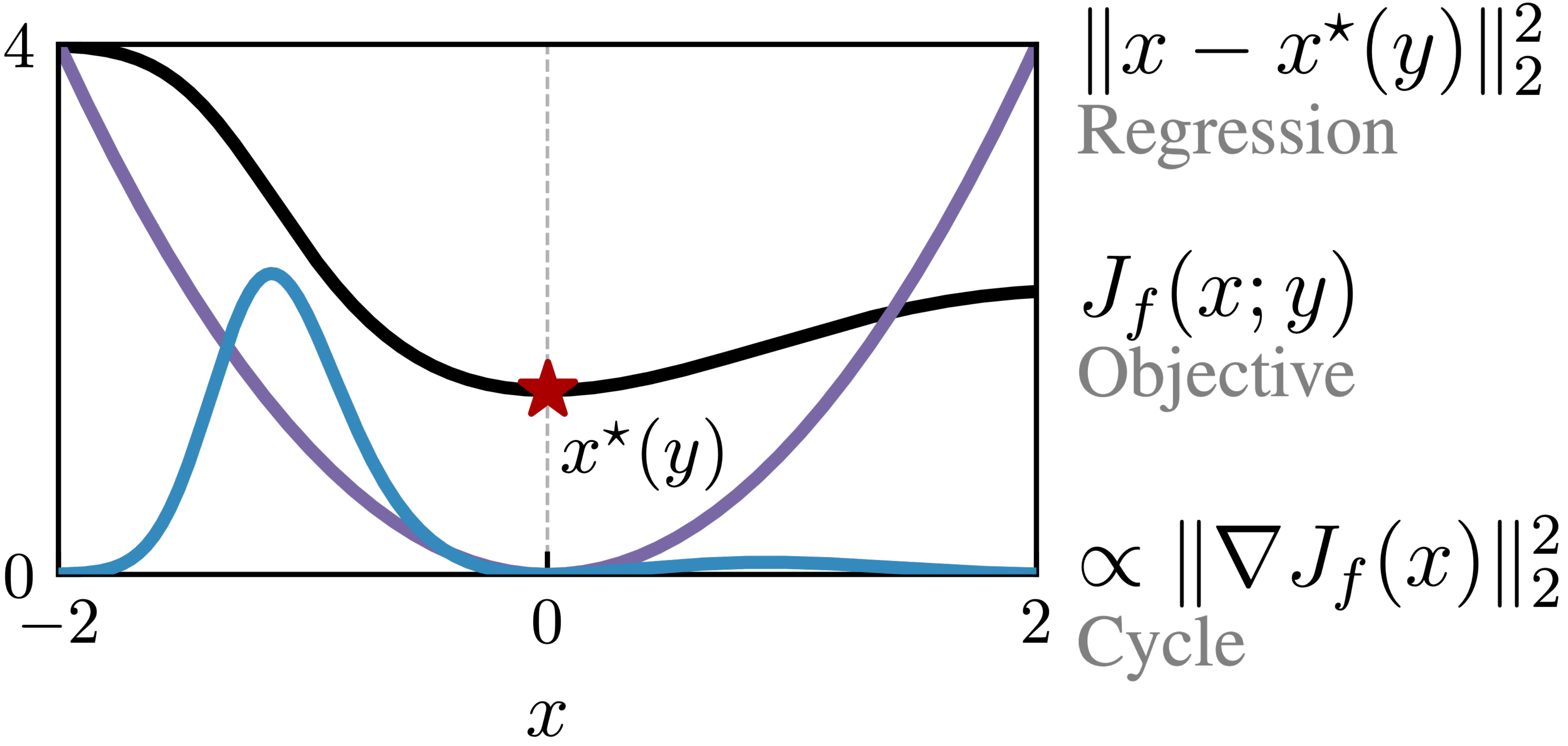
Conjugate amortization loss choices



Wasserstein-2 benchmark results

Do Neural Optimal Transport Solvers Work? Korotin et al., NeurIPS 2021.

Takeaway: amortization choice important, fine-tuning significantly helps

HD benchmarks: Unexplained Variance Percentage (UVP, lower is better)

Baselines from Korotin et al. (2021a)

	Amortization loss	Conjugate solver	$n = 2$	$n = 4$	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
*[W2]	Cycle	None	0.1	0.7	2.6	3.3	6.0	7.2	2.0	2.7
*[MMv1]	None	Adam	0.2	1.0	1.8	1.4	6.9	8.1	2.2	2.6
*[MMv2]	Objective	None	0.1	0.68	2.2	3.1	5.3	10.1	3.2	2.7
*[MM]	Objective	None	0.1	0.3	0.9	2.2	4.2	3.2	3.1	4.1

Potential model: the input convex neural network described in app. B.3 **Amortization model:** the MLP described in app. B.2

Amortization loss	Conjugate solver	$n = 2$	$n = 4$	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
Cycle	None	0.28 ±0.09	0.90 ±0.11	2.23 ±0.20	3.03 ±0.06	5.32 ±0.14	8.79 ±0.16	5.66 ±0.45	4.34 ±0.14
Objective	None	0.27 ±0.09	0.78 ±0.12	1.78 ±0.26	2.00 ±0.11	>100	>100	>100	>100
Cycle	L-BFGS	0.26 ±0.09	0.77 ±0.11	1.63 ±0.28	1.15 ±0.14	2.02 ±0.10	4.48 ±0.89	1.65 ±0.10	5.93 ±9.43
Objective	L-BFGS	0.26 ±0.09	0.79 ±0.12	1.63 ±0.30	1.12 ±0.11	1.92 ±0.19	4.40 ±0.79	1.64 ±0.11	2.24 ±0.13
Regression	L-BFGS	0.26 ±0.09	0.78 ±0.12	1.64 ±0.29	1.14 ±0.12	1.93 ±0.20	4.41 ±0.74	1.69 ±0.11	2.21 ±0.15
Cycle	Adam	0.26 ±0.09	0.79 ±0.11	1.62 ±0.29	1.14 ±0.12	1.95 ±0.21	4.55 ±0.62	1.88 ±0.26	>100
Objective	Adam	0.26 ±0.09	0.79 ±0.14	1.62 ±0.31	1.08 ±0.14	1.89 ±0.19	4.23 ±0.76	1.59 ±0.12	1.99 ±0.15
Regression	Adam	0.35 ±0.07	0.81 ±0.12	1.61 ±0.32	1.09 ±0.11	1.85 ±0.20	4.42 ±0.68	1.63 ±0.08	1.99 ±0.16

Potential model: the non-convex neural network (MLP) described in app. B.4 **Amortization model:** the MLP described in app. B.2

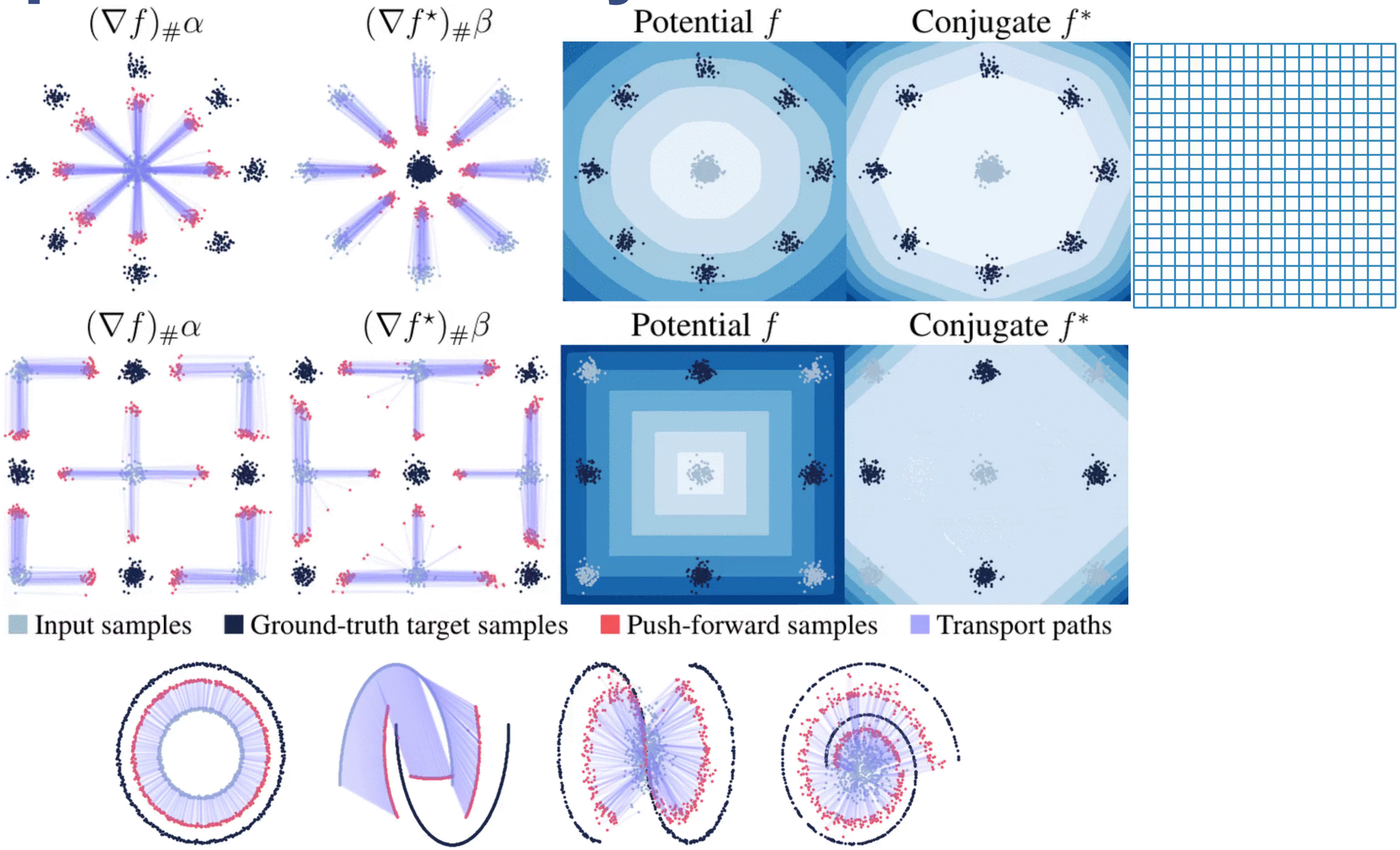
Amortization loss	Conjugate solver	$n = 2$	$n = 4$	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$	$n = 256$
Cycle	None	0.05 ±0.00	0.35 ±0.01	1.51 ±0.08	>100	>100	>100	>100	>100
Objective	None	>100	>100	>100	>100	>100	>100	>100	>100
Cycle	L-BFGS	>100	>100	>100	>100	>100	>100	>100	>100
Objective	L-BFGS	0.03 ±0.00	0.22 ±0.01	0.60 ±0.03	0.80 ±0.11	2.09 ±0.31	2.08 ±0.40	0.67 ±0.05	0.59 ±0.04
Regression	L-BFGS	0.03 ±0.00	0.22 ±0.01	0.61 ±0.04	0.77 ±0.10	1.97 ±0.38	2.08 ±0.39	0.67 ±0.05	0.65 ±0.07
Cycle	Adam	0.18 ±0.03	0.69 ±0.56	1.62 ±2.82	>100	>100	>100	>100	>100
Objective	Adam	0.06 ±0.01	0.26 ±0.02	0.63 ±0.07	0.81 ±0.10	1.99 ±0.32	2.21 ±0.32	0.77 ±0.05	0.66 ±0.07
Regression	Adam	0.22 ±0.01	0.28 ±0.02	0.61 ±0.07	0.80 ±0.10	2.07 ±0.38	2.37 ±0.46	0.77 ±0.06	0.75 ±0.09
Improvement factor over prior work		**3.3**	**3.1**	**3.0**	**1.8**	**2.7**	**1.5**	**3.0**	**4.4**

CelebA benchmarks: UVP

	Amortization loss	Conjugate solver	Potential Model	Early Generator	Mid Generator	Late Generator
*[W2]	Cycle	None	ConvICNN64	1.7	0.5	0.25
*[MM]	Objective	None	ResNet	2.2	0.9	0.53
*[MM-R†]	Objective	None	ResNet	1.4	0.4	0.22
	Cycle	None	ConvNet	>100	26.50 ±60.14	0.29 ±0.59
	Objective	None	ConvNet	>100	0.29 ±0.15	0.69 ±0.90
	Cycle	Adam	ConvNet	0.65 ±0.02	0.21 ±0.00	0.11 ±0.04
	Cycle	L-BFGS	ConvNet	0.62 ±0.01	0.20 ±0.00	0.09 ±0.00
	Objective	Adam	ConvNet	0.65 ±0.02	0.21 ±0.00	0.11 ±0.05
	Objective	L-BFGS	ConvNet	0.61 ±0.01	0.20 ±0.00	0.09 ±0.00
	Regression	Adam	ConvNet	0.66 ±0.01	0.21 ±0.00	0.12 ±0.00
	Regression	L-BFGS	ConvNet	0.62 ±0.01	0.20 ±0.00	0.09 ±0.01
		Improvement factor over prior work		**2.3**	**2.0**	**2.4**

† the *reversed* direction from Korotin et al. (2021a), i.e. the potential model is associated with the β measure

Transport between synthetic measures



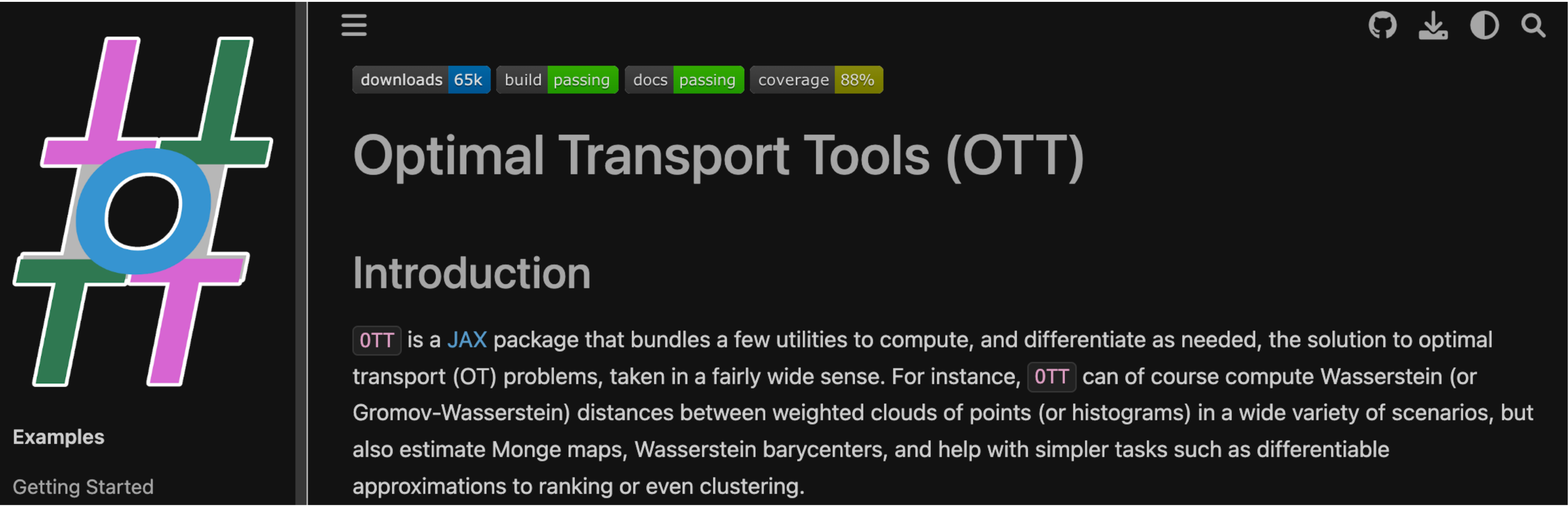
Learning flows via continuous OT

Continuous OT for flows:

1. Works **only from samples** (no likelihoods needed)
2. No need to explicitly enforce invertibility
3. No need to compute the log-det of the Jacobian

$$p_Y(y) = p_X(f^{-1}(y)) \left| \frac{\partial f^{-1}(y)}{\partial y} \right|$$

github.com/ott-jax/ott



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Optimal Transport Tools (OTT)

Introduction

`OTT` is a JAX package that bundles a few utilities to compute, and differentiate as needed, the solution to optimal transport (OT) problems, taken in a fairly wide sense. For instance, `OTT` can of course compute Wasserstein (or Gromov-Wasserstein) distances between weighted clouds of points (or histograms) in a wide variety of scenarios, but also estimate Monge maps, Wasserstein barycenters, and help with simpler tasks such as differentiable approximations to ranking or even clustering.

Examples

Getting Started

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