GENEVA SCHOOL OF ECONOMICS AND MANAGEMENT

UNIVERSITÉ DE GENÈVE

Theoretical and computational aspects of robust optimal transportation, with applications to **statistics** and machine learning

Davide La Vecchia
(with Y. Ma, H. Liu & M. Lerasle)

London, Aug-2023

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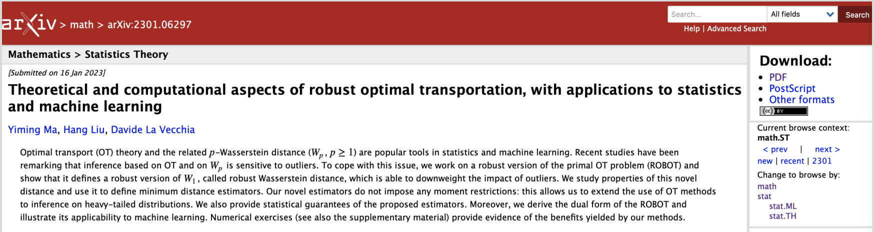

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[Submitted on 16 Jan 2023]

Theoretical and computational aspects of robust optimal transportation, with applications to statistics and machine learning

Yiming Ma, Hang Liu, Davide La Vecchia

Optimal transport (OT) theory and the related p-Wasserstein distance (W_p, $p \geq 1$) are popular tools in statistics and machine learning. Recent studies have been remarking that inference based on OT and on W_p is sensitive to outliers. To cope with this issue, we work on a robust version of the primal OT problem (ROBOT) and show that it defines a robust version of W_1, called robust Wasserstein distance, which is able to downweight the impact of outliers. We study properties of this novel distance and use it to define minimum distance estimators. Our novel estimators do not impose any moment restrictions: this allows us to extend the use of OT methods to inference on heavy-tailed distributions. We also provide statistical guarantees of the proposed estimators. Moreover, we derive the dual form of the ROBOT and illustrate its applicability to machine learning. Numerical exercises (see also the supplementary material) provide evidence of the benefits yielded by our methods.

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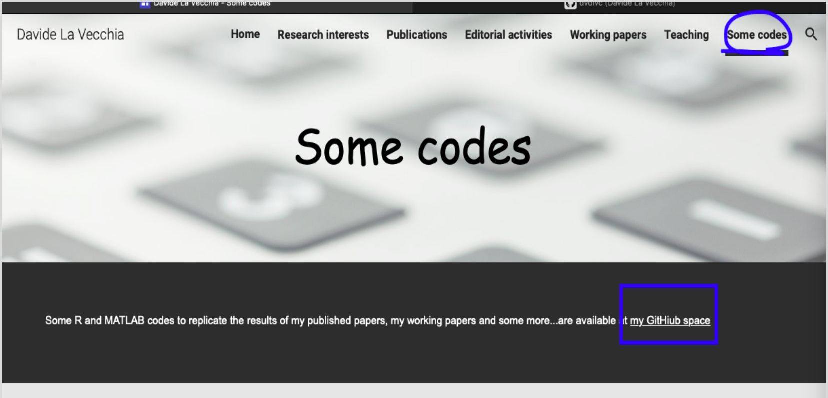

Outline

- A few words about Monge-Kantorovich OT problem and the related Wasserstein distance $\{W_p, p \geq 1\}$
- Motivation: robustness issues of $\{W_p, p \geq 1\}$
- Our solution:
  - Robust OT (ROBOT) and Robust Wasserstein distance $\{W^{(\lambda)}, \lambda > 0\}$
  - Minimum Robust Wasserstein distance estimation
  - Implementation aspects and statistical guarantees
- Synthetic data examples
- Take home message

A few words about Monge-Kantorovich OT problem

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Let α *and* β *denote two probability measures over (for simplicity)* $(\mathbb{R}^d, \mathcal{B}^d)$, *for* $d \geq 1$. *Let* $c : \mathbb{R}^{2d} \to \mathbb{R}$ *be a Borel-measurable cost function such that* $c(x, y)$ *represents the cost of transporting* x *to* y. *Then, find a measurable transport map* $\mathcal{T} : \mathbb{R}^d \to \mathbb{R}^d$ *that achieves*

$$\inf_{\mathcal{T} \in M} \int_{\mathbb{R}^d} c[x, \mathcal{T}(x)] \, \mathrm{d}\alpha \tag{1}$$

where

$$M := \{\mathcal{T} : X \to Y\},$$

with $X \sim \alpha$, $Y \sim \beta$. *The map* $\mathcal{T}\#\alpha = \beta$ *does the push forward of* α *to* β.

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$\Rightarrow$ The map solution to (1) is called the optimal transportation map.

Monge's problem remained open until the 1940s, when it was revisited by **Leonid Vitaliyevitch Kantorovich** (1912-1986; Nobel Prize in Economics in 1975) for the economic problem of optimal allocation of resources; see e.g. Villani (2008), Santambrogio (2015), Galichon (2016).

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In the Kantorovich primal problem, the objective is to find the optimal transportation plan γ, which solves

$$\inf_{\gamma\in\Gamma(\alpha,\beta)} \int_{\mathbb{R}^d\times\mathbb{R}^d} c(x,y)\,\mathrm{d}\gamma(x,y), \tag{2}$$

where the infimum is over all coupling (X, Y) of (α, β), belonging to $\Gamma(\alpha, \beta)$, the set of probability measures γ on $\mathbb{R}^d \times \mathbb{R}^d$, satisfying

$$\boxed{\gamma(A\times\mathbb{R}^d) = \alpha(A) \text{ and } \gamma(\mathbb{R}^d\times B) = \beta(B),}$$

for measurable sets $A, B \subset \mathbb{R}^d$:

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for measurable sets $A, B \subset \mathbb{R}^d$: **we impose exact marginal constraints!**

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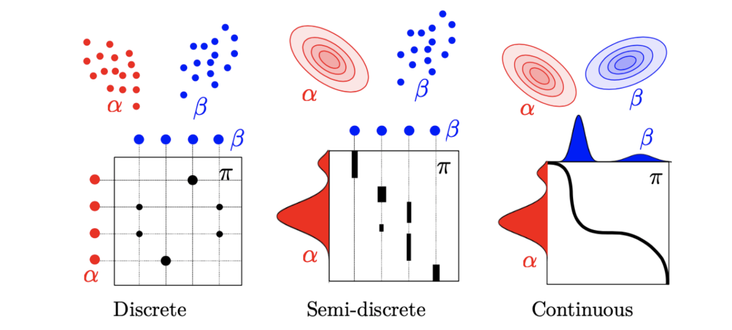
Remark

Solving the optimal transport problem (2) with $c = d^p$, introduces a distance between α and β:

$$W_p(\alpha,\beta) = \left(\inf_{\gamma \in \Gamma(\alpha,\beta)} \int d^p(x,y) \, \mathrm{d}\gamma(x,y) \right)^{1/p}, \tag{3}$$

which is the Wasserstein distance of order p ($p \geq 1$): W_1 and W_2 are widely-applied in many scientific areas.

We can make use of this theory to transport different types of measures, as depicted in Peyré & Cuturi (2019)



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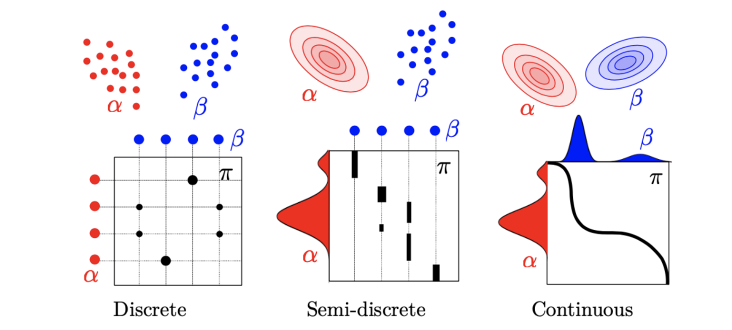

Some examples:

- PDEs: Jacoby equation, Monge-Ampére equation
- Differential geometry: geodesic, curvature, exponential mapping
- Machine learning (ML) and computer science: image processing, adversarial learning
- Statistics: Wasserstein distance based procedures

Motivation

The ability to lift the ground distance d^p is one of the perks of W_p and it makes it a suitable tool in statistics and ML. Interestingly, this desirable feature becomes a negative aspect as far as robustness is concerned.

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Example (Robustness issues and a preview of the solution)

Given two measure μ (original) and ν (target), OT embeds the distributions geometry: when the underlying distribution is contaminated by outliers, **the marginal constraints force OT** to transport outlying values, inducing an undesirable extra cost, which entails large changes in W_p.

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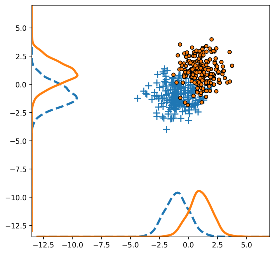

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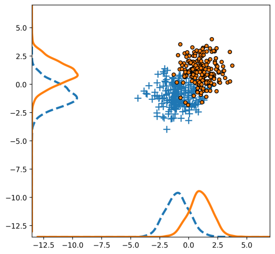

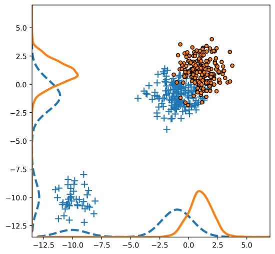

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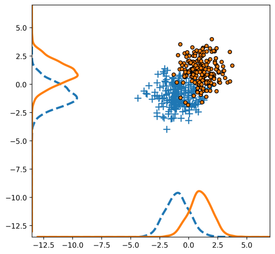

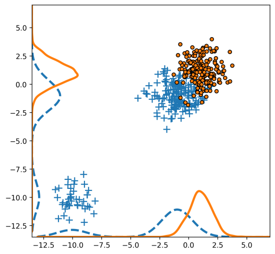

$W_1 = 3.00,\ W_2 = 3.02,\ W^{(\lambda)} = 2.93$ $\qquad$ $W_1 = 5.32,\ W_2 = 6.62$ and $W^{(\lambda)} = 3.31$

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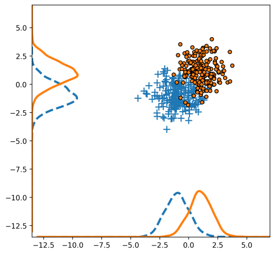

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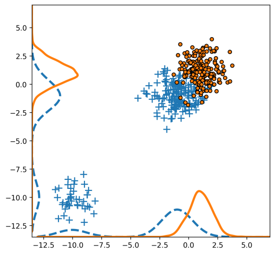

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where $\lambda = 3$. Let's meet $W^{(\lambda)}$...

Our solution: a quick look

Robust OT (ROBOT) problem is defined in Mukherjee et al. (2021):

$$\underbrace{\min_{\gamma,s} \int \boxed{c(x,y)}\, \gamma(x,y)\mathrm{d}x\mathrm{d}y}_{\text{standard OT}} + \underbrace{\lambda \|s\|_{\mathrm{TV}}}_{\text{penalization}}$$

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where $\lambda > 0$ is a **regularization parameter**, which controls for the role of s. The latter introduces a modification of the measure μ:

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Remark

Mukherjee et al. (2021) prove that solving (4) *is equivalent to*

$$\inf \left\{ \int \boxed{c_\lambda(x,y)})\mathrm{d}\gamma(x,y) : \gamma \in \Gamma(\mu,\nu) \right\}, \tag{5}$$

which is similar to the original OT problem, but the cost function $c(x,y) = d(x,y)$ *is replaced by* $\boxed{c_\lambda = \min\{c, 2\lambda\}}$ *that is bounded from above by* 2λ.

We prove that, similarly to OT, for $c_\lambda(x, y)$,

$$W^{(\lambda)}(\mu, \nu) := \inf_{\gamma \in \Gamma(\mu,\nu)} \left\{ \int c_\lambda(x, y) \, \mathrm{d}\gamma(x, y) \right\} \tag{6}$$

is the Robust Wasserstein distance and it is such that, if $W_1(\mu, \nu)$ exists, we have

$$\lim_{\lambda \to \infty} W^{(\lambda)}(\mu, \nu) = W_1(\mu, \nu).$$

Given a class of parametric models $\{\mu_\theta, \theta \in \Theta \subset \mathbb{R}^k\}$, to this distance, we associate the *minimum robust Wasserstein estimator* (MRWE)

$$\hat{\theta}_n^\lambda = \operatorname*{argmin}_{\theta \in \Theta} \underbrace{W^{(\lambda)}(\mu_\theta, \hat{\mu}_n)}_{\text{loss function}},$$

where $\hat{\mu}_n$ is the empirical measure.

Remark

- *Computational aspects: As discussed in Bernton et al. 2019 for minimizing W_p, typically there is no explicit expression for the probability measure characterizing the parametric model (e.g. in complex generative models) and for $W^{(\lambda)}$.*

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$$\hat{\theta}^{\lambda}_{n,m} = \underset{\theta \in \Theta}{\operatorname{argmin}} \ \mathrm{E}_m \left[W^{(\lambda)} \left(\hat{\mu}_{\theta,m}, \hat{\mu}_n, \right) \right], \tag{7}$$

where the expectation $\mathrm{E}_m[\cdot]$ is taken over the distribution $\mu_\theta^{(m)}$, which represents the measure of a m-dimensional sample simulated from μ_θ.

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- *Statistical guarantees: Intuitively, the* **consistency** *can be conceptualized as follows. The empirical measure converges to $\mu_\star$: $W^{(\lambda)}(\hat{\mu}_n, \mu_\star) \to 0$ as $n \to \infty$. Therefore, the* arg min *of $W^{(\lambda)}(\hat{\mu}_n, \mu_\star)$ converges to the* arg min *of $W^{(\lambda)}(\mu_\star, \mu_\theta)$, which is denoted by $\theta_\star$. The same can be said for the minimum of the MERWE, provided that $m \to \infty$.*

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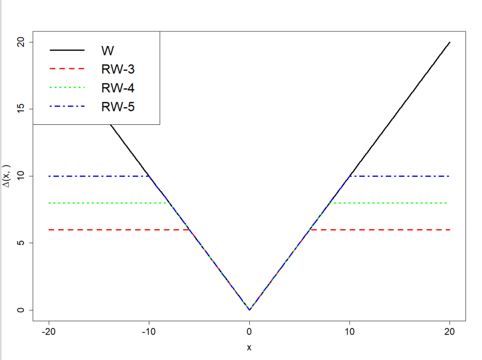
As far as robustness is concerned, plotting the loss function $W^{(\lambda)}$ and W_1 yields



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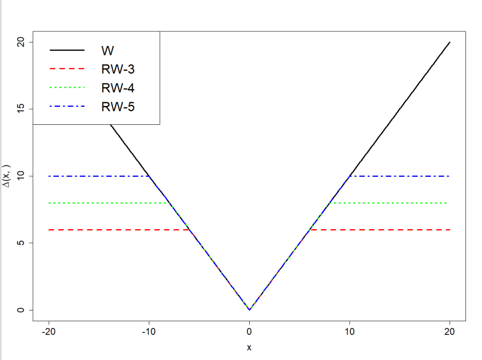

Remark

The cost c_λ determines, in the language of robust statistics, the so-called "hard rejection": it bounds the influence of outlying values (to be contrasted with the behavior of Huber loss, which downweights outliers to preserve efficiency at the reference model); see Ronchetti (2022).

Using **synthetic data**, we illustrate the performance of MERWE considering the problem of estimation of a (location) parameter in the univariate setting. Specifically, we study the following settings:

- Finite moments (sum of log-normal r.v.s, with and w/o ε of contamination), for different sample sizes
- Infinite moments of different order (symmetric α-stable r.v.s with different values of α, with and w/o ε of contamination)

In all cases, we compare the MERWE (based on $W^{(\lambda)}$) to MEWE (based on the extant W_1): our goal is to illustrate the robustness of MERWE.

Finite moments:

SETTINGS	$n = 100$				$n = 200$				$n = 1000$			
	BIAS		MSE		BIAS		MSE		BIAS		MSE	
	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE
$\varepsilon = 0.1, \eta = 1$	0.049	0.092	0.003	0.009	0.041	0.092	0.002	0.011	0.036	0.085	0.001	0.007
$\varepsilon = 0.1, \eta = 4$	0.035	0.089	0.001	0.012	0.029	0.096	0.001	0.015	0.013	0.098	≈ 0	0.017
$\varepsilon = 0.2, \eta = 1$	**0.071**	**0.157**	**0.007**	**0.028**	0.086	0.177	0.008	0.033	**0.081**	**0.172**	**0.006**	**0.030**
$\varepsilon = 0.2, \eta = 4$	0.046	0.204	0.003	0.045	0.034	0.202	0.001	0.042	0.017	0.194	≈ 0	0.038
$\varepsilon = 0$	**0.036**	**0.034**	**0.001**	**0.001**	0.022	0.021	≈ 0	≈ 0	**0.012**	**0.010**	≈ 0	≈ 0

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$\varepsilon = 0.1, \eta = 1$	0.049	0.092	0.003	0.009	0.041	0.092	0.002	0.011	0.036	0.085	0.001	0.007
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$\varepsilon = \mathbf{0.2}, \eta = \mathbf{1}$	**0.071**	**0.157**	**0.007**	**0.028**	0.086	0.177	0.008	0.033	**0.081**	**0.172**	**0.006**	**0.030**
$\varepsilon = 0.2, \eta = 4$	0.046	0.204	0.003	0.045	0.034	0.202	0.001	0.042	0.017	0.194	≈ 0	0.038
$\varepsilon = \mathbf{0}$	**0.036**	**0.034**	**0.001**	**0.001**	0.022	0.021	≈ 0	≈ 0	**0.012**	**0.010**	≈ 0	≈ 0

Remark

- *In small samples $n = 100$, the MERWE has smaller bias and MSE than the MEWE, in all settings. Similar results are available in moderate samples, $n = 200$*

Finite moments:

SETTINGS	$n = 100$				$n = 200$				$n = 1000$			
	BIAS		MSE		BIAS		MSE		BIAS		MSE	
	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE
$\varepsilon = 0.1, \eta = 1$	0.049	0.092	0.003	0.009	0.041	0.092	0.002	0.011	0.036	0.085	0.001	0.007
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$\varepsilon = 0.2, \eta = 1$	**0.071**	**0.157**	**0.007**	**0.028**	0.086	0.177	0.008	0.033	**0.081**	**0.172**	**0.006**	**0.030**
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Remark

- *In small samples $n = 100$, the MERWE has smaller bias and MSE than the MEWE, in all settings. Similar results are available in moderate samples, $n = 200$*
- *For $n = 1000$, MERWE and MEWE have similar performance when $\varepsilon = 0$ (no contamination), whilst the MERWE still has smaller MSE for $\varepsilon > 0$. This implies that the MERWE maintains good efficiency with respect to MEWE at the reference model.*

Infinite moments:

SETTINGS	Cauchy				Stable ($\alpha = 0.5$)				Stable ($\alpha = 1.1$)			
	BIAS		MSE		BIAS		MSE		BIAS		MSE	
	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE	MERWE	MEWE
$\varepsilon = 0.1, \eta = 1$	0.084	1.531	0.010	3.627	0.087	3.178	0.011	13.730	0.089	0.658	0.011	1.029
$\varepsilon = 0.1, \eta = 4$	0.205	1.529	0.047	3.656	0.163	3.173	0.034	13.706	0.206	0.745	0.047	1.050
$\varepsilon = 0.2, \eta = 1$	**0.180**	**1.502**	**0.037**	**3.601**	0.170	3.155	0.036	12.838	**0.181**	**0.675**	**0.037**	**0.941**
$\varepsilon = 0.2, \eta = 4$	0.459	1.820	0.223	4.690	0.383	3.140	0.165	12.713	0.484	1.072	0.244	1.801
$\varepsilon = 0$	**0.045**	**1.550**	**0.003**	**3.740**	0.044	3.118	0.003	12.600	**0.041**	**0.612**	**0.002**	**0.893**

Remark

The MEWE has larger bias and MSE than the ones yielded by the MERWE. This aspect is particularly evident for the distributions with undefined first moment, namely the Cauchy distribution. If we increase α to 1.1, the absence of the second moment still entails a worse performance of MEWE wrt to the MERWE.

We propose RWGAN-1 and RWGAN-2, which are two RWGAN deep learning models: both approaches are based on dual version of ROBOT. We compare these two methods with routinely-applied Wasserstein GAN (WGAN) and with the robust WGAN introduced by Balaji et al 2020.

Using **syntetic data**, we study the robustness of RWGAN-1 and RWGAN-2. We consider reference samples generated from a simple model, which includes some outliers:

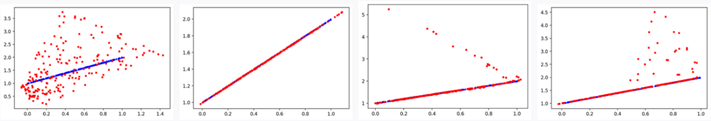
$$\begin{aligned} X_{i_1}^{(n)} \sim \mathrm{U}(0,1), X_{i_2}^{(n)} = X_{i_1}^{(n)} + 1, \\ X_i^{(n)} = (X_{i_1}^{(n)}, X_{i_2}^{(n)}), i = 1, 2, \ldots, n_1, \\ X_i^{(n)} = (X_{i_1}^{(n)}, X_{i_2}^{(n)} + \eta), i = n_1 + 1, n_1 + 2, \ldots, n, \end{aligned} \tag{8}$$

with η representing the size of outliers. We set $n = 1000$ and try four different settings by changing values of $\varepsilon = (n - n_1)/n$ and η.

WGAN	RWGAN-1	RWGAN-2	RWGAN-B

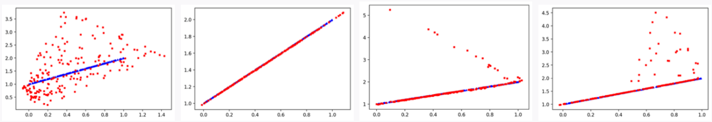
WGAN RWGAN-1 RWGAN-2 RWGAN-B

10%



(a) $W^1 = 0.5864$ (b) $W^1 = 0.0514$ (c) $W^1 = 0.1560$ (d) $W^1 = 0.1771$

	WGAN	RWGAN-1	RWGAN-2	RWGAN-B



10%

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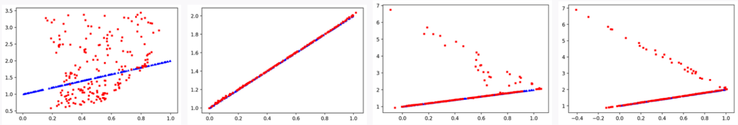
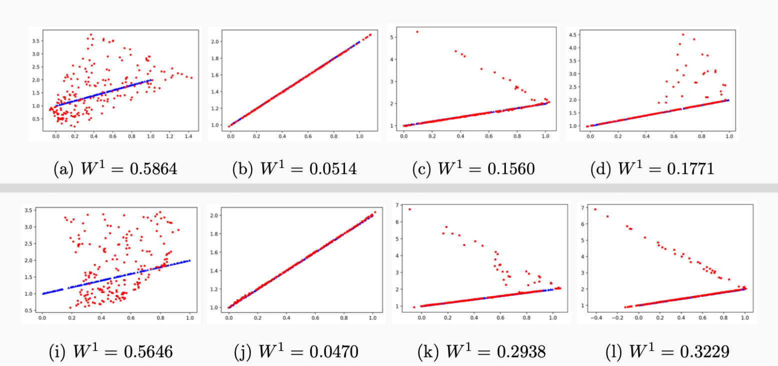


20%

(i) $W^1 = 0.5646$ (j) $W^1 = 0.0470$ (k) $W^1 = 0.2938$ (l) $W^1 = 0.3229$

	WGAN	RWGAN-1	RWGAN-2	RWGAN-B



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20%: (i) $W^1 = 0.5646$ (j) $W^1 = 0.0470$ (k) $W^1 = 0.2938$ (l) $W^1 = 0.3229$

Remark

WGAN is greatly affected by outliers. Differently, RWGAN-2 and RWGAN-B are able to generate data roughly consistent with the uncontaminated distribution, but they still produce some abnormal points when the proportion and size of outliers increase. RWGAN-1 performs better than its competitors and generates data that agree with the uncontaminated distribution, even when the proportion and size of outliers are large.

Take home message

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