Computing Kantorovich-Wasserstein Distances on d-dimensional histograms using $(d+1)-$partite graphs

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Abstract

TASK: *To compute the distance between two d-dimensional histograms having n bins. For instance, images are 2-dimensional histograms with n bins (pixels)*

PROBLEM: *The mathematical tool used to compute this distance requires the solution of an optimization problem with up to n^2 variables*

IDEA: *To exploit the structure of the cost function in order to reduce the number of variables of the optimization problem*

1. Optimal Transport

The optimal transport is a tool that is nowadays used to compute distances between images. For example the W_2 distance is used in image processing, but it is still a problem to compute W_2 efficiently.

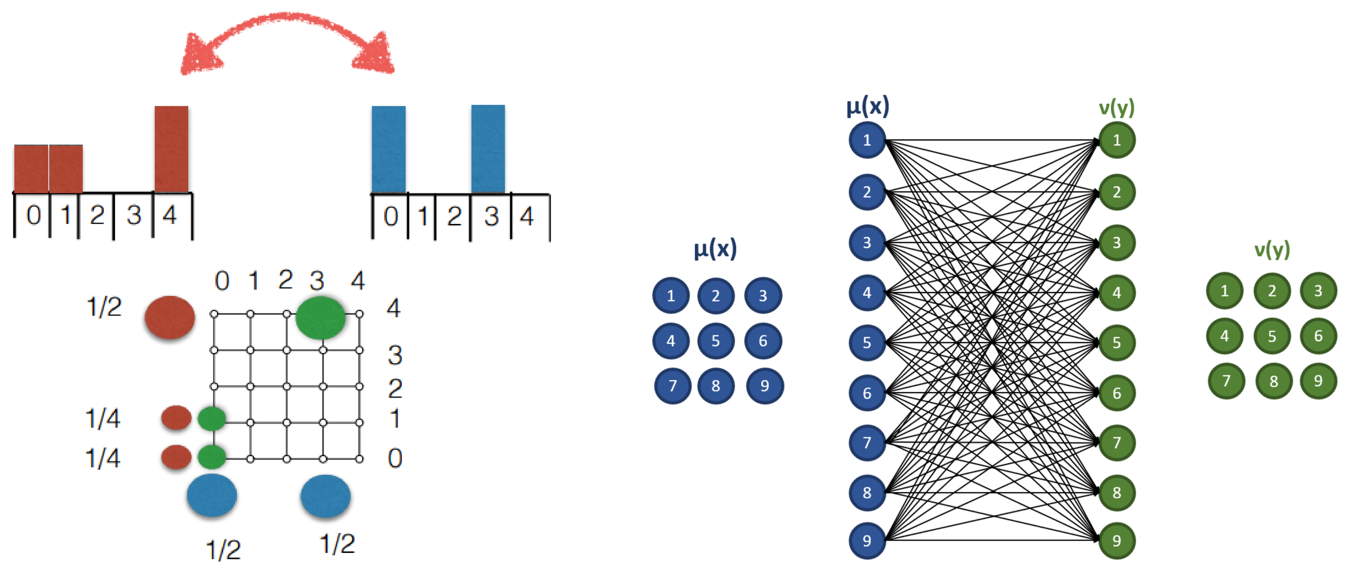


Figure 1: *Left: Blablabla. Right: blablabla*

The problem outline is the following: given two different configurations, that we will represent with two probability measures, we want to rearrange one into the other one.
For the sake of clarity and brevity we will work with $2D$ grids.

We want to find the optimal way to map a probability μ to a probability ν where moving a unit mass from x to y costs $c(x,y) = (x_1 - y_1)^2 + (x_2 - y_2)^2$, so we consider

$$W_2(\mu,\nu) := \min \sum_{x \in X} \sum_{y \in Y} c(x,y)\pi_{x,y}$$

where the minimum is taken over all the probability measures $\pi_{x,y}$ such that

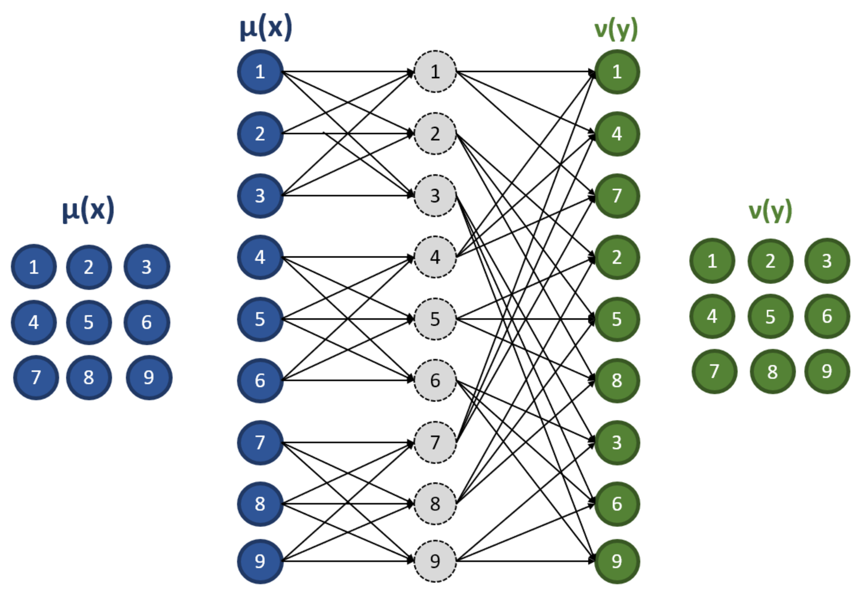
$$\sum_{x \in X} \pi_{x,y} = \nu_y, \quad \text{and} \quad \sum_{y \in Y} \pi_{x,y} = \mu_x.$$

This can be done only for some images (we can compute this quantity only when they have equal mass), but actually it can applied to each image, also to histograms, if we normalize them.

2. Our Reformulation

The standard approach to compute W_2 distances between $2D$ histograms with $n = N^2$ bins can be seen as an Uncapacitated Min Cost Flow problem on a bipartite graph, with $2n$ nodes and n^2 arcs, and can then be solved in $O(n^3 \log(n))$ time.

Those huge numbers are due to the large amount of connections we need, as showed in the following figure.



In our paper we present a novel approach to this computation that exploits the structure of the cost function to reduce the number of connections needed.

In fact, since the cost function is the sum of two independent contributes, we can describe each transport from a generic point to another one as the concatenation of two transports along the two main directions.
As a consequence of this fact, we can show that the W_2 distance can be computed as a flux problem on a $3-$partite graph, as illustrated in the following picture.
In this way, rather than connect each bin to each bin, we effectuate two connections: the first one between each bin and each other bin aligned along the first main direction and the second one between bins aligned along the second main direction.

This simple change of formulation reduces drastically the computational cost, but there is even more:

- This reasoning is easily adaptable to grids of any dimension d and the method escalates very well with it: while the old method required n^2 connections, this methods only requires $dn^{1+\frac{1}{d}}$.
- We can also adapt this method to each cost function that is separable, *i.e.* can be written as sum of independent contributions.
- As showed in the next section, this method outperforms all known approximated methods and still provides us the exact computation.

3. Numerical Results

Table 1: *Comparison on Flow Cytometry data with increasing value of d.*

			Bipartite Graph			$(d+1)$-partite Graph		
N	d	n	$\lvert V\rvert$	$\lvert A\rvert$	Runtime	$\lvert V\rvert$	$\lvert A\rvert$	Runtime
16	2	256	512	65 536	0.024 (0.01)	768	8 192	0.003 (0.00)
	3	4 096	8 192	16 777 216	38.2 (14.0)	16 384	196 608	0.12 (0.02)
	4	65 536		*out-of-memory*		327 680	4 194 304	4.8 (0.84)
32	2	1 024	2 048	1 048 756	0.71 (0.14)	3072	65 536	0.04 (0.01)
	3	32 768		*out-of-memory*		131 072	3 145 728	5.23 (0.69)

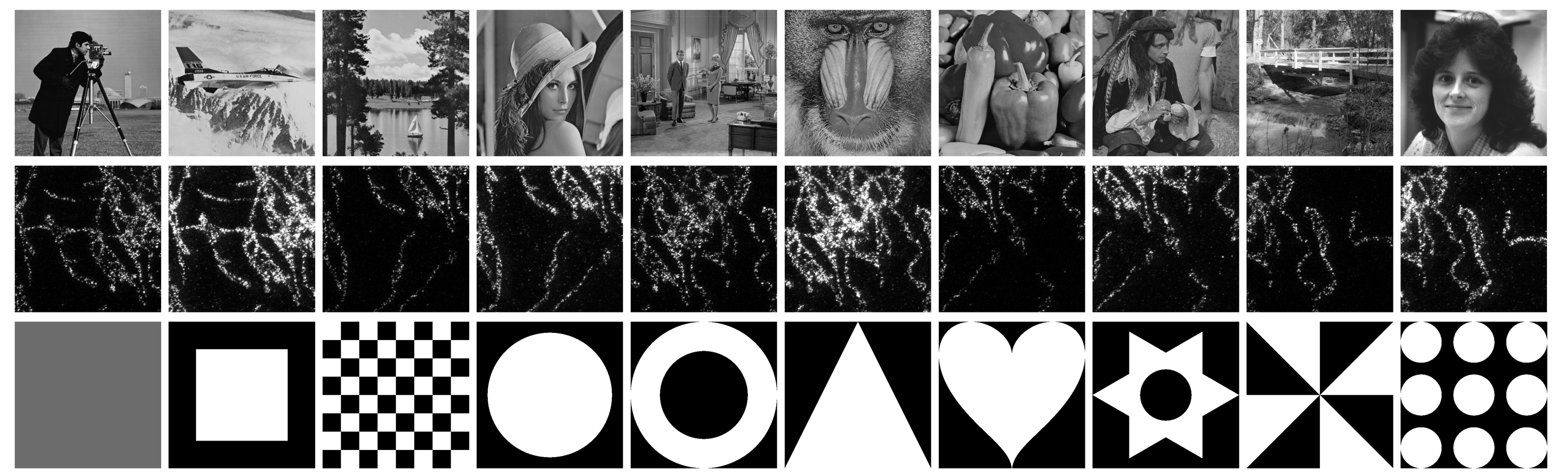


Figure 3: *DOTmark benchmark: Classic, Microscopy, and Shapes images.*

Table 2: *Comparison of different approaches on 32×32 images. The runtime (in seconds) is given as "Mean (StdDev)". The gap to the optimal value opt is computed as $\frac{UB - opt}{opt} \cdot 100$, where UB is the upper bound computed by Sinkhorn's algorithm. Each row reports the averages over 45 instances.*

	EMD[2]	Sinkhorn [1]				Bipartite	3-partite
		$\lambda = 1$		$\lambda = 1.5$			
Image Class	Runtime	Runtime	Gap	Runtime	Gap	Runtime	Runtime
Classic	24.0 (3.3)	6.0 (0.5)	17.3%	8.9 (0.7)	9.1%	0.54 (0.05)	0.07 (0.01)
Microscopy	35.0 (3.3)	3.5 (1.0)	2.4%	5.3 (1.4)	1.2%	0.55 (0.03)	0.08 (0.01)
Shapes	25.2 (5.3)	1.6 (1.1)	5.6%	2.5 (1.6)	3.0%	0.50 (0.07)	0.05 (0.01)

	Improved Sinkhorn [3, 4]						3-partite
	$\lambda = 1$		$\lambda = 1.25$		$\lambda = 1.5$		
Image Class	Runtime	Gap	Runtime	Gap	Runtime	Gap	Runtime
CauchyDensity	0.22 (0.15)	2.8%	0.33 (0.23)	2.0%	0.41 (0.28)	1.5%	0.07 (0.01)
Classic	0.20 (0.01)	17.3%	0.31 (0.02)	12.4%	0.39 (0.03)	9.1%	0.07 (0.01)
GRFmoderate	0.19 (0.01)	12.6%	0.29 (0.02)	9.0%	0.37 (0.03)	6.6%	0.07 (0.01)
GRFrough	0.19 (0.01)	58.7%	0.29 (0.01)	42.1%	0.38 (0.02)	31.0%	0.05 (0.01)
GRFsmooth	0.20 (0.02)	4.3%	0.30 (0.04)	3.1%	0.38 (0.04)	2.2%	0.08 (0.01)
LogGRF	0.22 (0.05)	1.3%	0.32 (0.08)	0.9%	0.40 (0.13)	0.7%	0.08 (0.01)
LogitGRF	0.22 (0.02)	4.7%	0.33 (0.03)	3.3%	0.42 (0.04)	2.5%	0.07 (0.02)
Microscopy	0.18 (0.03)	2.4%	0.27 (0.04)	1.7%	0.34 (0.05)	1.2%	0.08 (0.02)
Shapes	0.11 (0.04)	5.6%	0.16 (0.06)	4.0%	0.20 (0.07)	3.0%	0.05 (0.01)
WhiteNoise	0.18 (0.01)	76.3%	0.28 (0.01)	53.8%	0.37 (0.02)	39.2%	0.04 (0.00)

References

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