The Wasserstein transform

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Abstract

We introduce the Wasserstein transform, a method for enhancing and denoising datasets defined on general metric spaces. The construction draws inspiration from Optimal Transportation ideas. We establish precise connections with the mean shift family of algorithms and establish the stability of both our method and mean shift under data perturbation.

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Figure 1: In this illustration $\alpha$ is the empirical probability measure associated to the point cloud $X$ shown in the figure, and $d_X$ is the Euclidean distance. With the truncation kernel, the Wasserstein transform $W_\varepsilon$ will calculate the dissimilarity (via $d_{W,1}$) of the $\varepsilon$-neighborhoods (shown as light red disks) corresponding to all pairs of points to produce a new distance $d_\alpha^{(\varepsilon)}$ on $X$. For example, for the pair of left most points, $A$ and $B$, their respective $\varepsilon$-neighborhoods are not only similar, but also the distance between these regions is small so $d_\alpha^{(\varepsilon)}(A, B)$ will be small between those two points. Something similar is true for the pair $C$ and $D$. In contrast, despite the fact that the points $B$ and $C$ are very close to eachother, their $\varepsilon$-neighborhoods are structurally different: the neighborhood of $B$ is essentially 2-dimensional whereas that of $C$ is 1-dimensional. This will result in $d_\alpha^{(\varepsilon)}(B, C)$ being large. Similarly, since the $\varepsilon$-neighborhood of $E$ is 0-dimensional and that of $G$ is 1-dimensional, despite being very close to eachother $d_\alpha^{(\varepsilon)}(E, G)$ will be large. Finally, $d_\alpha^{(\varepsilon)}(E, F)$ will equal the ground distance between $E$ and $F$ since their respective neighborhoods consist of a single point.

1 Introduction

Optimal transport (OT) is concerned with finding cost efficient ways of deforming a given source probability distribution into a target distribution [Vil03, Vil08, San15]. In recent years, ideas from OT have found applications in machine learning and data analysis in general. Applications range from image equalization [Del04], shape interpolation [SDGP+15], image/shape [SPKST16, RTG98] and document classification [KSKW15, RCPT16], semi-supervised learning [SRGB14], to population analysis of Gaussian processes [MF17] and domain adaptation [CFTR17].

In line with previous applications of OT, we represent datasets as probability measures on an ambient metric space. We introduce the so called Wasserstein transform which takes this input dataset and alters its interpoint distance information in order to both enhance features, such as clusters, present in the data, and to denoise the data. As our main theoretical contribution, we prove the stability of our construction to perturbations in the input data (i.e. changes in the input probability measure).

We also interpret our proposed feature enhancing method as both a generalization and a strengthening of mean shift [Che95, FH75] which can operate on general metric

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spaces. Although mean shift has been generalized to data living on Riemannian manifolds [SM09, SSCO06], our interpretation departs from the ones in those papers in that we do not attempt to estimate a local mean or median of the data but, instead, we use the local density of points to iteratively directly adjust the distance function on the metric space. This is done without appealing to any intermediate embedding into a Euclidean space. As a further contribution, through this connection we can prove that mean shift is stable to data perturbations.

2 Optimal transport concepts

Given a compact metric space \((X, d_X)\) one of the fundamental concepts of OT [Vil03] is the so called Wasserstein distance on the set of all probability measures \(P(X)\) on \(X\). The \(\ell^1\)-Wasserstein distance \(d_{W,1}(\alpha, \beta)\) between probability measures \(\alpha, \beta \in P(X)\) is obtained by solving the following optimization problem:

\[
d_{W,1}(\alpha, \beta) := \min_{\mu \in \Pi(\alpha, \beta)} \int_{X \times X} d_X(x, x') d\mu(x \times x'),
\]

where \(\Pi(\alpha, \beta)\) is the set of all couplings between the probability measures \(\alpha\) and \(\beta\): namely, \(\mu\) in \(\Pi(\alpha, \beta)\) is a probability measure on \(X \times X\) whose marginals are \(\alpha\) and \(\beta\), respectively.

**Remark 2.1** (Wasserstein distance between delta measures). A simple but important remark [Vil03] is that for points \(x, x' \in X\), if one considers the Dirac measures supported at those points (which will be probability measures), \(\delta_x\) and \(\delta_{x'}\), then \(d_{W,1}(\delta_x, \delta_{x'}) = d_X(x, x')\).

**Remark 2.2.** It is known [RTG98] that in \(\mathbb{R}^d\), \(\|\text{mean}(\alpha) - \text{mean}(\beta)\| \leq d_{W,1}(\alpha, \beta)\) for any \(\alpha, \beta \in P(\mathbb{R}^d)\). In words, in Euclidean spaces, the Wasserstein distance between two probability measures is bounded below by the Euclidean distance between their respective means, which reflects the fact that \(\alpha\) and \(\beta\) can certainly have the same means but can still be quite different.

3 The Wasserstein transform

Given a compact metric space \((X, d_X)\), we introduce a subset \(P_f(X)\) of \(P(X)\), which consists of those probability measures on \(X\) with full support: the support \(\text{supp}(\alpha)\) of a probability measure \(\alpha\) is the largest closed subset such that every open neighborhood of a point in \(\text{supp}(\alpha)\) has positive measure. Given an ambient metric space \(X = (X, d_X)\), we interpret a given probability measure \(\alpha \in P_f(X)\) as the data. For example, given point cloud \(X = \{x_1, \ldots, x_n\} \subset \mathbb{R}^d\) one could choose \(\alpha = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}\) be its empirical measure. The ambient space distance between data points (in this case the Euclidean distance) is not always directly useful, and by absorbing information about the spatial density of data points, the Wasserstein transform introduced below produces a new metric on the data points which can be used in applications to reveal and concentrate interesting features present but not apparent in the initial presentation of the data. The essential idea behind the Wasserstein transform is to first capture local information of the data and then induce a new distance function between pairs of points based on the dissimilarity between their respective neighborhoods. Localization operators are gadgets that capture these neighborhoods.
3.1 Localization operators

One can always convert a point in a metric space into a Dirac measure supported at that point. More generally, a point in a metric space can be replaced by any reasonable probability measure which includes information about the neighborhood of the point – this leads to the notion of localization operators for probability measures.

**Definition 1.** Let \((X, d_X)\) be a metric space – referred to as the ambient metric space. A localization operator \(L\) is a map from \(P_f(X)\) to Markov kernels over \(X\), i.e., given \(\alpha \in P_f(X)\), \(L\) produces \(L(\alpha) = (X, m_\alpha^L(\cdot))\), where for every \(x \in X\), \(m_\alpha^L(x)\) is a probability measure on \(X\).

The following are two simple examples. (a) Given \(\alpha\) in \(P_f(X)\), let \(m_\alpha^L(x) \equiv \alpha, \forall x \in X\), which assigns to all points in \(X\) the reference probability measure \(\alpha\). This is a trivial example in that it does not localize the measure \(\alpha\) at all. (b) For any \(\alpha\) in \(P_f(X)\), let \(m_\alpha^L(x) = \delta_x, \forall x \in X\). This is a legitimate localization operator but it does not retain any information from \(\alpha\).

Local truncations, mean shift, and kernel based localization operators (in Euclidean spaces) are three typical interesting examples of localization operators, which will be discussed in the following sections.

3.2 The Wasserstein transform

After specifying a localization operator \(L\) and given \(\alpha \in P_f(X)\), one associates each point \(x\) in \(X\) with a probability measure \(m_\alpha^L(x)\), and then obtains a new metric space by considering the Wasserstein distance between each pair of these measures.

\[
\text{Wasserstein Transform of } \alpha
\]

\[
(X, d_X) \xrightarrow{L} (X, d_{W,1}^L) \xrightarrow{W_L} W_L(\alpha) = (X, d_\alpha^L)
\]

**Definition 2 (The Wasserstein transform).** Let \((X, d_X)\) be a given ambient metric space and let \(\alpha \in P_f(X)\). Given a localization operator \(L\), the Wasserstein transform \(W_L\) applied to \(\alpha\) gives the distance function \(d_\alpha^L\) on \(X\) defined by

\[
d_\alpha^L(x, x') := d_{W,1}^L (m_\alpha^L(x), m_\alpha^L(x')) , \forall x, x' \in X.
\]

By \(W_L(\alpha)\) we will denote the (pseudo) metric space \((X, d_\alpha^L)\).

Even if in this paper we consider only the case of the \(\ell^1\)-Wasserstein transform, it is possible to formulate a similar transform using the notion of \(\ell^p\)-Wasserstein distance.

**Remark 3.1 (Iterating the Wasserstein transform).** The Wasserstein transform can be iterated any desired number of times with the purpose of successively enhancing features.
and/or reducing noise. After applying the Wasserstein transform once to $\alpha \in \mathcal{P}_f(X)$, the ambient metric space $(X, d_X)$ is transformed into $(X, d_\alpha^1)$. Then we can apply the Wasserstein transform again to $\alpha$ on the ambient space $(X, d_\alpha^1)$ etc. This fact is useful in applications such as clustering, see Section 5.

### 3.3 Local truncations

We now concentrate on a particular type of localization operator that we call local truncation. Given $\alpha \in \mathcal{P}_f(X)$ and a scale parameter $\varepsilon > 0$, consider for each $x \in X$ the probability measure

$$m_\alpha^\varepsilon(x) := \frac{\alpha(B_\varepsilon(x))}{\alpha(B_\varepsilon(x))},$$

arising from restricting $\alpha$ to the closed ball $B_\varepsilon(x)$ and then renormalizing to obtain a new probability measure. In other words, for each set $A \subset X$, the measure of that set is $m_\alpha^\varepsilon(x)(A) = \frac{\alpha(B_\varepsilon(x) \cap A)}{\alpha(B_\varepsilon(x))}$. When $X$ is finite, $X = \{x_1, \ldots, x_n\}$, and $\alpha$ is its empirical measure, this formula becomes

$$m_\alpha^\varepsilon(x)(A) = \frac{\#\{i | x_i \in A \text{ and } d_X(x_i, x) \leq \varepsilon\}}{\#\{i | d_X(x_i, x) \leq \varepsilon\}}.$$

We denote the resulting Wasserstein transform by $W_\varepsilon$, and in this case, for each $\alpha$, the new metric produced by $W_\varepsilon(\alpha)$ will be denoted as $d_\alpha^\varepsilon$. See Figure 1 for an intuitive explanation.

**Remark 3.2** (Behavior across scales). Notice that as $\varepsilon \to \infty$ one has $m_\alpha^\varepsilon(x) = \alpha$ for any $x \in X$. However, for $\varepsilon \to 0$, $m_\alpha^\varepsilon(x) \to \delta_x$. In words, $\varepsilon$ acts as a localization parameter: for small $\varepsilon$ the renormalized measures absorb local information, whereas for large values the renormalized measures for different points become indistinguishable. Thus we have the following for any pair $x, x'$ of points in $X$:

1. As $\varepsilon \to 0$ one has $d_\alpha^\varepsilon(x, x') \to d_X(x, x')$; and
2. As $\varepsilon \to \infty$ one has $d_\alpha^\varepsilon(x, x') \to 0$.

Using the fact that the Wasserstein distance on $\mathbb{R}$ admits a closed form expression [Vil03] we are able to prove the following Taylor expansion.

**Remark 3.3.** If $X \subset \mathbb{R}$ and the probability measure $\alpha$ has a density $f$, we have the asymptotic formula for $d_\alpha^\varepsilon(x, x')$ when $\varepsilon \to 0$:

$$d_\alpha^\varepsilon(x, x') = x' - x + \frac{1}{3} \left[ \frac{f'(x')}{f(x')} - \frac{f'(x)}{f(x)} \right] \varepsilon^2 + O(\varepsilon^3), \text{ for } x' > x \text{ and } f(x), f(x') \neq 0.$$

The interpretation is that after one iteration of the Wasserstein transform $W_\varepsilon$ of $\alpha$, pairs of points $x$ and $x'$ on very dense areas (reflected by large values of $f(x)$ and $f(x')$) will be at roughly the same distance they were before applying the Wasserstein transform. However, if one of the points, say $x'$ is in a sparse area (i.e. $f(x')$ is small), then the Wasserstein transform will push it away from $x$. It is also interesting what happens when $x$ and $x'$ are both critical points of $f$: in that case the distance does not change (up to order $\varepsilon^2$). See Figure 3.
Proof of Remark 3.3. It’s shown in page 73 of [Vil03] that given two probability measures \( \alpha, \beta \in \mathcal{P}(\mathbb{R}) \), we have

\[
d_{W,1}(\alpha, \beta) = \int_{-\infty}^{\infty} |F(t) - G(t)|dt,
\]

where \( F \) and \( G \) are the cumulative distribution functions of \( \alpha \) and \( \beta \) respectively. Now let’s also use \( F \) and \( G \) to represent the cumulative distribution functions of \( m^{(c)}_{\alpha}(x) \) and \( m^{(c)}_{\alpha}(x') \) respectively. Then we have explicitly

\[
F(t) = \begin{cases} 
0, & t \leq x - \varepsilon \\
\frac{\alpha((x', t])}{\alpha((x - \varepsilon, x + \varepsilon])}, & x - \varepsilon \leq t < x + \varepsilon \\
1, & x + \varepsilon \leq t
\end{cases}
\]

and

\[
G(t) = \begin{cases} 
0, & t \leq x' - \varepsilon \\
\frac{\alpha((x', t])}{\alpha((x - \varepsilon, x + \varepsilon])}, & x' - \varepsilon \leq t < x' + \varepsilon \\
1, & x' + \varepsilon \leq t
\end{cases}
\]

Now suppose \( \varepsilon \) is small enough such that \( x + \varepsilon \leq x' - \varepsilon \), then we have \( F = G \) on \( (-\infty, x - \varepsilon] \cup [x' + \varepsilon, \infty) \) and thus

\[
\int_{-\infty}^{\infty} |F(t) - G(t)|dt = \left( \int_{-\infty}^{x-\varepsilon} + \int_{x-\varepsilon}^{x+\varepsilon} + \int_{x'+\varepsilon}^{\infty} \right) |F(t) - G(t)|dt
\]

\[= \int_{x-\varepsilon}^{x'+\varepsilon} |F(t) - G(t)|dt \]

\[= \int_{x-\varepsilon}^{x'-\varepsilon} F(t)dt + \int_{x'-\varepsilon}^{x'+\varepsilon} |1 - G(t)|dt \]

\[= x' - x + \int_{x-\varepsilon}^{x'+\varepsilon} \frac{\alpha((x - \varepsilon, t])}{\alpha((x - \varepsilon, x + \varepsilon])} dt - \int_{x'-\varepsilon}^{x'+\varepsilon} \frac{\alpha((x' - \varepsilon, t])}{\alpha((x' - \varepsilon, x' + \varepsilon])} dt \]

Now recalling that \( \alpha \) has density function \( f \), and using its Taylor expansion, we have

\[
H(x) = \frac{\int_{x-\varepsilon}^{x'+\varepsilon} \int_{x-\varepsilon}^{t} f(s) ds dt}{\int_{x-\varepsilon}^{x'+\varepsilon} f(s)ds} = \frac{\int_{-\varepsilon}^{t} \int_{-\varepsilon}^{t} f(x + s) ds dt}{\int_{-\varepsilon}^{t} f(x + s)ds} \]

\[= \frac{\int_{-\varepsilon}^{\varepsilon} \int_{-\varepsilon}^{\varepsilon} \left( f(x) + f'(x)s + \frac{f''(x)}{2}s^2 + O(s^3) \right) ds dt}{\int_{-\varepsilon}^{\varepsilon} \left( f(x) + f'(x)s + \frac{f''(x)}{2}s^2 + O(s^3) \right) ds} \]

\[= \frac{2\varepsilon^2 f(x) + 2\varepsilon^3 f'(x) + \varepsilon^4 f''(x) + O(\varepsilon^5)}{2\varepsilon f(x) + \frac{\varepsilon^3}{3} f''(x) + O(\varepsilon^4)} \]

\[= \varepsilon - \frac{f''(x)}{3f(x)} \varepsilon^2 + O(\varepsilon^3). \]
Figure 2: After applying one iteration of the Wasserstein transform, both the distance between $A, C$ and the distance between $C, E$ should remain almost the same since these are all critical points of $f$. According to the formula in Remark 3.3, since $f'$ has negative sign at $B$ and $B$ lies to the right of $A$, $B$ will be pushed towards $A$, while $D$ will be pushed away from $A$ since $f'(D) > 0$ and it lies to the right of $A$. Similarly both $D$ and $F$ are pushed towards $E$.

Similarly, 

$$H(x') = \varepsilon - \frac{f'(x')}{3f(x')} \varepsilon^2 + O(\varepsilon^3).$$

Therefore

$$d'_{\alpha}(x, x') = d_{W,1}(m^{(\varepsilon)}_{\alpha}(x), m^{(\varepsilon)}_{\alpha}(x'))$$

$$= x' - x + H(x) - H(x')$$

$$= d^{(\varepsilon)}_{\alpha}(x, x') = x' - x + \frac{1}{3} \left[ \frac{f'(x')}{f(x')} - \frac{f'(x)}{f(x)} \right] \varepsilon^2 + O(\varepsilon^3).$$

\[\square\]

### 3.4 The Wasserstein transform as a generalization of Mean Shift to any metric space

Mean Shift \cite{Che95, FH75} is a clustering method for Euclidean data which operates by iteratively updating each data point until convergence according to a rule that moves points towards the mean/barycenter of their neighbors. More specifically, given a point cloud $X = \{x_1, \ldots, x_n\}$ in $\mathbb{R}^d$, a kernel function $K : \mathbb{R}_+ \rightarrow \mathbb{R}_+$, and a scale parameter $\varepsilon > 0$, then in the $k$th iteration the $i$th point is shifted as follows:

$$x_i(k + 1) = \frac{\sum_{j=1}^{n} K\left( \frac{\|x_j(k) - x_i(k)\|}{\varepsilon} \right) x_j(k)}{\sum_{j=1}^{n} K\left( \frac{\|x_j(k) - x_i(k)\|}{\varepsilon} \right)}$$

where $x_i(0) = x_i$.

The kernels of choice are the Gaussian kernel $K(t) = e^{-t^2/2}$, the Epanechnikov kernel $K(t) = \max\{1 - t, 0\}$, or the truncation kernel $K(t)$ (which equals 1 if $t \in [0, 1]$ and is zero otherwise).

To see how the Mean Shift method lies in the framework of the Wasserstein Transform, let us firstly introduce a new type of localization operator. We assume that the ambient space $X$ is a convex compact subset of $\mathbb{R}^d$ endowed with Euclidean distance. Given any localization operator $L$, define a new localization operator $L^{\text{ns}}$ as follows: for $\alpha \in \mathcal{P}_f(\mathbb{R}^d)$, and $x \in X$,
$m^L_{\alpha}(x) := \delta_{\text{mean}(m^L_{\alpha}(x))}$. In words, at a fixed point $x$, $L^{ms}$ applied to a measure $\alpha$ at $x$ first localizes $\alpha$ via $L$ to obtain $m^L_{\alpha}(x)$, and then further localizes this measure by only retaining information about its mean. The fact that we can actually compute the mean (or barycenter) of a probability measure is enabled by the assumption that the ambient space is (a convex) subset of Euclidean space.

Since by Remark 2.1, the Wasserstein distance between delta measures equals the ground distance between their support points, then, considering the Wasserstein transform $W_{L^{ms}}(\alpha)$ arising from $L^{ms}$, we have for all $x, x' \in X$ that

$$d^{L^{ms}}_{\alpha}(x, x') = \|\text{mean}(m^L_{\alpha}(x)) - \text{mean}(m^L_{\alpha}(x'))\|.$$

The cost of computing the Wasserstein transform $W_L$ is larger than that of computing its mean shift version $W_{L^{ms}}$ since the former requires solving an optimal transportation problem (OTP) for every pair of points, whereas the latter only involves computing Euclidean distances. Nevertheless, recent advances [PC+17, Cut13, GCPB16] have yielded very efficient methods for tackling large scale OTPs, see Section 5.

The connection with mean shift. Now, given any kernel function $K$ and $\varepsilon > 0$ as in the case of mean shift one obtains an associated kernel based localization operator $L_{K,\varepsilon}$ such that for any $x \in X$ and $A \subset X$,

$$m^{L_{K,\varepsilon}}_{\alpha}(x)(A) := \frac{\int_A K\left(\frac{\|x-x'\|}{\varepsilon}\right) d\alpha(x')}{\int_{\mathbb{R}^d} K\left(\frac{\|x-x'\|}{\varepsilon}\right) d\alpha(x')}.$$

Now, if for a point cloud $X = \{x_1, \ldots, x_n\}$ in $\mathbb{R}^d$ we consider $\alpha$ to be the empirical measure induced by $X$, that is, $\alpha = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}$, then, for the localization operator $m^{L_{K,\varepsilon}}_{\alpha}$ defined above, we obtain, for $x \in X$, the following formula which agrees with the result of applying one iteration of mean shift to the points in $X$:

$$\text{mean}(m^{L_{K,\varepsilon}}_{\alpha}(x)) = \frac{\sum_{i=1}^n K\left(\frac{\|x-x_i\|}{\varepsilon}\right) x_i}{\sum_{i=1}^n K\left(\frac{\|x-x_i\|}{\varepsilon}\right)}.$$

Now, that the metric space $W_{L_{K,\varepsilon}}(\alpha)$ contains the same information as the collection of mean shift points above follows from the fact that any finite set in $\mathbb{R}^d$ can be reconstructed up to rigid transformations from its interpoint distance matrix.

Remark 3.4 (The Wasserstein transform as a strengthening of mean shift). Note that in general, because of Remark 2.2 one has that whenever $X \subset \mathbb{R}^d$ is convex and compact, and $\alpha \in \mathcal{P}(\mathbb{R}^d)$, then for all $x, x' \in X$,

$$\|\text{mean}(m^\varepsilon(\alpha)(x)) - \text{mean}(m^\varepsilon(\beta)(x'))\| \leq d^{\varepsilon(\alpha)}(x, x'),$$

which indicates that the mean shift procedure provides a lower bound for the result of applying the Wasserstein transform to a dataset represented by $\alpha$. In other words, the Wasserstein transform retains, via $d^{\varepsilon(\alpha)}$, more information about the dataset than mean shift.
4 Stability under perturbations of \( \alpha \)

The goal of this section is to establish the stability of the Wasserstein transform \( W_\varepsilon(\alpha) \) under perturbations in the probability measure \( \alpha \) representing the dataset. As a byproduct of this, we will also obtain a novel stability result for mean shift.

As before we fix a compact metric space \( (X, d_X) \) (the ambient space). Probability measures on \( X \) are required to satisfy a mild doubling type condition.

**Definition 3.** Given \( \Lambda > 0 \), we say that a Borel measure \( \alpha \) on \( X \) satisfies the \( \Lambda \)-doubling condition if for all \( x \in \text{supp}(\alpha), r_1 \geq r_2 > 0 \) one has

\[
\frac{\alpha(B_{r_1}(x))}{\alpha(B_{r_2}(x))} \leq \left( \frac{r_1}{r_2} \right)^\Lambda.
\]

**Remark 4.1.** Suppose \( \alpha \in P_f(X) \) and \( \text{diam}(X) < D \). If \( \alpha \) satisfies the \( \Lambda \)-doubling condition, then we have \( \alpha(B_r(x)) \geq \psi_{\Lambda, D}(r) \), for all \( x \in X \) and \( r > 0 \), where \( \psi_{\Lambda, D}(r) := \min \left( 1, \left( \frac{r}{D} \right)^\Lambda \right) \).

**Proof.** Take \( r_1 = D, r_2 = r \) in Definition 3, we have when \( r \leq D \)

\[
\frac{\alpha(B_D(x))}{\alpha(B_r(x))} \leq \left( \frac{D}{r} \right)^\Lambda.
\]

Notice that \( X = B_D(x), \) hence we have \( \alpha(B_D(x)) = \alpha(X) = 1 \). Therefore

\[
\alpha(B_r(x)) \geq \left( \frac{r}{D} \right)^\Lambda \geq \min \left( 1, \left( \frac{r}{D} \right)^\Lambda \right).
\]

When \( r > D \), obviously we have \( \alpha(B_r(x)) = \alpha(X) = 1 \geq \min \left( 1, \left( \frac{r}{D} \right)^\Lambda \right) \).

**Setup and assumptions.** We henceforth assume that the diameter of \( X \) satisfies \( \text{diam}(X) := \max_{x, x' \in X} d_X(x, x') < D \) for some \( D > 0 \). Additionally, we assume that two (fully supported) probability measures \( \alpha \) and \( \beta \) in \( P_f(X) \) are given and satisfy the doubling condition for some \( \Lambda > 0 \). Also, since our results below are for local truncations, we fix a scale parameter \( \varepsilon > 0 \).

For each \( \eta \geq 0 \) define \( \Phi_{\Lambda, D, \varepsilon}(\eta) := \frac{\eta}{\psi_{\Lambda, D}(\varepsilon)} + \left[ (1 + \frac{\eta}{\varepsilon})^\Lambda - 1 \right] \).

**Remark 4.2.** Notice that \( \Phi_{\Lambda, D, \varepsilon}(\eta) \) is an increasing function of \( \eta \) and furthermore that \( \lim_{\eta \to 0} \Phi_{\Lambda, D, \varepsilon}(\eta) = 0 \).

Then, we have the following stability result for the localization (via local truncations) of two different probability measures on the same ambient space. The stability is expressed in terms of the Wasserstein distance itself.

**Theorem 4.3** (Stability of local truncations).

\[
\sup_{x \in X} d_{W,1} \left( m^{(\varepsilon)}_{\alpha}(x), m^{(\varepsilon)}_{\beta}(x) \right) \leq (1 + 2\varepsilon)\Phi_{\Lambda, D, \varepsilon} \left( \sqrt{d_{W,1}(\alpha, \beta)} \right). \]
By Remark 4.2, Theorem 4.3 indicates that if $\alpha$ and $\beta$ are similar in terms of the Wasserstein distance, then for every point $x \in X$ the localized measures $m_\alpha^{(\varepsilon)}(x)$ and $m_\beta^{(\varepsilon)}(x)$ will also be similar. As a consequence of Theorem 4.3 we obtain the following two theorems:

**Theorem 4.4** (Stability of $d_\alpha^{(\varepsilon)}$).

$$\sup_{x,x' \in X} \|d_\alpha^{(\varepsilon)}(x,x') - d_\beta^{(\varepsilon)}(x,x')\| \leq 2(1+2\varepsilon)\Phi_{\Lambda,D,\varepsilon}\left(\sqrt{d_{W,1}(\alpha,\beta)}\right).$$

**Proof.** By applying the triangle inequality for the Wasserstein distance [1], we have for any $x, x' \in X$

$$\|d_\alpha^{(\varepsilon)}(x,x') - d_\beta^{(\varepsilon)}(x,x')\| = \|d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\alpha^{(\varepsilon)}(x')) - d_{W,1}(m_\beta^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x'))\|
\leq \|d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\alpha^{(\varepsilon)}(x')) - d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x'))\|
+ \|d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x')) - d_{W,1}(m_\beta^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x'))\|
\leq d_{W,1}(m_\alpha^{(\varepsilon)}(x'), m_\beta^{(\varepsilon)}(x')) + d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x))$$

Therefore by taking supremum on both sides and invoking Theorem 4.3 we obtain the claim.

**Theorem 4.5** (Stability of mean shift for local truncations). Assume that $(X,d_X)$ is a subspace of $\mathbb{R}^n$ with Euclidean distance. Then, for mean shift arising from local $\varepsilon$-truncations we have:

$$\sup_{x \in X} \|\text{mean}(m_\alpha^{(\varepsilon)}(x)) - \text{mean}(m_\beta^{(\varepsilon)}(x))\| \leq (1+2\varepsilon)\Phi_{\Lambda,D,\varepsilon}\left(\sqrt{d_{W,1}(\alpha,\beta)}\right).$$

**Proof.** By Remark 3.4 and Theorem 4.3 we have $\forall x \in X$,

$$\|\text{mean}(m_\alpha^{(\varepsilon)}(x)) - \text{mean}(m_\beta^{(\varepsilon)}(x))\| \leq d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x)) \leq (1+2\varepsilon)\Phi_{\Lambda,D,\varepsilon}\left(\sqrt{d_{W,1}(\alpha,\beta)}\right).$$

### 4.1 The proof of Theorem 4.3

**Proof of Theorem 4.3.** To analyze $d_{W,1}(m_\alpha^{(\varepsilon)}(x), m_\beta^{(\varepsilon)}(x))$, it is more convenient to first analyze the Prokhorov distance [GS02], and then convert the result to a Wasserstein distance bound by the lemma below. The Prokhorov distance $d_P(\alpha, \beta)$ equals $\inf\{\delta > 0 : \alpha(A) \leq \beta(A^\delta) + \delta, \forall A \subset X\}$. Here $A^\delta$ is the $\delta$-fattening of $A$: the set of points in $X$ which are at distance less than $\delta$ from a point in $A$. Though seemingly asymmetric, $d_P$ is actually symmetric [GS02].

**Lemma 4.6** (Theorem 2 of [GS02]). Given a metric space $(X,d_X)$ with bounded diameter, then $\forall \alpha, \beta \in \mathcal{P}_f(X)$, we have the following relation between the Wasserstein and Prokhorov distances:

$$(d_P(\alpha, \beta))^2 \leq d_{W,1}(\alpha, \beta) \leq (1 + \text{diam}(X))d_P(\alpha, \beta).$$
Remark 4.7. If $\alpha$ and $\beta$ are not fully supported, then by restricting the metric $d$ to $S = \text{supp}(\alpha) \cup \text{supp}(\beta) \subset X$, the rightmost inequality above can be improved to $d_{W,1}(\alpha, \beta) \leq (1 + \text{diam}(S))d_P(\alpha, \beta)$.

Claim 1. For any $x \in X$, we have $d_P\left(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)\right) \leq \Phi_{\Lambda, D, \epsilon}(d_P(\alpha, \beta))$.

Proof of Claim 1. Suppose $d_P(\alpha, \beta) < \eta$ for some $\eta > 0$. Fix $x \in X$ and assume WLOG that $\beta(B_\epsilon(x)) \leq \alpha(B_\epsilon(x))$. Then invoke the expression $d_P\left(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)\right) = \inf\{\delta > 0 : m^{(c)}_{\alpha}(x)(A) \leq m^{(c)}_{\beta}(x)(A^\delta) + \delta, \forall A \subset X\}$. For any $A \subset X$ we have the following inclusions:

\[
(A \cap B_\epsilon(x))^\eta \subset A^n \cap (B_\epsilon(x))^\eta \subset A^n \cap B_{\epsilon + \eta} = A^n \cap \left(B_\epsilon(x) \cup (B_{\epsilon + \eta}(x) \setminus B_\epsilon(x))\right)
\]

\[
\subset A^n \cap B_\epsilon(x) \cup A^n \cap B_{\epsilon + \eta}(x) \setminus B_\epsilon(x) \subset A^n \cap B_\epsilon(x) \cup B_{\epsilon + \eta}(x) \setminus B_\epsilon(x).
\]

Then by monotonicity of measure and the fact that $d_P(\alpha, \beta) < \eta$, we have

\[
m^{(c)}_{\alpha}(x)(A) = \frac{\alpha(A \cap B_\epsilon(x))}{\alpha(B_\epsilon(x))} \leq \frac{\beta((A \cap B_\epsilon(x))^\eta) + \eta}{\beta(B_\epsilon(x))} \leq \frac{\beta((A \cap B_\epsilon(x))^\eta) + \eta}{\beta(B_\epsilon(x))}
\]

\[
\leq \frac{\beta(A^n \cap B_\epsilon(x)) + \beta(B_{\epsilon + \eta}(x) \setminus B_\epsilon(x))}{\beta(B_\epsilon(x))} + \frac{\eta}{\beta(B_\epsilon(x))} - 1
\]

\[
\leq m^{(c)}_{\beta}(x)(A^n) + \left(1 + \frac{\eta}{\epsilon}\right)^{\Lambda} - 1 + \frac{\eta}{\beta(B_\epsilon(x))} \leq m^{(c)}_{\beta}(x)(A^\eta) + \xi,
\]

where $\xi := \Phi_{\Lambda, D}(\eta) = \left(1 + \frac{\eta}{\epsilon}\right)^{\Lambda} - 1 + \frac{\eta}{\psi_{\Lambda, D}(\epsilon)}$, and the last inequality follows from Remark 4.1. Note that since $\left(1 + \frac{\eta}{\epsilon}\right)^{\Lambda} - 1 \geq 0$, and $\psi_{\Lambda, D}(\epsilon) \leq 1$, then $\xi \geq \eta$. Thus, from the inequality above, and since $A^n \subset A^\delta$, then $m^{(c)}_{\alpha}(x)(A) \leq m^{(c)}_{\beta}(x)(A^n) + \xi \leq m^{(c)}_{\beta}(x)(A^\delta) + \xi$. Therefore $d_P(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)) \leq \xi = \Phi_{\Lambda, D}(\eta)$. Then by letting $\eta \rightarrow d_P(\alpha, \beta)$ we have $d_P(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)) \leq \Phi_{\Lambda, D, \epsilon}(d_P(\alpha, \beta))$, where the RHS is independent of $x$, so the proof is done.

We now finish the proof of Theorem 4.3. Since $\text{supp}(m^{(c)}_{\alpha}(x))$ and $\text{supp}(m^{(c)}_{\beta}(x))$ are both contained in $B_\epsilon(x)$ and $\text{diam}(B_\epsilon(x)) \leq 2\epsilon$, we have from Remark 4.7 that $d_{W,1}(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)) \leq (1 + 2\epsilon)d_P\left(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)\right)$. Now, from this inequality, by Claim 1 above we in turn obtain $d_{W,1}(m^{(c)}_{\alpha}(x), m^{(c)}_{\beta}(x)) \leq (1 + 2\epsilon)\Phi_{\Lambda, D, \epsilon}(d_P(\alpha, \beta))$. Finally, since $\Phi_{\Lambda, D, \epsilon}(\eta)$ is an increasing function of $\eta$, by Lemma 4.6 we obtain the statement of the theorem.

5 Implementation and experiments

In the case of the local truncation transform $W_\epsilon$, for each pair of points $x, x' \in X$, the computation of $d^{(c)}_{\alpha}(x, x') = d_{W,1}(m^{(c)}_{\alpha}(x), m^{(c)}_{\alpha}(x'))$ only requires knowledge of the rectangular chunk of $d_X$ consisting of those points in $B_\epsilon(x) \times B_\epsilon(x')$ and, as such, the size of each instance of $d_{W,1}$ can be controlled by choosing $\epsilon$ to be sufficiently small. The solution of
Figure 3: Top left: A dumbbell shape consisting of two disk shaped blobs each with 100 points and separated by a thin chain of 30 points in the plane with Euclidean distance. The diameter of the initial shape was approximately 4. From left to right: 0, 1, 2, 3, and 4, iterations of \( W_\epsilon \) for \( \epsilon = 0.3 \). The top row shows MDS plots of the successive metric spaces thus obtained (color is by class: first blob, chain, and second blob), the middle row shows their distance matrices (ordered so that first we see the points in one blob, then the points on the connecting chain, and then the points of the second blob. The third row shows the corresponding single linkage dendrograms. Notice how the the MDS plot/distance matrices/dendrograms at iteration 5 exhibit clearly defined clusters.

The associated Kantorovich optimal transport problem is carried via entropic regularization using the Sinkhorn code from [sink]. The computation of the matrix \( \left( d_\alpha^{(\epsilon)}(x, x') \right)_{x, x' \in X} \) is an eminently parallelizable task. In our implementation we ran this on a 24 core server via Matlab’s parallel computing toolbox.

**Ameliorating the chaining effect.** In this application we considered the case of clustering two well defined disk shaped blobs (each containing 100 points) connected by a thin trail consisting of 30 points. This is a standard scenario in which standard single linkage hierarchical clustering fails to detect the existence of two clusters due to the so called **chaining effect**. However, successive applications of the Wasserstein transform \( W_\epsilon \) (corresponding to local truncations) consistently improve the quality of the dendrograms. See Figure 3. See Figure 4 for a study of the effects of increasing \( \epsilon \) and the number of iterations on this dataset. As already suggested by the interpretation in Figure 1 \( \epsilon \)-neighborhoods of points in the interior of the dumbbell are essentially two dimensional, whereas \( \epsilon \)-neighborhoods of points on the chain are one dimensional – this means that their Wasserstein distance will be quite large, thus having the effect of separating the clusters in the sense of \( d_\alpha^{(\epsilon)} \).
Figure 4: In this figure we computed 14 different iterations of the dumbbell dataset for $\varepsilon = 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, \text{ and } 0.4$. Notice how distance matrices corresponding to the lower right corner show a very well defined block structure indicative of the presence of two large clusters (the blobs) and a smaller one (the points originally corresponding to the chain).
Denoising of a circle: mean shift vs. $W_\varepsilon$. The top row shows the result of applying mean shift with the truncation kernel; the bottom row shows 2D MDS plots of the results obtained from applying the local truncation Wasserstein transform $W_\varepsilon$. In each case $\varepsilon$ was chosen to be 0.3 relative to the diameter at each iteration. The first column shows the initial dataset which is the same for both cases. From left to right we show increasing number of iterations. Notice how $W_\varepsilon$ is able to better resolve the shape of the circle; in particular, it is better at displacing interior points towards the high density area around the circle.

Denoising of a circle. In this example we study the case of 800 points uniformly spaced on a circle with radius 1 and centered at the origin in the plane. This circle is heavily corrupted by 1200 outliers chosen uniformly at random in the unit square $[-1, 1] \times [-1, 1]$. This type of preprocessing may help in applications where one wishes to detect voids/loops in data which may signal periodicity [Per16, EGK14]. We compare the performance of $W_\varepsilon$ with mean shift (with the same kernel and same parameter $\varepsilon$). See Figure 5. This shows that $W_\varepsilon$ can be a useful preprocessing step before applying nonlinear dimensionality reductions or manifolds learning techniques to a dataset.

6 Conclusions

We have introduced the Wasserstein transform as a method that takes a dataset represented by a distance matrix and a probability measure and iteratively alters the distance matrix with the goal of enhancing features and/or removing noise. We established the stability of our method under data perturbations, and exhibited a connection with the mean shift algorithm. This connection established the stability of mean shift as well.

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