Flow-based Alignment Approaches for Probability Measures in Different Spaces

Tam Le[*] RIKEN AIP

Nhat Ho[*] The University of Texas at Austin

Makoto Yamada Kyoto University & RIKEN AIP

Abstract

Gromov-Wasserstein (GW) is a powerful tool to compare probability measures whose supports are in different metric spaces. However, GW suffers from a computational drawback since it requires to solve a complex non-convex quadratic program. In this work, we consider a specific family of cost metrics, namely, tree metrics for supports of each probability measure, to develop efficient and scalable discrepancies between the probability measures. Leveraging a tree structure, we propose to align *flows* from a root to each support instead of pair-wise tree metrics of supports, i.e., flows from a support to another support, in GW. Consequently, we propose a novel discrepancy, named *Flow-based Alignment* (FlowAlign), by matching the flows of the probability measures. FlowAlign is computationally fast and scalable for large-scale applications. Further exploring the tree structure, we propose a variant of FlowAlign, named *Depth-based Alignment* (DepthAlign), by aligning the flows hierarchically along each depth level of the tree structures. Theoretically, we prove that both FlowAlign and DepthAlign are pseudo-metrics. We also derive tree-sliced variants of the proposed discrepancies for applications without prior knowledge about tree structures for probability measures, computed by averaging FlowAlign/DepthAlign using random tree metrics, adaptively sampled from supports of probability measures. Empirically, we test our proposed approaches against other variants of GW baselines on a few benchmark tasks.

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1 Introduction

Optimal transport (OT) theory provides a powerful set of tools to compare probability measures. OT has recently gained considerable interests in machine learning community (Cuturi, 2013; Perrot et al., 2016; Genevay et al., 2016; Muzellec and Cuturi, 2018; Luise et al., 2019; Mena and Niles-Weed, 2019; Paty and Cuturi, 2019; Togninalli et al., 2019), and played an increasingly important role in several research areas, such as computer graphics (Solomon et al., 2015; Bonneel et al., 2016; Lavenant et al., 2018; Solomon and Vaxman, 2019), domain adaptation (Courty et al., 2016, 2017; Bhushan Damodaran et al., 2018; Redko et al., 2019), and deep generative models (Arjovsky et al., 2017; Gulrajani et al., 2017; Genevay et al., 2018; Kolouri et al., 2019; Nadjahi et al., 2019; Wu et al., 2019).

When probability measures are discrete and their supports are in the same space, OT distance can be recasted as a linear programming, which can be solved by standard interior-point method algorithms. However, these algorithms are not efficient when the number of supports is large. In order to account for the scalability of the OT distance, Cuturi (2013) initiated a new research line by regularizing the OT with the entropy of the transport plans. Several efficient algorithms have been recently proposed to solve the entropic OT (Altschuler et al., 2017; Dvurechensky et al., 2018; Lin et al., 2019; Altschuler et al., 2019).

When probability measures are discrete and their supports are in different spaces, the classical OT distance is no longer valid to measure their discrepancy. In his seminal work, Mémoli (2011) introduced Gromov-Wasserstein (GW) distance to compare probability measures whose supports are in different metric spaces. Due to its flexibility, the GW distance has been used in several applications, including quantum chemistry (Peyré et al., 2016), computer graphics (Solomon et al., 2016), cross-lingual embeddings (Alvarez-Melis and Jaakkola, 2018; Grave et al., 2019), graph partitioning and matching (Xu et al., 2019a,b), and deep generative mod-

[*]: The first two authors contributed equally.

els (Bunne et al., 2019). However, the GW is a complex non-convex quadratic program and NP-hard for arbitrary inputs (Peyré and Cuturi, 2019, §10.6.3). Therefore, its computation is very costly, which hinders applications in large-scale settings where the number of supports is large.

Reposing on the entropic regularization idea from OT, Peyré et al. (2016) proposed an entropic GW (EGW) discrepancy. The EGW can be efficiently solved by the Sinkhorn algorithm under certain cases of regularization parameter and a specific family of loss functions. Nevertheless, EGW requires the regularization to be sufficiently large for a fast computation, which leads to a poor approximation of GW. Following the direction of leveraging entropic regularization, Xu et al. (2019a,b) proposed algorithmic approaches to further speed up GW for graph data. Another approach for scaling up the computation of GW is sliced GW (SGW) (Vayer et al., 2019), which relies on a one-dimensional projection of supports of the probability measures. Consequently, similar to sliced-Wasserstein, SGW albeit fast limits its capacity to capture high-dimensional structure in a distribution of supports (Le et al., 2019b; Liutkus et al., 2019). Additionally, SGW can be *only* either applied for discrete measures with the same number of supports and uniform weights, or required an artifact zero-padding for probability measures having different number of supports (Vayer et al., 2019).

Contributions. In this work, we consider a particular family of cost metrics, namely tree metrics for a space of supports of each probability measure, and aim for developing efficient and scalable discrepancies for probability measures in different spaces that can be applied as fast alternative approaches for GW, especially in large-scale applications.

Although it is well-known that one can leverage tree metrics to speed up a computation of arbitrary metrics (Bartal, 1996, 1998; Charikar et al., 1998; Indyk, 2001; Fakcharoenphol et al., 2004), our goal is rather to sample tree metrics for spaces of supports, and use them as cost metrics, similar to tree-sliced-Wasserstein (TSW) (Le et al., 2019b). However, different to TSW, one may *not* apply this idea straightforwardly by only using tree metrics as cost metrics for GW to develop scalable discrepancy for probability measures in different tree metric spaces. Therefore, by exploiting a tree structure, we propose to align *flows* from a root to each support instead of pair-wise tree metrics of supports, i.e., flows from a support to another, in GW for the probability measures. Consequently, we propose a novel discrepancy, named *Flow-based Alignment* (FlowAlign), by matching the flows of the probability measures. FlowAlign is fast for computation and scalable for large-scale applications. To further explore the tree structures, we propose to align the flows hierarchically along each depth level of the tree structures, named *Depth-based Alignment* (DepthAlign). We then prove that both FlowAlign and DepthAlign are pseudo-metrics, i.e., they are symmetric and satisfy the triangle inequality.

For applications without prior knowledge about tree structures for probability measures, we derive tree-sliced variants of FlowAlign/DepthAlign, computed by averaging FlowAlign/DepthAlign using random tree metrics, sampled by a fast adaptive method, e.g., clustering-based tree metric sampling (Le et al., 2019b, §4). We empirically illustrate that the proposed discrepancies compares favorably with state-of-the-art variants of GW baselines, e.g., EGW (Peyré et al., 2016) and SGW (Vayer et al., 2019), in applications. Especially, FlowAlign is several orders faster than EGW and at least as fast as SGW while remedies the curse of dimensionality in SGW by leveraging tree structures.

Organization. The paper is organized as follows: we review tree metrics and GW in §2. We propose two novel discrepancies: FlowAlign and DepthAlign for probability measures in different tree metric spaces in §3 and §4 respectively. In §5, we derive their tree-sliced variants for practical applications, and then give discussions and related work in §6. We evaluate the proposed discrepancies against other baselines on some benchmark tasks in §7 before concluding in §8. We have released code for our proposal[1].

Notation. We denote $[n] = \{1, 2, \ldots, n\}$, $\forall n \in \mathbb{N}_+$. For $x \in \mathbb{R}^d$, let $\|x\|_1$ be the ℓ_1-norm of x, and δ_x be the Dirac function at x. For probability measure μ, we denote $\text{supp}(\mu)$ and $|\mu|$ for the set and the number of support(s) of μ respectively.

2 Reminders on Tree Metric and GW

In this section, we first recall tree metric space and then briefly review GW between probability measures in different tree metric spaces.

2.1 Tree metric space

For a tree metric space $(\mathcal{T}, d_\mathrm{T})$, d_T is a tree metric on tree $\mathcal{T}$. The *tree metric* d_T between two nodes in $\mathcal{T}$ is equal to a length of the (unique) path between them (Semple and Steel, 2003, §7, p.145–182). Given node $x \in \mathcal{T}$, let $\Gamma(x)$ be the set of nodes in the subtree of $\mathcal{T}$ rooted at x, i.e., $\Gamma(x) = \{z \in \mathcal{T} \mid x \in \mathcal{P}(r, z)\}$ where $\mathcal{P}(r, z)$ is the (unique) path between root r and node z

[1] https://github.com/lttam/FlowBasedAlignment-GW

in $\mathcal{T}$, $\mathcal{S}(x)$ be the set of child nodes of x, and $|\mathcal{S}(\cdot)|$ is the cardinality of set $\mathcal{S}(\cdot)$. Given edge e, we write u_e and v_e for the nodes that are respectively at a shallower (i.e., closer to r) and deeper (i.e., further away from r) level of edge e, and w_e be the non-negative length of that edge. We illustrate those notions in Figure 1.

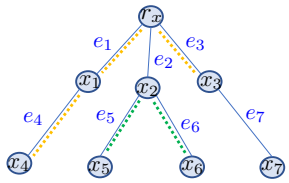

Figure 1: An illustration for a tree metric space. x_2 is at depth level 2. $\mathcal{P}(x_3, x_4)$ contains e_3, e_1, e_4 (the orange dot path), $\Gamma(x_2) = \{x_2, x_5, x_6\}$ (the green dot subtree), and $\mathcal{S}(r_x) = \{x_1, x_2, x_3\}$. For edge e_5, $v_{e_5} = x_5$ and $u_{e_5} = x_2$.

Throughout the paper, we consider two probability measures $\mu = \sum_{i\in[k]} a_i \delta_{x_i}$ (with k supports) and $\nu = \sum_{j\in[k']} b_j \delta_{z_j}$ (with k' supports) where $\text{supp}(\mu)$ and $\text{supp}(\nu)$ are in different tree metric spaces $(\mathcal{T}_X, d_{\mathcal{T}_X})$ and $(\mathcal{T}_Z, d_{\mathcal{T}_Z})$[2] respectively; $a_i, b_j \in \mathbb{R}_+, \forall i \in [k], j \in [k']$ such that $\sum_{i\in[k]} a_i = \sum_{j\in[k']} b_j = 1$. Our goal is to define discrepancies for these probability measures.

2.2 Gromov-Wasserstein with Tree Metrics

Mémoli (2011) defined Gromov-Wasserstein $\mathcal{GW}$ between μ, ν as

$$\mathcal{GW}^2(\mu,\nu) := \min_{T\in\Pi(\mu,\nu)} \sum_{i,j,i',j'} |d_{\mathcal{T}_X}(x_i, x_{i'}) - d_{\mathcal{T}_Z}(z_j, z_{j'})|^2 T_{ij} T_{i'j'}, \quad (1)$$

where $\Pi(\mu,\nu)$ is a set of the transport plans $T \in \mathbb{R}_+^{k\times k'}$ such that $\sum_{j\in[k']} T_{ij} = a_i \;|_{i\in[k]}, \sum_{i\in[k]} T_{ij} = b_j \;|_{j\in[k']}$. Intuitively, GW aligns pair-wise tree metrics of supports $d_{\mathcal{T}_X}(x_i, x_{i'}) \;|_{i,i'}$ and $d_{\mathcal{T}_Z}(z_j, z_{j'}) \;|_{j,j'}$ for μ and ν.

However, one may not scale up GW by straightforwardly using tree metrics as cost metrics as in Equation (1) like TSW (Le et al., 2019b). Therefore, we propose to leverage tree structure to align *flows* from a root to each support instead of pair-wise tree metrics of supports, i.e., flows from a support to another, in GW to develop scalable discrepancy for the probability measures. Consequently, we propose two novel discrepancies: FlowAlign and DepthAlign, detailed in §3 and §4 respectively.

3 Flow-based Alignment Discrepancy

In this section, we propose a novel, efficient and scalable discrepancy, named Flow-based Alignment (FlowAlign), for probability measures in different tree metric spaces.

[2] $d_{\mathcal{T}_X}, d_{\mathcal{T}_Z}$ are tree metrics on tree $\mathcal{T}_X, \mathcal{T}_Z$ respectively.

3.1 Definition of FlowAlign

Different from GW, FlowAlign exploits tree structures for the alignment.

Definition 1. *The Flow-based Alignment discrepancy $\mathcal{A}_f$ between μ, ν is defined as*

$$\mathcal{A}_f^2(\mu,\nu) := \min_{r_x, r_z, T\in\Pi(\mu,\nu)} \sum_{i,j} |d_{\mathcal{T}_X}(r_x, x_i) - d_{\mathcal{T}_Z}(r_z, z_j)|^2 T_{ij}. \quad (2)$$

Intuitively, FlowAlign considers the matching for *flows* from a root to each support for probability measures based on (i) the flow lengths (i.e., tree metrics from a root to each support), and (ii) the flow masses (i.e., weights on supports corresponding to the flows). Moreover, FlowAlign also takes into account the root alignment for corresponding tree structures of tree metric spaces since the *flows* depend on which node in the tree structure has a role as the tree root. Therefore, instead of matching *pairs of supports* as in GW for probability measures in different spaces, FlowAlign exploits tree structures of the tree metric spaces to align *both tree root and supports* for the probability measures. To the best of our knowledge, our work is the first approach leveraging tree metric to align probability measures supported in different metric spaces (i.e., alternative approach for GW based on flows)[3].

One should distinguish FlowAlign from tree-(sliced)-Wasserstein which directly matches *supports* for probability measures in the *same* tree metric space. Additionally, the goal of FlowAlign is to match the probability measures μ, ν like GW, by exploiting the tree structures $(\mathcal{T}_X, d_{\mathcal{T}_X})$, $(\mathcal{T}_Z, d_{\mathcal{T}_Z})$, but not to compare trees $\mathcal{T}_X, \mathcal{T}_Z$ themselves like tree edit distance (Zhang and Shasha, 1989).

Theorem 1. *FlowAlign is a pseudo-distance. It satisfies symmetry and the triangle inequality.*

See the supplementary (§A) for the proof of Theorem 1. When $\mathcal{A}_f^2(\mu,\nu) = 0$, we can find roots r_x^* and r_z^* such that $\tilde{\mu}^* \equiv \tilde{\nu}^*$ where $\tilde{\mu}^* = \sum_i a_i \delta_{d_{\mathcal{T}_X}(r_x^*, x_i)}$ and $\tilde{\nu}^* = \sum_j b_j \delta_{d_{\mathcal{T}_Z}(r_z^*, z_j)}$. It demonstrates that μ and ν have similar weights on supports (i.e., flow masses) while the tree metrics of their supports to the corresponding root r_x^* or r_z^* (i.e., flow lengths) are identical.

While GW with tree metrics relies on *pair-wise supports alignment* to match probability measures, FlowAlign uses *flow alignment* based on geometric

[3] After our preprint, Mémoli et al. (2021) leveraged ultrametric—a special case of tree metrics—to study basic topological and geometric properties of Sturm's distance (Sturm et al., 2006) and Gromov-Wasserstein.

structures of trees. We next attempt to draw relations between them when the deepest levels of trees $\mathcal{T}_X$ and $\mathcal{T}_Z$ are equal to two.

Proposition 1. *If the deepest levels of trees $\mathcal{T}_X$ and $\mathcal{T}_Z$ are two, then $\mathcal{GW}(\mu,\nu) \leq 2\mathcal{A}_f(\mu,\nu)$.*

See the supplementary (§A) for the proof of Proposition 1.

In practical applications without prior knowledge about tree structures for probability measures, $\mathcal{T}_X$ and $\mathcal{T}_Z$ are sampled from support data points, e.g., by clustering-based tree metric sampling (Le et al., 2019b). We argue that the farthest-point clustering (Gonzalez, 1985) within the clustering-based tree metric sampling ensures that FlowAlign is invariant to rotation and translation, detailed in the supplementary (§B).

3.2 Efficient computation for FlowAlign

A naive implementation for FlowAlign $\mathcal{A}_f$ has a complexity $\mathcal{O}(N^3 \log N)$ where N is the number of nodes in tree, if one exhaustively searches the optimal pair of roots for $\mathcal{T}_X$ and $\mathcal{T}_Z$[4]. In this section, we present an efficient computation approach which reduces this complexity into nearly $\mathcal{O}(N^2)$.

Consider $\mathcal{A}_f$ between μ,ν in $\mathcal{T}_X, \mathcal{T}_Z$ rooted at r_x, r_z respectively. When one changes into the new root $\bar{r}_z$ for $\mathcal{T}_Z$, illustrated in Figure 2, there are two cases that can happen:

Case 1 : $\bar{r}_z$ is in the subtree rooted at a node in $\mathcal{S}(r_z)$, which is disjoint from $\text{supp}(\nu)$, illustrated in the left-bottom tree of Figure 2. Then, $\forall z_i \in \text{supp}(\nu)$, we have

$$d_{\mathcal{T}_Z}(\bar{r}_z, z_i) = d_{\mathcal{T}_Z}(r_z, z_i) + d_{\mathcal{T}_Z}(\bar{r}_z, r_z).$$

Therefore, the path-length order from the root is preserved.

Case 2 : $\bar{r}_z$ is in the subtree rooted at a node in $\mathcal{S}(r_z)$, containing some supports of ν, denoted as Ω_ν, illustrated in the right-bottom tree of Figure 2. Then, $\forall z_j \in \text{supp}(\nu) \setminus \Omega_\nu$, we have

$$d_{\mathcal{T}_Z}(\bar{r}_z, z_j) = d_{\mathcal{T}_Z}(r_z, z_j) + d_{\mathcal{T}_Z}(\bar{r}_z, r_z).$$

Thus, the path-length order from the root (except those for $z_i \in \Omega_\nu$) is preserved. For supports in Ω_ν (illustrated in the supplementary (§B)), there are three following sub-cases:

• **Case 2a**: For supports $z_i \in \Omega_\nu$ which $\bar{r}_z \in \mathcal{P}(r_z, z_i)$, then

$$d_{\mathcal{T}_Z}(\bar{r}_z, z_i) = d_{\mathcal{T}_Z}(r_z, z_i) - d_{\mathcal{T}_Z}(r_z, \bar{r}_z).$$

[4]More details about (aligned-root) FlowAlign complexity are given in §3.3, and in the supplementary (§C).

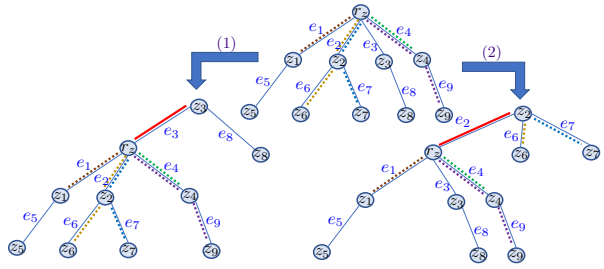

Figure 2: An illustration for an efficient computation for FlowAlign. Given $\nu = b_1\delta_{z_1} + b_2\delta_{z_6} + b_3\delta_{z_7} + b_4\delta_{z_4} + b_5\delta_{z_9}$, when the new root $\bar{r}_z = z_3$ (z_3 is in the subtree rooted at z_3 which is disjoint from $\text{supp}(\nu)$), the order of $d_{\text{T}}(r_z, z_i)\,|_{z_i \in \nu}$ is the same as that of $d_{\text{T}}(z_3, z_i)\,|_{z_i \in \nu}$, and $d_{\text{T}}(z_3, z_i) = d_{\text{T}}(r_z, z_i) + d_{\text{T}}(r_z, z_3), \forall z_i \in \text{supp}(\nu)$ (**Case 1**: the left-bottom tree). When $\bar{r}_z = z_2$ (z_2 is in the subtree rooted at z_2, and containing supports $\Omega_\nu = \{z_6, z_7\}$ of ν), the order of $d_{\text{T}}(r_z, z_i)\,|_{z_i \in \text{supp}(\nu) \setminus \Omega_\nu}$ is the same as that of $d_{\text{T}}(z_3, z_i)\,|_{z_i \in \text{supp}(\nu) \setminus \Omega_\nu}$, and $d_{\text{T}}(z_2, z_i) = d_{\text{T}}(r_z, z_i) + d_{\text{T}}(r_z, z_3), \forall z_i \in \text{supp}(\nu) \setminus \Omega_\nu$ (**Case 2**: the right-bottom tree).

So, the path-length order from the root of those supports are preserved.

• **Case 2b**: For supports $z_i \in \Omega_\nu$ which $z_i \in \mathcal{P}(r_z, \bar{r}_z)$, then

$$d_{\mathcal{T}_Z}(\bar{r}_z, z_i) = d_{\mathcal{T}_Z}(r_z, \bar{r}_z) - d_{\mathcal{T}_Z}(r_z, z_i).$$

Therefore, the path-length order from the root of those supports are reversed.

• **Case 2c**: For supports $z_i \in \Omega_\nu$ which $\bar{r}_z \notin \mathcal{P}(r_z, z_i)$ and $z_i \notin \mathcal{P}(r_z, \bar{r}_z)$, then one needs to find the corresponding closest common ancestor ζ_i of $\bar{r}_z$ and z_i, i.e., ζ_i is on both paths $\mathcal{P}(r_z, \bar{r}_z)$ and $\mathcal{P}(r_z, z_i)$, and

$$d_{\mathcal{T}_Z}(\bar{r}_z, z_i) = d_{\mathcal{T}_Z}(r_z, \bar{r}_z) + d_{\mathcal{T}_Z}(r_z, z_i) - 2d_{\mathcal{T}_Z}(r_z, \zeta_i).$$

Note that the path-length order from the root of supports having the same ζ_i is preserved.

Therefore, one only needs to merge the ordered path-lengths from the root in those above cases with the complexity nearly $\mathcal{O}(N)$ (except the degenerated instance where each above case contains only one support).

Thus, one may not need to sort for tree metrics between $\bar{r}_z$ and each support of ν by leveraging the sorted order of the tree metrics between r_z and each support. Moreover, those computational steps can be done separately for each tree. Consequently, the complexity of $\mathcal{A}_f$ reduces from $\mathcal{O}(N^3 log N)$ into nearly $\mathcal{O}(N^2)$. More details can be seen in the supplementary (§C).

3.3 Aligned-root FlowAlign

We consider a special case of FlowAlign where roots have been already aligned[5]. Therefore, we can leave out minimization step with roots in Definition 1, and name it as aligned-root FlowAlign.

Definition 2. *Assume that root r_x in $\mathcal{T}_X$ is aligned with root r_z in $\mathcal{T}_Z$. Then, the aligned-root Flow-based Alignment discrepancy $\widehat{\mathcal{A}}_f$ between μ, ν is defined as*

$$\widehat{\mathcal{A}}_f^2(\mu,\nu;r_x,r_z) := \min_{T\in\Pi(\mu,\nu)} \sum_{i,j} \left|d_{\mathtt{T}_X}(r_x,x_i) - d_{\mathtt{T}_Z}(r_z,z_j)\right|^2 T_{ij}. \tag{3}$$

The $\widehat{\mathcal{A}}_f$ in Equation (3) is equivalent to the univariate Wasserstein distance (1d-OT) between $\tilde{\mu} := \sum_i a_i \delta_{d_{\mathtt{T}_X}(r_x,x_i)}$ and $\tilde{\nu} := \sum_j b_j \delta_{d_{\mathtt{T}_Z}(r_z,z_j)}$, which is equal to the integral of the absolute difference between the generalized quantile functions of these two univariate probability distributions (Santambrogio, 2015, §2). Therefore, one only needs to *sort* flow lengths $d_{\mathtt{T}_X}(r_x,x_i)\ |_i$, and $d_{\mathtt{T}_Z}(r_z,z_j)\ |_j$ for the computation of $\widehat{\mathcal{A}}_f$, i.e., linearithmic complexity. Due to sharing the same structure as 1d-OT, $\widehat{\mathcal{A}}_f$ inherits the same properties as those of the 1d-OT. More precisely, $\widehat{\mathcal{A}}_f$ is symmetric and satisfies the triangle inequality. Additionally, $\widehat{\mathcal{A}}_f(\mu,\nu;r_x,r_z) = 0$ is equivalent to $\tilde{\mu} \equiv \tilde{\nu}$. Furthermore, one can extend the squared loss (in Equation (2) and Equation (3)) into functions which are a nonnegative convex function g applied to the difference $(x-z)$ between two tree metrics, i.e., $g(x-z)$. See the supplementary (§B) for an illustration of $\widehat{\mathcal{A}}_f$.

Note that in practical applications, we usually do not have prior knowledge about tree structures for probability measures. Therefore, we need to sample tree metrics for each support data space. Moreover, by leveraging geometrically spatial information, we choose means of support data distributions as roots when using the clustering-based tree metric sampling (Le et al., 2019b) as a heuristic for sampling likely suboptimal *aligned-root tree metrics*. Consequently, we can reduce the complexity of FlowAlign by using aligned-root FlowAlign.

Aligned-root FlowAlign barycenter. The aligned-root FlowAlign can be handily used for a barycenter problem, especially in large-scale applications. Given m probability measures $\mu_i\ |_{i\in[m]}$ in different tree metric spaces $(\mathcal{T}_{X_i}, d_{\mathtt{T}_{X_i}})\ |_{i\in[m]}$ with aligned-roots $r_{x_i}\ |_{i\in[m]}$ respectively, and corresponding weights $p_i\ |_{i\in[m]}$, the aligned-root FlowAlign barycenter aims to find a flow-based tree structure[6] $\Delta_{\bar{\mu}} := \{d_{\mathtt{T}_X}(r_x,x_i), a_i\}_{i\in[\mathtt{k}]}$ of an optimal probability measure $\bar{\mu}$ with at most $\mathtt{k}$ supports in $(\mathcal{T}_X, d_{\mathtt{T}_X})$ that takes the form:

$$\Delta_{\bar{\mu}} \in \arg\min_{\Delta_{\hat{\mu}}} \left(\sum_{i=1}^{m} p_i \widehat{\mathcal{A}}_f^2(\hat{\mu},\mu_i;r_x,r_{x_i}) \right), \tag{4}$$

where the roots r_{x_i} in $\mathcal{T}_{X_i}\ |_{i\in[m]}$ are aligned with root r_x in $\mathcal{T}_X$. The barycenter problem in Equ. (4) is equivalent to the free-support 1d-OT barycenter efficiently solved, e.g., by using Alg. 2 in (Cuturi and Doucet, 2014).

4 Depth-based Alignment Discrepancy

FlowAlign only focuses on flows from a root to each support and tree root alignment, but ignores the depth level of supports in trees. In this section, we take into account the depth level of supports, and propose Depth-based Alignment (DepthAlign) discrepancy $\mathcal{A}_d$ by considering the alignment for flows hierarchically for each depth level along the tree structures. We first introduce some necessary definitions to define $\mathcal{A}_d$. Recall that, $\mathcal{S}(x)$ is a set of child nodes of x in $\mathcal{T}$.

Definition 3. *Given node x in $\mathcal{T}$, a 2-depth-level tree $\mathcal{T}_x^2$ is an induced subtree of $\mathcal{T}$, rooted as x and spanned by x and its children $\mathcal{S}(x)$.*

Let $V(\mathcal{T}_x^2)$ be the set of vertices of $\mathcal{T}_x^2$. Following Definition 3, $V(\mathcal{T}_x^2)$ contains x and all $\bar{x} \in \mathcal{S}(x)$. Moreover, given μ in $\mathcal{T}$, we have a corresponding $\mu_{\mathcal{T}_x^2}$ in $\mathcal{T}_x^2$, defined as $\mu_{\mathcal{T}_x^2} = \sum_i \bar{a}_i \delta_{\bar{x}_i}$ where $\bar{x}_i \in V(\mathcal{T}_x^2)$, and if $\bar{x}_i \neq x$ then

$$\bar{a}_i = \mu(\Gamma(\bar{x}_i))/\mu(\Gamma(x)),$$

otherwise

$$\bar{a}_i = 1 - \sum_{\bar{x}_j \in \mathcal{S}(x)} \mu(\Gamma(\bar{x}_j))/\mu(\Gamma(x)).$$

In order to define DepthAlign, we start with its special case when roots are aligned. Let $\mathcal{M}_h$ and $T_h^*(x,z)$ be a set of optimal aligned pairs and the optimal matching mass for the pair (x,z) at the depth level h respectively.

Definition 4. *Assume that root r_x in $\mathcal{T}_X$ is aligned with root r_z in $\mathcal{T}_Z$. Then, the aligned-root Depth-based Alignment $\widehat{\mathcal{A}}_d$ between μ, ν is defined as*

$$\widehat{\mathcal{A}}_d(\mu,\nu;r_x,r_z) := \sum_h \sum_{(x,z)\in\mathcal{M}_{h-1}} T_{h-1}^*(x,z) \widehat{\mathcal{A}}_f(\mu_{\mathcal{T}_x^2}, \nu_{\mathcal{T}_z^2}; x, z), \tag{5}$$

where h is the considered depth level, starting from 2 to the deepest level of the lower tree between $\mathcal{T}_X$ and $\mathcal{T}_Z$;

[5] By root alignment, we mean the optimal pair of roots in (r_x^*, r_z^*, T^*) in Equation (2).

[6] Recall that $\widehat{\mathcal{A}}_f$ is equivalent to 1d-OT, Δ_μ is a representation (e.g., supports and weights) in 1d-OT problem of a probability measure μ in $\widehat{\mathcal{A}}_f$ problem.

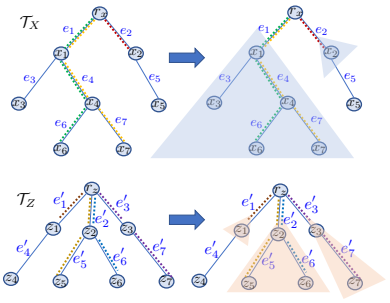

Figure 3: An illustration for aligned-root DepthAlign $\widehat{\mathcal{A}}_d$ between $\mu = a_1\delta_{x_6} + a_2\delta_{x_7} + a_3\delta_{x_2}$ on $\mathcal{T}_X$ and $\nu = b_1\delta_{z_1} + b_2\delta_{z_5} + b_3\delta_{z_6} + b_4\delta_{z_7}$ on $\mathcal{T}_Z$. In $\widehat{\mathcal{A}}_d$, we consider the optimal alignment at each depth level h. At $h = 1$, root r_x is trivially aligned for root r_z. Since r_x, r_z have their child nodes, the alignment (r_x, r_z) is recursive into $h = 2$. For μ in $\mathcal{T}_X$, r_x has 2 subtrees rooted at x_1, x_2. Thus, $V(\mathcal{T}^2_{r_x}) = \{r_x, x_1, x_2\}$, and $\mu_{\mathcal{T}^2_{r_x}} = (a_1 + a_2)\delta_{x_1} + a_3\delta_{x_2}$. Similarly, for ν in $\mathcal{T}_Z$, $\nu_{\mathcal{T}^2_{r_z}} = b_1\delta_{z_1} + (b_2 + b_3)\delta_{z_2} + b_4\delta_{z_3}$. The recursive procedure is repeated until the deepest level of the lower tree where only simple cases exist.

$\mathcal{M}_1 = \{(r_x, r_z)\}$; $T^*_1(r_x, r_z) = 1$. *Solving the optimal transport maps* $T^*_h(\cdot,\cdot)$ *of subproblems* $\widehat{\mathcal{A}}_f$ *at depth level* h *will form a set of optimal aligned pairs* $\mathcal{M}_h$.

Intuitively, at each depth level h, we consider the alignment for the corresponding 2-depth-level trees. Note that the 2-depth-level tree structures are at the same depth level h for both $\mathcal{T}_X$ and $\mathcal{T}_Z$, and one can consider $\widehat{\mathcal{A}}_f$ for such alignment. Moreover, at $h = 1$, $\widehat{\mathcal{A}}_d$ trivially matches r_x to r_z with optimal matching mass 1. Solving the optimal transport maps $T^*_h(\cdot,\cdot)$ of subproblems $\widehat{\mathcal{A}}_f$ at depth level h will form a set of optimal aligned pairs $\mathcal{M}_h$. Then, $T^*_h(\cdot,\cdot)$ and $\mathcal{M}_h$ are used in the next depth level $(h+1)$. Thus, the matching procedure is recursive along all depth levels in trees, illustrated in Figure 3. The simple case of the recursive procedure is that either at least one node of considered pair does not have child nodes, or sum of weights of child nodes in the corresponding 2-depth-level tree is equal to 0.

When roots of trees $\mathcal{T}_X$ and $\mathcal{T}_Z$ are not aligned yet, we optimize the root alignment as follow:

$$\mathcal{A}_d(\mu,\nu) := \min_{r_x, r_z} \widehat{\mathcal{A}}_d(\mu,\nu; r_x, r_z), \tag{6}$$

which is referred to as DepthAlign. Similar to FlowAlign, we have a following theorem:

Theorem 2. *DepthAlign is a pseudo-distance. It satisfies symmetry and the triangle inequality.*

See the supplementary (§A) for the proof of Theorem 2. When $\mathcal{A}_d(\mu,\nu) = 0$, we can find roots r^*_x and r^*_z such that all the hierarchical corresponding $\widehat{\mathcal{A}}_f(\mu_{\mathcal{T}^2}, \nu_{\mathcal{T}^2}; \cdot, \cdot)$ for each depth level along the trees are equal to 0. It demonstrates that μ and ν have similar weights on supports while their supports have similar depth levels, and for each depth level, the tree metrics of supports in the corresponding $\mu_{\mathcal{T}^2}, \nu_{\mathcal{T}^2}$ to the 2-depth-level-tree roots are identical, i.e., corresponding weight edges are identical.

DepthAlign computes a set of $\widehat{\mathcal{A}}_d$ subproblems hierarchically for each tree depth level. The number of $\widehat{\mathcal{A}}_d$ subproblems depends on the tree deepest level, and the number of assignments at each depth level. DepthAlign takes into account the depth level of each support which is not addressed in FlowAlign, but DepthAlign is much slower than FlowAlign.

5 Tree-sliced Variants by Sampling Tree Metrics

In practical applications, one usually do not have prior knowledge about tree structure for each probability measure. Computing FlowAlign/DepthAlign requires to choose or sample tree metrics for each space of supports. One way is to optimize tree metrics for probability measures from input data for a given task. However, this approach may be expensive and gives an extra cost for the computation of FlowAlign/DepthAlign.

Following the approach of TSW (Le et al., 2019b), we propose the tree-sliced variants for our proposed discrepancies, computed by averaging the corresponding FlowAlign/DepthAlign using randomly sampled tree metrics. We use fast adaptive methods, e.g., clustering-based tree metric sampling (Le et al., 2019b), to sample tree metrics from support data points of a given task.

Definition 5. *Given* μ, ν *supported on a set in which tree metric spaces* $\{(\mathcal{T}_{X_i}, d_{\mathcal{T}_{X_i}}) \mid i \in [n]\}$ *and* $\{(\mathcal{T}_{Z_i}, d_{\mathcal{T}_{Z_i}}) \mid i \in [n]\}$ *can be defined respectively, the tree-sliced variants of (aligned-root) FlowAlign/DepthAlign is defined as an average of corresponding (aligned-root) FlowAlign/DepthAlign for* μ, ν *on* $(\mathcal{T}_{X_i}, d_{\mathcal{T}_{X_i}})$, *and* $(\mathcal{T}_{Z_i}, d_{\mathcal{T}_{Z_i}})$ *respectively.*

As discussed in (Le et al., 2019b), the average over different random tree metrics can reduce quantization effects or clustering sensitivity problems in which data points may be clustered to adjacent but different clusters respectively in tree metric sampling. Moreover, the complexity of tree metric sampling is negligible. Indeed, for clustering-based tree metric sampling[7], its complexity is $\mathcal{O}(H_{\mathcal{T}} m \log \kappa)$ when one fixes the same number

[7] In principle, one can control the number of nodes in sampled trees by hyperparameters $(H_{\mathcal{T}}, \kappa)$ of the clustering-based tree metric sampling. We empirically follow suggestions in (Le et al., 2019b) to sample each tree containing about 4000 nodes.

of clusters κ for the farthest-point clustering (Gonzalez, 1985) and sets $H_{\mathcal{T}}$ for the predefined deepest level of tree $\mathcal{T}$, and m is the number of input data points.

Much like one-dimensional projections do not have interesting properties in a distortion viewpoint, but remain useful for SGW (or for sliced Wasserstein (Rabin et al., 2011)). We believe trees with high distortion can be useful for FlowAlign/DepthAlign (similar to TSW (Le et al., 2019b, §4)). Moreover, excessive efforts to optimize the problem in Equation (2) for each randomly sampled tree metric would be self-defeating since it would lead to overfitting within the computation of FlowAlign itself (see (Peyré and Cuturi, 2019, §8.4) and (Le et al., 2019b, §4)). Therefore, we apply the clustering-based tree metric sampling where we choose population means as tree roots as a heuristic based on geometrically spatial information to sample *aligned-root* tree metrics which are likely suboptimal in applications. Consequently, we can reduce the computational complexity of tree-sliced variants of FlowAlign/DepthAlign by using their aligned-root formulations with those randomly sampled *aligned-root* tree metrics.

6 Discussion and Related Work

For specific applications with prior knowledge about tree metrics for probability measures, one can apply FlowAlign, or consider DepthAlign if the known tree structure is important for the applications. Moreover, if roots of those known tree metrics are already aligned, one can use the corresponding aligned-root formulations to reduce the complexity. For general applications without prior knowledge about tree metrics for probability measures, one can use a heuristic to sample aligned-root tree metrics, e.g., by choosing a mean of support data as its root for the clustering-based tree metric sampling (Le et al., 2019b), and use the aligned-root formulations for an efficient computation.

Ultrametric (a.k.a, non-Archimedean or isosceles metric (Shkarin, 2004)) is a special case of tree metrics. Mémoli et al. (2019) employed ultrametric to study geometric and computational properties of Gromov-Hausdoff, and later basic topological and geometric properties of Sturm's distance (Sturm et al., 2006) and Gromov-Wasserstein in (Mémoli et al., 2021). Additionally, tree metrics are also used for other OT problems, e.g., tree-Wasserstein barycenter (Le et al., 2019a) and entropy partial transport (Le and Nguyen, 2021).

7 Experiments

We evaluate our proposed discrepancies for quantum chemistry and document classification with *random linear transformation* word embeddings[8]. We also carry out the large-scale FlowAlign barycenter problem within k-means clustering for point clouds of handwritten digits in `MNIST` dataset *rotated arbitrarily* in the plane as in (Peyré et al., 2016).

Setup. We consider two baselines: (i) SGW (Vayer et al., 2019) and (ii) EGW (Peyré et al., 2016). In all of our experiments, we do not have prior knowledge about tree metrics for probability measures. Therefore, we apply the clustering-based tree metric sampling (Le et al., 2019b) where means of support data points are chosen as tree roots, as a heuristic to sample *aligned-root* tree metrics from support data points. Thus, we can leverage the aligned-root formulations for both FlowAlign (FA) and DepthAlign (DA) to reduce their complexity. For SGW, we follow Vayer et al. (2019) to add artifact zero-padding for discrete measures having different numbers of supports, and use the binomial expansion to reduce its complexity. For EGW, we use the entropic regularization to optimize transport plan, but exclude it when computing GW, which gives comparative or better performances than those of standard EGW. We also apply the log-stabilized Sinkhorn (Schmitzer, 2019). We observe that the quality of EGW is better when entropic regularization becomes smaller, but the computation is considerably slower. In our experiments, the computation for EGW is either usually blown up, or too slow for evaluation when entropic regularization is less than or equal 1. We run experiments with Intel Xeon CPU E7-8891v3 (2.80GHz), and 256GB RAM. Reported time consumption for all methods has already included their corresponding preprocessing, e.g., tree metric sampling for FlowAlign and DepthAlign, or one-dimensional projection for SGW.

7.1 Applications

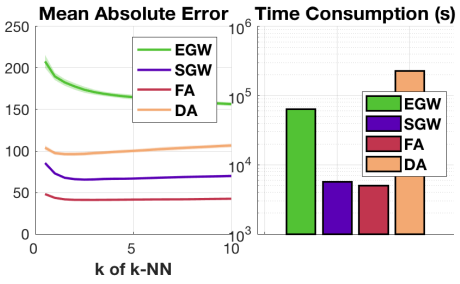

Figure 4: MAE and time consumption of k-NN regression on `qm7` for EGW (eps=5), SGW (10 slices), FA (10 tree-slices), and DA (1 tree-slice).

Quantum chemistry. We consider a regression problem on molecules for `qm7` dataset as in (Peyré et al., 2016). The task is to predict atomization energies for

[8] We apply different random linear transformation for word embedding in each document.

molecules based on similar labeled molecules instead of estimating them through expensive numerical simulations (Rupp et al., 2012; Peyré et al., 2016).

For simplicity, we only used the relative locations in $\mathbb{R}^3$ of atoms in molecules, *without information about atomic nuclear charges* as the experiments in (Rupp et al., 2012; Peyré et al., 2016). Therefore, a molecule with t atoms is represented as a probability measure $\mu = \frac{1}{t}\sum_{i=1}^{t}\delta_{x_i}$ where x_i is the relative location of atom i in $\mathbb{R}^3$. We randomly split 80%/20% for training and test sets, and repeat 20 times. As in (Peyré et al., 2016), we use k-nearest neighbor (k-NN) regression.

Document classification with non-registered word embeddings. We also evaluate our proposed discrepancies for document classification with non-registered word embeddings in `TWITTER`, `RECIPE`, `CLASSIC`, and `AMAZON` datasets. For each document in these datasets, we apply different *random linear transformation* for *word2vec* word embedding (Mikolov et al., 2013), pre-trained on Google News[9], containing about 3 million words/phrases. *word2vec* maps those words/phrases into $\mathbb{R}^{300}$. Following Kusner et al. (2015); Le et al. (2019b), we remove SMART stop words (Salton and Buckley, 1988), and drop words in documents if they are not in the pre-trained *word2vec*. Therefore, each document can be considered as an empirical measure where each word and its frequency are regarded as a support and its weight respectively. We randomly split 80%/20% for training and test sets, and repeat 20 times.

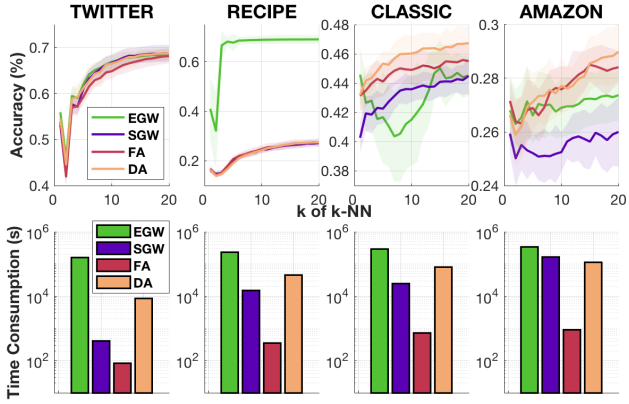

Figure 5: Accuracy and time consumption of k-NN classification on document datasets for EGW (eps=5 in `TWITTER`, and eps=10 in others), SGW (10 slices), FA (10 tree-slices), and DA (1 tree-slice).

Performance results, time consumption and discussions. The results of averaged mean absolute value (MAE) for different k in k-NN regression, and time consumption of quantum chemistry in `qm7` dataset are illustrated in Figure 4, while the results of averaged accuracy for different k in k-NN, and time consumption of document classification with non-registered word embeddings in `TWITTER`, `RECIPE`, `CLASSIC`, and `AMAZON` datasets are shown in Figure 5.

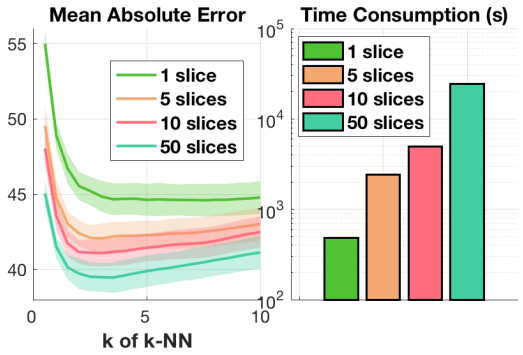

Figure 6: Trade-off between performances and time consumption for FlowAlign w.r.t. tree slices in `qm7`.

The computational time of FlowAlign is at least comparative to that of SGW, and several-order faster than that of EGW. Especially, in `CLASSIC`, it took 12 minutes for FlowAlign (10 slices), while 6.8 hours for SGW (10 slices), and 3.3 days for EGW (entropic regularization eps=10). Moreover, the performances of FlowAlign compare favorably with other baselines, except EGW in RECIPE dataset. FlowAlign performs better when the number of tree slices is increased, but its time consumption is also increased linearly. We show this trade-off on `qm7` in Figure 6. For DepthAlign, its performances are comparative with other baselines. However, DepthAlign is slow in practice due to solving a large number of sub-problems, i.e., aligned-root FlowAlign between corresponding 2-depth-level trees. For EGW, its performances are improved when the entropic regularization small enough for the problems, but its computational time is considerably increased which makes EGW unsuitable for large-scale applications. The value of entropic regularization is important for performances of EGW, e.g., EGW performs well in `RECIPE`, and is comparative with other approaches on other datasets. For SGW, its computational time is slow down when document lengths are large, e.g., in `AMAZON` dataset, since it requires to use extra artificial zeros padding and uniform weights for probability measures with different number of supports (i.e., documents with different lengths), while other approaches work with an original number of supports (i.e., unique words in documents), and general weights (i.e., frequencies of unique words) for supports in probability measures.

Similar to tree metric sampling for TSW (Le et al., 2019b), we observe that the clustering-based tree metric sampling for FlowAlign and DepthAlign is fast and its time consumption is negligible compared to that of either FlowAlign or DepthAlign. For examples, for each

[9] https://code.google.com/p/word2vec

tree metric sampling with the suggested parameters (e.g., the predefined deepest level $H_{\mathcal{T}} = 6$, and the number of clusters $\kappa = 4$ for the farthest-point clustering), it only took about $0.4, 1.5, 11.0, 17.5, 20.5$ seconds for `qm7`, `TWITTER`, `RECIPE`, `CLASSIC`, and `AMAZON` datasets respectively.

We further randomly sample 1 million pairs of distributions in `qm7` dataset and compare FlowAlign $\mathcal{A}_f$ using the optimization in Equation (2) (i.e., optimize the roots r_x, r_z and the transport plan T), and *aligned-root* FlowAlign $\widehat{\mathcal{A}}_f$ in Equation (3) with the heuristic of sampling *aligned-root* tree metrics by using clustering-based tree metric sampling where we choose population means as tree roots (i.e., only optimize the transport plan T with the sampled suboptimal *aligned-root* tree metrics). There are 68.12% of those randomly sampled suboptimal aligned-root tree metrics using the heuristic for $\widehat{\mathcal{A}}_f$ that are actually *optimal* when we optimize $\mathcal{A}_f$ with those sampled trees (the optimization problem for FlowAlign in Equation (2)), and the average relative difference $(\widehat{\mathcal{A}}_f - \mathcal{A}_f)/\mathcal{A}_f$ is 0.0244. Therefore, the sampled *aligned-root* tree metrics are likely suboptimal that not only help to reduce the complexity of the proposed discrepancies by using their aligned-root formulations, but also play as an efficient regularization for the computation of FlowAlign/DepthAlign in applications. Moreover, there is no need for paying too much efforts to optimize the proposed discrepancies with respect to each randomly sampled tree metric since it would lead to overfitting within the computation of FlowAlign/DepthAlign (Peyré and Cuturi, 2019, §8.4), (Le et al., 2019b, §4).

Further experimental results about performances and time consumptions of the discrepancies with different parameters (e.g., entropic regularization in EGW, and number of (tree) slices in SGW, FlowAlign and DepthAlign), and clustering-based tree metric sampling with different parameters (i.e., $H_{\mathcal{T}}, \kappa$ for tree depths and branches respectively) can be seen in the supplementary (§D).

We emphasize that the proposed discrepancies are novel for probability measures in different tree metric spaces, and we do not try to mimic or approximate either GW (with tree metrics) or EGW/SGW. Besides their relations in Proposition 1, we also thoroughly investigate their empirical relations in the supplementary (§G).

7.2 Large-scale FlowAlign barycenter within k-means clustering

We applied FlowAlign barycenter (§3.3), using Algorithm 2 in (Cuturi and Doucet, 2014) where we set `k` = 100 for the maximum number of supports in barycenters, into a larger machine learning pipeline such as k-means clustering on `MNIST` dataset where point clouds of handwritten digits are *rotated arbitrarily* in the plane as in (Peyré et al., 2016). For each handwritten digit, we randomly extracted 6000 point clouds. We evaluated k-means with FlowAlign for 60K, 120K, 240K, 480K, and 960K handwritten-digit point clouds where each handwritten digit is *randomly rotated* $1, 2, 4, 8$, and 16 times respectively. Furthermore, we grouped the handwritten digit 6 and digit 9 together due to applying random rotation. We used k-means++ initialization technique (Arthur and Vassilvitskii, 2007), set 20 for the maximum iterations of k-means, and repeated 10 times with different random seeds for k-means++ initialization. In Figure 7, we show the averaged time consumption and F_β measure (Manning et al., 2008) where β is chosen as in (Le and Cuturi, 2015) for the results of k-means clustering with FlowAlign. Note that, in these settings, the barycenter problem from EGW has extremely slow running time. A small experimental setup for performance comparison can be found in the supplementary (§D).

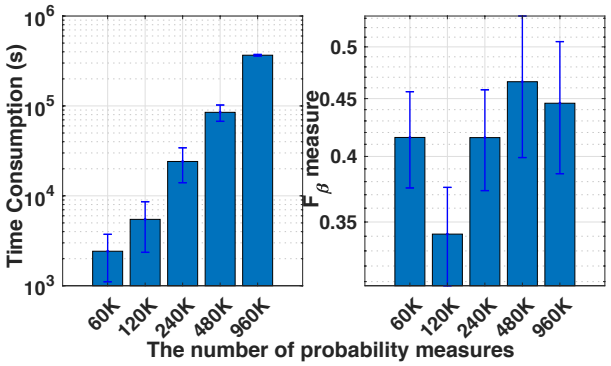

Figure 7: Time consumption and F_β measure for k-means clustering with FlowAlign for *randomly rotated* `MNIST`.

8 Conclusion

We proposed two discrepancies FlowAlign and DepthAlign for probability measures whose supports are in different tree metric spaces. The FlowAlign is not only several order faster than EGW and at least as fast as SGW while remedies its curse of dimensionality, but its performances also compare favorably with those of variants of GW baselines. Moreover, FlowAlign can be applied for large-scale applications (e.g., a million probability measures) which are usually prohibited for (entropic) GW. The questions about sampling efficiently tree metrics from support data points for the proposed discrepancies, or using them for more involved parametric inference are left for the future work.

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