Towards Optimal Transport with Global Invariances

David Alvarez-Melis Stefanie Jegelka Tommi S. Jaakkola dalvmel@mit.edu
 stefje@mit.edu
 tommi@mit.edu

Abstract

Many problems in machine learning involve calculating correspondences between sets of objects, such as point clouds or images. Discrete optimal transport (OT) provides a natural and successful approach to such tasks whenever the two sets of objects can be represented in the same space or when we can evaluate distances between the objects. Unfortunately neither requirement is likely to hold when object representations are learned from data. Indeed, automatically derived representations such as word embeddings are typically fixed only up to some global transformations, for example, reflection or rotation. As a result, pairwise distances across the two types of objects are ill-defined without specifying their relative transformation. In this work, we propose a general framework for optimal transport in the presence of latent global transformations. We discuss algorithms for the specific case of orthonormal transformations, and show promising results for unsupervised word alignment.

1 Introduction

Optimal transport (OT) plays dual roles across machine learning applications. On the one hand, it provides a well-founded, geometrically driven approach to realizing correspondences between sets of objects such as shapes in different images. Such correspondences can be used for image registration [Haker and Tannenbaum, 2001] or to interpolate between them [Solomon et al., 2015]. More generally, optimal transport extends to problems such as domain adaptation where we wish to transport a set of labeled source points to the realm of the target task [Courty et al., 2017a,b]. On the other hand, by solving the optimal transport problem we induce a theoretically well-characterized distance between sets of objects. This distance is expressed in the form of a transport cost and serves as a natural population difference measure. It can be therefore exploited as a source of feedback in adversarial training [Arjovsky et al., 2017, Bousquet et al., 2017]. Our focus in this paper is on the optimal coupling mediating the transport, i.e., realizing the latent correspondences between the objects.

One of the key deficiencies of traditional OT is that it assumes that the two sets of objects in question are represented in the same space. At minimum, it assumes that one should be able to measure meaningful pairwise distances across the two sets of objects. This is not always the case, especially when the objects are represented by learned vectors. For example, word embedding algorithms operate at the level of inner products or distances between word vectors [Artetxe et al., 2018a, Conneau et al., 2018]. The vector representations of words produced by such algorithms can be therefore arbitrarily rotated, sometimes even for different runs of the same algorithm on the same data. Such global

degrees of freedom left in the vector representations render direct pairwise distances between objects across the sets meaningless. Indeed, traditional OT is *locally greedy* as it focuses on minimizing individual movement of mass, oblivious to global transformations. As a concrete example, consider two identical sets of points where one set is subjected to a global rotation. The optimal transport coupling evaluated between the resulting sets may no longer recover the correct mapping between the points.

When the global (relative) transformation is known or can be easily evaluated separately, it can be incorporated in the computation of pairwise distances, thereby enabling the use of traditional OT. Unfortunately, only the type of transformation such as rotation is typically known, not the actual realization. In such cases, we would intuitively like the optimal transport problem to also solve for the best latent transformation together with the optimal coupling. In other words, we seek a formulation of optimal transport that remains invariant under classes of global transformations.

In this work, we propose a generalization of the discrete optimal transport problem that incorporates global invariances directly into the optimization problem. While our discussion is primarily focused on rigid transformations of euclidean space (arguably, the most common case encountered in practice), our framework is more general and opens the door to other types of invariances to be encoded. Moreover, our approach unifies previous methods for fusing OT with global transformations such as Procrustes mappings [Grave et al., 2018, Rangarajan et al., 1997, Zhang et al., 2017b], and reveals unexpected connections to the Gromov-Wasserstein distance [Mémoli, 2011], a recent similarity-based generalization of OT.

The main contributions of this work are thus:

- A modified formulation of the discrete optimal transport problem that allows for global geometric transformations incorporated into the cost objective
- Design and analysis of efficient algorithms for the case of rigid transformations
- An application of the framework to the problem of unsupervised word alignment, demonstrating performance comparable to the state-of-the-art at a fraction of the computational cost of alternative approaches

2 Related Work

The general problem of finding correspondences between two sets of features in a fully unsupervised way is well-studied and arises in various fields, under different names, such as manifold alignment [Wang and Mahadevan, 2009], feature set matching [Grauman and Darrell, 2005] and feature correspondence finding [Torresani et al., 2008]. Here, we focus our survey of related work on methods that combine correspondence search via soft correspondences (such as those derived from optimal transport distances) with explicit space alignment.

Perhaps the earliest such approach is by Rangarajan et al. [1997], who derive a framework to establish correspondences between shapes that rejects non-homologies (e.g., rotations) based on a entropy-regularized version of the optimal transport problem. The

resulting algorithm, which they refer to as the *Softassign Procrustes Algorithm*, proceeds iteratively by alternating between estimating optimal rotations and and Sinkhorn iterations. Their approach, however, only considers rotations, and is tailored to the 2-dimensional case, where rotations can be easily parametrized.

More recently, Zhang et al. [2017b] propose combining optimal transport distances with Procrustes alignment to find correspondences between word embedding spaces. They initialize their orthogonal mapping using an adversarial training phase, much like Conneau et al. [2018], and solve the optimization problem with alternating minimization. Our approach differs from theirs: by bootstrapping on the solution of a smaller problem to initialize the mapping, we avoid the need for a neural network initialization that is used in their approach. In addition, our annealing scheme on the entropic regularization leads to smooth convergence, with very little sensitivity to initialization.

Concurrently with our work, Grave et al. [2018] tackle the problem of unsupervised word embedding alignment with a similar optimization framework as the one proposed by Zhang et al. [2017b], combining Wasserstein distances (an instance of optimal transport distances) and Procrustes alignment. Their approach differs from Zhang et al. [2017b] in how they scale up optimization, by relying on a stochastic Sinkhorn solver [Genevay et al., 2018]. In addition, they initialize their approach by solving a convex relaxation of the the original problem.

Although driven by a similar motivation (word embedding alignment) and relying on similar principles (joint optimization of optimal transport coupling and feature mapping) as the work of Zhang et al. [2017b] and Grave et al. [2018], our approach differs from them in several aspects. First, we allow for more general types of invariance Schatten-norm classes, subsuming orthogonal invariance considered in prior work as a special case. Second, we dispense with the need for any ad-hoc initialization by introducing instead a convexity-annealing approach to optimization. Third, our approach remains robust to the choice of entropy regularization parameter λ . Curiously, the relaxation proposed by Grave et al. [2018] as initialization corresponds to solving a hybrid version of two instances of our framework for $p = \infty$ (since they optimize over orthogonal matrices) and p = 2 (since their relaxed objective uses the Frobenius norm).

A different generalization of the optimal transport problem aimed at addressing lack of intrinsic correspondence between the spaces to be aligned is the Gromov-Wasserstein distance [Mémoli, 2011]. While our framework recovers the Gromov-Wasserstein distance in certain scenarios (see 4.2), it is best understood as a compromise between the the classic formulation of optimal transport that requires the spaces to be fully registered, and the Gromov-Wasserstein distance, which completely forgoes explicit computation of distances across spaces and instead relies on comparison of intra-space similarities. Thus, our approach is best suited to settings where indeed distances can be computed across spaces, but they need to be made invariant to a known specific class of transformations (e.g., orthogonal, low-rank, etc). A further difference is that our approach produces, as intrinsic part of optimization, a mapping which can be used to transport *out-of-sample points* from one space to the other, which both the usual optimal transport and Gromov-Wasserstein

¹The preprint of Grave et al. [2018] was brought to our attention while completing this manuscript.

distances lack.

3 Motivation: Correspondences between feature spaces

Notation. Throughout this work, we denote vectors and matrices with bold font (e.g., \mathbf{x} , \mathbf{X}), their entries without it (x_i, X_{ij}) , and sets as X, Y. We use super-indices to enumerate vectors, and subindices to denote their entries. For matrices \mathbf{A} , \mathbf{B} , we denote by $\langle \mathbf{A}, \mathbf{B} \rangle$ their Frobenius inner product, i.e., $\langle \mathbf{A}, \mathbf{B} \rangle = \operatorname{tr}(\mathbf{A}^T\mathbf{B}) = \sum_{i,j} [\mathbf{A}]_{ij} [\mathbf{B}]_{ij}$, and by $\|\cdot\|_*$ the nuclear (trace, Ky-Fan) matrix norm.

In the unsupervised feature correspondence problem we are given two sets of examples, say $X = \{\mathbf{x}^{(i)}\}_{i=1}^n$ and $Y = \{\mathbf{y}^{(j)}\}_{j=1}^m$, with $\mathbf{x}^{(i)} \in \mathcal{X} \subset \mathbb{R}^{d_x}$ and $\mathbf{y}^{(j)} \in \mathcal{Y} \subset \mathbb{R}^{d_y}$. Here \mathcal{X} and \mathcal{Y} are potentially distinct feature spaces. For simplicity of presentation, we will assume for now that m = n and $d_x = d_y$.

As stated before, our goal is to learn correspondences between the two collections X and Y, in the challenging case where no previous instance-wise correspondences are known—i.e., the problem is fully unsupervised—and the spaces \mathcal{X} and \mathcal{Y} are unregistered—i.e., the *global* correspondence between these two representation spaces is unknown. This problem can be thought of as consisting of two sub-problems: (i) finding correspondences between the items in X and Y, via an assignment $\mathcal{A}: [1,n] \mapsto [1:m]$ such that $\mathbf{x}^{(i)} \leftrightarrow \mathbf{y}^{(j)}$ if point $\mathbf{x}^{(i)}$ corresponds to $\mathbf{y}^{(j)}$ and (ii) finding a global correspondence of spaces \mathcal{X} and \mathcal{Y} , e.g., via a mapping $T: \mathcal{X} \to \mathcal{Y}$ such that $T(\mathbf{x}) = \mathbf{y}$ for every correspondence pair (\mathbf{x}, \mathbf{y}) . As with the assignment approach, requiring this condition to be satisfied exactly for all points is likely to too strong an assumption. Hence, we instead seek T that minimizes $d(T\mathbf{x}^{(i)}, \mathbf{y}^{(j)})$ with respect to some metric d.

Individually, these two problems (namely, finding instance-wise correspondences and estimating global mappings between feature spaces) are well-studied and understood. Below, we briefly discuss popular approaches to tackle each of them. Then, in Section 4, we show how they can be combined to enforce invariances in the optimal transport problem, leading naturally to a flexible class of problems which can be solved efficiently.

3.1 Space alignment from paired samples

The problem of estimating mappings between euclidean spaces based on finite samples usually assumes known correspondences between these finite samples. Formally, given collections $X = \{\mathbf{x}^{(i)}\}_{i=1}^n$ and $Y = \{\mathbf{y}^{(j)}\}_{j=1}^m$, let \mathbf{X} and \mathbf{Y} be matrices whose columns correspond to these elements. Assume we seek to find a mapping that approximately maps columns of \mathbf{X} into the columns of \mathbf{Y} in that order (i.e., the i-th column of \mathbf{X} is to be mapped to the i-th column of \mathbf{Y}). Then, a general formulation in matrix notation of this problem can be expressed as

$$\min_{T \in \mathcal{F}} \|\mathbf{X} - T(\mathbf{Y})\|^2 \tag{1}$$

where \mathcal{F} is some class of functions and $\|\cdot\|$ is a matrix norm, typically taken to be the Frobenius norm $\|A\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2}$. Naturally, the difficulty of finding T, as well as the quality of the alignment implied by it, both depend on the choice of space \mathcal{F} . Depending

on the constraints imposed on the function space from which such a mapping is to be estimated, the problem can take many different—often seemingly disconnected—forms.

A classic approach constrains the type of admissible transformations to linear, unitary operators—i.e., orthogonal matrices for real spaces. The orthogonal Procrustes problem,² a classic matrix approximation problem in linear algebra, reads:

$$\min_{\mathbf{P}\in O(n)} \|\mathbf{X} - \mathbf{PY}\|_F^2 \tag{2}$$

The restriction that **P** be orthogonal effectively restricts the type of admissible transformations to rotations and reflections. Despite its simplicity, the Procrustes problem is a popular tool, used in various applications, from statistical shape analysis [Goodall, 1991] to market research and others [Gower et al., 2004]. Its main advantage is that it has a closed-form solution, in terms of the singular value decomposition (SVD) of XY^T , as first shown by Schönemann [1966]. Namely, given an SVD decomposition $U\Sigma V^T$ of XY^T , the orthogonal matrix minimizing problem (2) is:

$$\mathbf{P}^* = \mathbf{U}\mathbf{V}^T$$

the proof is simple, and a direct consequence of a well-known property of the singular value decomposition (SVD):

Lemma 3.1. If $\mathbf{A} \in \mathbb{R}^{n \times m}$ and $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$ is an SVD of \mathbf{A} , then

$$\underset{\mathbf{P}\in O(n)}{\operatorname{argmin}}\langle \mathbf{P}, \mathbf{A}\rangle = \mathbf{U}\mathbf{V}^T$$

As mentioned before and evidence by objective (2), the Procrustes approach is intrinsically a *supervised* method, since it completely relies on the fact that the columns of **X** and **Y** are paired, i.e., there is an a-priori known matching between instances of the two domains. Thus, its application to the problem of feature alignment requires either an —ideally small— set of true paired examples [Zhang et al., 2016] or a method to generate pseudo-pairs [Conneau et al., 2018].

3.2 Finding correspondences between aligned spaces

Optimal transport is popular approach for finding correspondences between vectors, enjoying strong theoretical results and fast algorithms. The original formulation of the problem dates back to Gaspar Monge, who was interested in finding optimal ways to transport coal from mines to factories. Optimal transport considers two measures μ and ν over spaces \mathcal{X} and \mathcal{Y} respectively, and a transportation cost $c: \mathcal{X} \times \mathcal{Y} \to \mathbb{R}^+$. It seeks to minimize the cost of *transporting* space \mathcal{X} to \mathcal{Y} while preserving the measure μ onto ν . In its original discrete formulation, μ and ν are empirical distributions:

$$\mu = \sum_{i=1}^{n} p_i \delta_{\mathbf{x}^{(i)}}, \quad \nu = \sum_{j=1}^{m} q_j \delta_{\mathbf{y}^{(j)}}$$
(3)

²The problem owes its name to Procrustes (Προχρούστης), a rogue smith in the Greek mythology who infamously made his victims fit in an iron bed by stretching or cutting their limbs.

so the cost function need only be specified for every pair $(\mathbf{x}^{(i)}, \mathbf{y}^{(j)})$, i.e., it is a matrix $\mathbf{C} \in \mathbb{R}^{n \times m}$. Monge's formulation involves finding a transport map $T : \mathcal{X} \to \mathcal{Y}$, with $T(\mathbf{x}^{(i)}) = \mathbf{y}^{(i)}$ for every i, which realizes:

$$\min_{T} \sum_{i=1}^{n} c(\mathbf{x}^{(i)}, T(\mathbf{x}^{(i)})) \tag{4}$$

The solution to this problem might not exist, and even if it does, finding it corresponds to solving an assignment problem, known to be NP-hard. A relaxation of this problem by Kantorovich considers instead "soft" assignments defined in terms of probabilistic *transportation couplings* $\Gamma \in \mathbb{R}^{n \times m}_+$ whose marginals recover μ and ν . Formally, Kantorovich's formulation seeks Γ in the transportation polytope

$$\Pi_{\mu,\nu} = \{ \Gamma \in \mathbb{R}_+^{n \times m} \mid \Gamma \mathbf{1} = \mathbf{p}, \ \Gamma^T \mathbf{1} = \mathbf{q} \}. \tag{5}$$

that solves

$$\min_{\Gamma \in \Pi_{u,v}} \langle \Gamma, \mathbf{C} \rangle. \tag{6}$$

We refer to (6) as the discrete optimal transport (DOT) problem. If n = m, and μ and ν are uniform measures, $\Pi_{\mu,\nu}$ is the Birkhoff polytope of size n, and the solutions of problem (6), which lie in the corners of this polytope, are permutation matrices.

DOT is a linear program, and thus can be solved exactly in $O(n^3 \log n)$ with interior point methods. In practice, a version with entropic smoothing has proven more efficient [Cuturi, 2013]:

$$\min_{\Gamma \in \Pi} \langle \Gamma, C \rangle - \frac{1}{\lambda} H(\Gamma). \tag{7}$$

This is a strictly convex optimization problem, whose solution of this strictly has the form $\Gamma^* = \operatorname{diag}(u) \operatorname{\mathbf{K}} \operatorname{diag}(v)$, with $\operatorname{\mathbf{K}} = e^{-\frac{C}{\lambda}}$ where the exponential is computed entry-wise [Peyré and Cuturi, 2018], and can be obtained efficiently via the Sinkhorn-Knopp algorithm, an iterative matrix-scaling procedure [Cuturi, 2013]. Besides significant speedups, the smoothed problem often leads to better empirical results in downstream applications that benefit from soft alignments, e.g., when correspondences are computed between noisy features for which sparse correspondences might be too strict.

Optimal transport is an obvious choice for the problem of finding correspondences between spaces in a fully unsupervised way. Instead of relying on a-priori alignment of instances of the two spaces as the Procrustes problem does, DOT instead infers a geometrically-optimal correspondence matrix between all the instances. However, naive application of DOT often fails in applications where the two spaces $\mathcal X$ and $\mathcal Y$ are not registered: i.e., when there is no a priori meaningful notion of distance between them. This the case, for example, when $\mathcal X$ and $\mathcal Y$ are learnt euclidean feature spaces for which absolute positions are meaningless and the only relevant aspect is the relative positions of elements in the space. Thus, even if the elements of these spaces are of the same dimension, computing euclidean distance between them is meaningless, since there is no guarantee that their coordinate axes are consistent with each other. This the case for the motivating

application of word embedding alignment, where the embedding spaces across languages (and even across different runs of the same algorithm) are not aligned.

In the absence of a native alignment between spaces, we seek a notion of distance that is invariant to global transformations of the space, e.g., to rotations, or more generally, the action of operators in a certain function class. Yet, optimal transport is locally greedy: it tries to find optimal—i.e., little displacement—matchings and is oblivious to such global invariances. In the next section we propose a framework to endow OT with invariance to a general class of global transformations.

4 Transporting with Global Geometric Invariances

Our goal in this work is to extend the DOT problem (6) to enforce invariance with respect to certain classes of transformations. Formally, we assume there exists an unknown function f in a pre-specified class \mathcal{F} which characterizes the global correspondence between spaces $\mathcal{X} \subseteq \mathbb{R}^d$ and $\mathcal{Y} \subseteq \mathbb{R}^d$, i.e., for which $\mathcal{X} = \{\mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = f(\mathbf{y}), \, \mathbf{y} \in \mathcal{Y}\}$ is the preimage of \mathcal{Y} . Naturally, the choice of \mathcal{F} should be informed by the application domain.

In this setting, given collections $\{\mathbf{x}^{(i)}\}_{i=1}^n$, $\mathbf{x}^{(i)} \in \mathcal{X}$ and $\{\mathbf{y}^{(j)}\}_{j=1}^m$, $\mathbf{y}^{(j)} \in \mathcal{Y}$ and associated empirical measures μ, ν , we seek to simultaneously find the best global transformation of the space (within \mathcal{F}) and the best local correspondences between the two collections, as defined by the optimal transport problem. In other words, we seek to jointly optimize $f \in \mathcal{F}$ and $\Gamma \in \Pi(\mu, \nu)$ to minimize the transportation cost between the two empirical distributions. Formally, given a choice of invariance set, for any $f \in \mathcal{F}$ let $f(\mathbf{Y})$ denote the matrix of size $d \times m$ whose columns are $f(\mathbf{y}^{(j)})$. The problem we wish to solve is

$$\min_{\Gamma \in \Pi(\mu,\nu)} \min_{f \in \mathcal{F}} \langle \Gamma, C(\mathbf{X}, f(\mathbf{Y})) \rangle \tag{8}$$

In this work, we focus on invariances defined by linear operators with bounded norm:

$$\mathcal{F}_p := \{ \mathbf{P} \in \mathbb{R}^{d \times d} \mid ||\mathbf{P}||_p \le k_p \}$$
(9)

where $\|\cdot\|_p$ is the Schatten ℓ_p -norm, that is, $\|\mathbf{P}\|_p = \|\sigma(\mathbf{P})\|_p$ where $\sigma(\mathbf{P})$ is a vector containing the singular values of \mathbf{P} . In addition, k_p is a norm- and problem-dependent constant.³ This choice of invariance sets follows both modeling and computational motivations. As for the former, Schatten norms allow for immediate interpretation of the elements of \mathcal{F}_p in terms of their spectral properties. For example, choosing p=1 encourages solutions with sparse spectra (e.g., projections, useful when the support of one of the two distributions is known to be contained in a lower-dimensional subspace), while $p=\infty$ instead seeks solutions with uniform spectra (e.g., unitary matrices, to enforce invariance to rigid transformations, cf. Section 4.1). Intermediate values of p interpolate between these two extremes. Surprisingly, the choice p=2 recovers a recent popular generalization of the optimal transport problem motivated by a similar goal: the Gromov-Wasserstein distance [Mémoli, 2011], as we show in Section 4.2. Thus, the proposed Schatten invariance framework offers significant flexibility. In terms of computation, Schatten norms

³In the most common case, k_p would be chosen to ensure the identity mapping is contained in this set.

exhibit various desirable properties, such as isometric invariance, submultiplicativity, and easy characterization via duality, all of which play an important role in deriving efficient optimization algorithms below.

Here, we will formulate the problem for the case where the ground metric c is the squared euclidean distance, i.e, $c(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2^2$, which is arguably the most common choice in practice. In this case, the objective (8) (for a fixed f) corresponds to the (squared) 2-Wasserstein distance between μ and ν . With this choice of ground metric, let \mathbf{u}, \mathbf{v} be vectors with entries $u_i = \|\mathbf{x}^{(i)}\|_2^2$, and $v_j = \|\mathbf{P}\mathbf{y}^{(j)}\|_2^2$ respectively. Then, it is easy to show that (8) becomes:

$$\max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} 2\langle \Gamma, \mathbf{X}' \mathbf{P} \mathbf{Y} \rangle - \langle \mathbf{u}, \mu \rangle - \langle \mathbf{v}, \nu \rangle$$
 (10)

This objective has a clear interpretation. The first term, which can be equivalently written as $\langle \mathbf{X}\Gamma, \mathbf{PY}\rangle$, measures agreement between $\mathbf{X}\Gamma$, the source points mapped according to the barycentric mapping implied by Γ , and \mathbf{PY} , the target points mapped according to \mathbf{P} . The other two terms, which can be interpreted as empirical expectations $\hat{\mathbb{E}}_{\mathbf{x}\sim\mu}\|\mathbf{x}\|_2^2$ and $\hat{\mathbb{E}}_{\mathbf{y}\sim\nu}\|\mathbf{Py}\|_2^2$, act as a counterbalance, normalizing the objective and preventing artificial maximization of the similarity term by arbitrary scaling of the mapped vectors.

In general, the problem (10) is concave in either variable if the other one is fixed. Hence, we can solve it via an alternating optimization approach, updating \mathbf{P} and Γ in alternation. Since only the first term depends on Γ , optimizing (10) for a fixed \mathbf{P} is a usual transportation problem, for which we discuss optimization in Section 4.4. On the other hand, the problem in \mathbf{P} for a fixed Γ is a concave maximization over a compact and convex set, which given the fact that computing projections onto Schatten ℓ_p -norm balls is tractable, can be solved efficiently with Frank-Wolfe-type algorithms [Jaggi, 2013].

While the approach outlined above provides a tractable way to solve problem (10) in general, we show next that under conditions that hold in many cases in practice, we can do even better. For this, we recall that neither of the last two terms in problem (10) depends on Γ , while only the last one depends on \mathbf{P} . The following lemma shows that under simple conditions imposed on the invariance set, we can remove dependency of this last term on \mathbf{P} and thus simplify the objective into a linear one. All proofs are provided in the Appendix.

Lemma 4.1. If any of the following conditions holds;

- 1. $\forall P \in \mathcal{F}$, P is angle-preserving (i.e., $\forall x, y \langle Px, Py \rangle = \langle x, y \rangle$).
- 2. $\exists k \geq 0 : \|\mathbf{P}\|_F = k \quad \forall \mathbf{P} \in \mathcal{F} \text{ and the matrix } \mathbf{Y} \text{ is } \nu\text{-whitened (i.e., } \mathbf{Y} \operatorname{diag}(\mathbf{q})^2 \mathbf{Y}' = \mathbf{I}_d),$

then problem (10) is equivalent to

$$\max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} \langle \Gamma, \mathbf{X}' \mathbf{P} \mathbf{Y} \rangle = \max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} \langle \mathbf{X} \Gamma \mathbf{Y}', \mathbf{P} \rangle \tag{11}$$

Assumption (1) in Lemma 4.1 is a reasonable requirement to impose on **P** as it guarantees it preserves geometric relations across spaces. On the other hand, whitening is a common pre-processing step in feature representation learning [Hyvärinen and Oja,

2000] and correspondence problems [Artetxe et al., 2018b]. Thus, the conditions 4.1 often hold in practice.

The following result, a generalization of Lemma 3.1, shows that when optimizing over Schatten ℓ_p -norm balls, the inner problem in (11) admits a closed form solution in terms of a singular value decomposition.

Lemma 4.2. Let **M** be a matrix with SVD $\mathbf{M} = \mathbf{U}\Sigma\mathbf{V}'$ and let $\Sigma = \operatorname{diag}(\boldsymbol{\sigma})$, then

$$\underset{P:\|P\|_p \le k}{\operatorname{argmax}} \langle P, M \rangle = U \operatorname{diag}(s) V'$$
(12)

where **s** is such that $\|\mathbf{s}\|_p \leq k$ and attains $\mathbf{s}'\boldsymbol{\sigma} = k\|\boldsymbol{\sigma}\|_q$, for $\|\cdot\|_q$ the dual norm of $\|\cdot\|_p$.

Therefore, Lemma 4.2 states the inner problem in (11) boils down to finding maximizers of the support function of vector-valued ℓ_p balls, which can be done in closed form for any $p \geq 1$ by choosing $s_i \propto \sigma_i^{q-1}$ [Jaggi, 2013]. This, in turn, greatly simplifies the alternating optimization approach. For a fixed Γ , we can use Lemma 4.2 to obtain a closed-from solution \mathbf{P}^* . On the other hand, for a fixed \mathbf{P} , optimizing Γ yields a classic discrete optimal transport problem with a cost matrix $\tilde{C} = -\mathbf{X}'\mathbf{P}\mathbf{Y}$. Naturally, this is mathematically equivalent to solving (for fixed \mathbf{P}) the original problem (8) instead, which has a simpler interpretation as an optimal transport problem for distributions supported in the points $\mathbf{x}^{(i)}$ and $\mathbf{P}\mathbf{y}^{(j)}$. Either way, we can obtain a solution with off-the-shelf optimal transport optimization algorithms.

Next, we briefly discuss what Lemma 4.2 implies for the three most interesting cases of invariance sets \mathcal{F}_p , namely p = 1,2 and ∞ . Then, we discuss optimization of the general problem in detail in Section 4.4.

4.1 The case $p = \infty$

The Schatten ℓ_{∞} -norm is the spectral norm $||A||_{\infty} = \sigma_{\max}(A)$. Since the identity map has unit spectral norm, to guarantee it is contained in \mathcal{F}_{∞} , it suffices to set k=1. Note that combining either condition in Lemma 4.1 with this implies that $\mathcal{F}_{\infty} = O(n)$, the set of orthogonal matrices. Indeed, the extreme points of the spectral unit ball are precisely the orthogonal matrices, so optimizing a linear objective such as (11) over the orthogonal matrices or the entire ball is equivalent. We therefore see that this choice of norm naturally allows us to encode invariance to rigid transformations: rotations and reflections. Using the dual characterization of Schatten norms, we see that

$$\max_{\mathbf{P}\in\mathcal{F}_{\infty}}\langle\mathbf{X}\Gamma\mathbf{Y}',\mathbf{P}\rangle = \max_{\mathbf{P}:\|\mathbf{P}\|_{\infty}\leq 1}\langle\mathbf{X}\Gamma\mathbf{Y}',\mathbf{P}\rangle = \|\mathbf{X}\Gamma\mathbf{Y}'\|_{*}$$
(13)

so that (11) becomes a single-block optimization problem:

$$\max_{\Gamma \in \Pi(\mu,\nu)} \|\mathbf{X} \Gamma \mathbf{Y}'\|_* \tag{14}$$

Albeit succinct, this alternative representation of the problem is not easier to solve. Despite having eliminated \mathbf{P} , the objective is now non-convex with respect to Γ (maximization

of a convex function). Nevertheless, this formulation offers an interesting geometric interpretation. When $\mu = \frac{1}{n}\mathbb{I}_n$ and $\nu = \frac{1}{m}\mathbb{I}_m$, then $\hat{Y} := \gamma \mathbf{Y}^T$ is an $n \times d$ matrix of vectors transported (from \mathcal{Y} to \mathcal{X}) according to the optimal barycentric mapping. Then, $\mathbf{X}\hat{\mathbf{Y}}$ is the $d \times d$ (shifted) cross-covariance matrix of the d features in \mathcal{X} and \mathcal{Y} space, i.e., $[\mathbf{X}\hat{\mathbf{Y}}]_{ij} = \text{cov}(x_i, y_j)$. Its nuclear norm indicates the strength of correlation of these features. Therefore, problem (14) essentially seeks a transport coupling that maximizes the correlation of feature dimensions after transportation. We leave exploration of direct techniques to optimize (14) for future work. Here instead we rely on the generic alternating minimization scheme described in the previous section. In this case, maximizing \mathbf{P} over the set of orthogonal matrices for a fixed Γ is exactly a traditional Procrustes problem whose solution is given by⁴

$$\mathbf{P}^* = \mathbf{U}\mathbf{V}' \tag{15}$$

where $\mathbf{U}\Sigma\mathbf{V}'$ is an SVD decomposition of $\mathbf{X}\Gamma\mathbf{Y}'$.

4.2 The case p = 2

The Schatten ℓ_2 -norm is the Frobenius norm $||A||_F = \sqrt{\sum_i \sigma(A)_i^2}$. Since $||I_d||_F = \sqrt{d}$, we take the invariance set to be

$$\mathcal{F}_2 = \left\{ \mathbf{P} \mid \|\mathbf{P}\|_F = \sqrt{d} \right\} \tag{16}$$

note that in this case condition (2) in Lemma 4.1 is satisfied by construction. As before, we use the Schatten norm duality to note that

$$\max_{\mathbf{P}\in\mathcal{F}_2}\langle \mathbf{X}\Gamma\mathbf{Y}',\mathbf{P}\rangle = \max_{\mathbf{P}:\|\mathbf{P}\|_F \le \sqrt{d}}\langle \mathbf{X}\Gamma\mathbf{Y}',\mathbf{P}\rangle = \sqrt{d}\|\mathbf{X}\Gamma\mathbf{Y}'\|_F$$
(17)

the problem is therefore now a Frobenius-norm maximization:

$$\max_{\Gamma \in \Pi(\mu,\nu)} \|\mathbf{X}\Gamma\mathbf{Y}'\|_{F} \tag{18}$$

with a similar intuition, but different metric, as that obtained for the $p = \infty$ case. However, this subtle difference has important consequences, among which is the following unexpected connection.

Lemma 4.3. *Consider the Gromov-Wasserstein problem for discrete measures* μ *and* ν [Mémoli, 2011, Peyré et al., 2016]:

$$\min_{\Gamma \in \Pi(\mu,\nu)} \sum_{i,j,k,l} L(\mathbf{C}_{ik}^{x}, \mathbf{C}_{jl}^{y}) \Gamma_{ij} \Gamma_{kl}$$
(19)

where the intra-space similarity matrices C^x and C^y as cosine distances between the columns of X and Y respectively, and L is chosen to be the ℓ_2 distance. Then, problem (18) is a lower bound on (19).

While we conjecture that under some conditions these two problems can be shown to be exactly equivalent, we leave a proof of this for future work.

⁴This can be verified as a particular case of Lemma 4.2, noting that s := 1 satisfies the stated requirements with $p = \infty$ and q = 1.

4.3 The case p = 1

The Schatten ℓ_1 -norm is the nuclear norm $||A||_* = \sum_{i=1}^n \sigma_i(A)$. As before, to ensure the identity mapping is contained in the invariance set we note that $||I_d||_* = d$, so the invariance set of interest is

$$\mathcal{F}_1 = \{ \mathbf{P} \mid \|\mathbf{P}\|_* = d \} \tag{20}$$

Note that adding either condition in Lemma 4.1 yields, again, the set of orthonormal matrices.⁵ Therefore, this case ends up being equivalent to the $p = \infty$ case.

4.4 Optimization

As stated above, we propose to solve problem (11) with alternating maximization on Γ and \mathbf{P} . For a fixed Γ , we can use Lemma 4.2 to obtain a closed-from solution \mathbf{P}^* at the cost of an $d \times d$ SVD, i.e., $O(d^3)$. On the other hand, for a fixed \mathbf{P} , the optimal Γ^* solving problem (11) can be found with linear programming methods in $O(N^3)$ time, where $N=n\times m$. However, this might be undesirable both computationally, and conceptually, as in most interesting applications the true correspondences between source and target points will likely not be exact (such as a word translating to multiple words on the other language, cf. Section 4), so the permutation recovered by the traditional optimal transport problem might be too rigid. Instead, a dense mapping that allows for one-to-many mappings might better model these soft correspondences. Thus, we can add an entropic regularization term to (11), as described in Section 3.2, yielding the problem:

$$\max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} \langle \Gamma, \mathbf{X}' \mathbf{P} \mathbf{Y} \rangle + \lambda H(\Gamma)$$
 (21)

This smoothed formulation allows for efficient computation of Γ^* using the Sinkhorn-Knopp algorithm [Cuturi, 2013]. Alternatively, the original (non-regularized) problem (11) can still be solved exactly by using the fact that the Sinkhorn-Knopp algorithm can yield an ϵ -approximate solution of this problem in $O(N \log N \epsilon^{-3})$ time [Altschuler et al., 2017], combined with the use of inexact alternating minimization methods that allow for approximate solution of the subproblems at each step (e.g., [Eckstein and Yao, 2017, Mokhtari et al., 2015]). Besides providing an alternative algorithmic approach, this observation could be used to prove convergence rates for problem (11). We leave this approach as an avenue of future work, focusing here instead on explicitly optimizing the regularized formulation (21).

The success of most alternating optimization optimization methods with non-convex objectives heavily depends on good initialization [Hardt, 2014, Jain et al., 2013]. Thus, it is no surprise that a key component of fully unsupervised approaches to feature alignment is finding good quality initializations. For example, for the problem of unsupervised word embedding alignment, state-of-the-art methods rely on some additional and often heuristic step to generate an initial solution, such as adversarially-trained neural networks [Conneau et al., 2018, Zhang et al., 2017a,b], robust self-learning [Artetxe et al., 2018b] or

⁵This can be easily verified by noting that the intersection of the Schatten ℓ_2 and ℓ_1 norm balls, defined in terms of intersections of the ℓ_2 and ℓ_1 vector norm balls, occurs in the extremal points of the latter

others. As shown by Artetxe et al. [2018b], adversarially-initialized approaches are often very sensitive to initialization, and even fail on the same problem over runs with different random seeds.

Problem (21) (as well as problem (11)) is not jointly concave on Γ and \mathbf{P} , so it faces a similar challenge in terms of sensitivity to initialization. Note however, that the value of the entropic regularization controls the extent of non-concavity of the problem: strong regularization leads to more a more concave objective, while on the contrary, $\lambda \to 0$ leads to increasingly more non-concave objective. We propose to leverage this observation to alleviate sensitivity to initialization by using an annealing scheme on the regularization term. Starting from a large value of λ , we decay this value in each iteration by setting $\lambda_t = \alpha \times \lambda_{t-1}$ with $\alpha < 1$. We do so for as long as the optimal transport problem can be solved without causing numerical instability. We stop the method when the value of the objective converges. The advantage of this annealing approach is that it avoids ad-hoc initialization, and eliminates the need for hyperparameter tuning on λ , since any sufficiently large choice of λ_0 achieves the same same objective. In *all* our experiments, we use the exact same values of initial regularization $\lambda_0 = 1$ and decay factor $\alpha = 0.99$.

While the procedure described so far leads to high-quality solutions for small and mid-sized problems, scaling up to very large sets of points—as required by the motivating application of word embedding alignment consisting of hundreds of thousands of words—can be prohibitive. We address this by dividing the problem into two phases. In the first stage, we solve a smaller problem (by taking a subsample of k points on each domain thus leading to smaller Γ and faster OT solution, but same size of P). Once the first phase reaches convergence, we scale up to the full-size problem. Note that while this might resemble other approaches that also consider a reduced set of points in their initialization step [Conneau et al., 2018, Grave et al., 2018], a crucial difference is that here we rely on the same optimization problem (21) in both stages, albeit with increasing sample size.

5 Experimental Setting

5.1 The task: Unsupervised word translation

We evaluate our framework in a recent and popular instance of the feature alignment problem: unsupervised word translation. The task consists of finding correspondences between the word embeddings of different languages without parallel data, and using these to translate words between them. While the general problem of unsupervised word translation (also known as bilingual lexical induction) goes back to Rapp [1995] and Fung [1995], the word-embedding approach was recently proposed prompted by the observation that mono-lingual word embeddings exhibit similar geometric properties across languages [Mikolov et al., 2013].

Most early work assumed some limited amount of supervision (e.g., a small list of translation seeds) for this task, recent work has shown that unsupervised methods can perform on-par and often above early supervised methods [Artetxe et al., 2018a, Conneau et al., 2018]. While successful, the mappings arise from multiple steps of processing, requiring either careful initial guesses or post-mapping refinements, including mitigating

the effect of frequent words on neighborhoods. The associated adversarial training schemes can be also challenging to tune properly [Artetxe et al., 2018a].

Here, we argue that word embedding alignment is an ideal task for the framework of the optimal transport with invariances. Indeed, word embeddings are estimated primarily in a relational manner to the extent that the algorithms are naturally interpreted as metric recovery methods [Hashimoto et al., 2016]. Thus, word embedding spaces are intrinsically invariant to all rigid transformations that preserve inner products (or distances, depending on the case), causing absolute positions of vectors to be irrelevant. Hence, for this task we use the $p = \infty$ invariance set scenario described in Section 4.1.

Compared to other methods that rely only on estimating an orthogonal map by solving the Procrustes problem (either for a small amount of parallel data, [Artetxe et al., 2017, Zhang et al., 2016] or by generating pseudo-matches through an initial unsupervised step [Artetxe et al., 2018a, Conneau et al., 2018]), our optimal-transport based framework goes beyond orthogonal mappings into more flexible correspondence estimation, while having a simple and direct optimization objective.

By evaluating on the word embedding alignment task we seek to validate our frame-work in a setting that involves the archetypal global invariance—to rotations—and for which previous work has established very strong unsupervised baselines. In the next section, we focus our evaluation on understanding the optimization dynamics of the proposed approach and evaluating its performance on benchmark cross-lingual word embedding tasks. Our focus is not on solely on performance, but rather in demonstrating that the proposed approach offers a viable fast, principled and robust alternative to state-of-the-art multi-step methods on this task, delivering comparable performance.

5.2 Datasets and Methods

Dataset We evaluate our method on two standard benchmark tasks for cross-lingual embeddings. First, we consider the dataset of Conneau et al. [2018], which consists of word embeddings trained with fastText on Wikipedia and parallel dictionaries for 110 language pairs. Here, we focus on five of the language pairs for which they report results: English (En) to Spanish (Es), French (Fr), German (De) and Russian (Ru). We do not report results on Esperanto (Eo) as dictionaries for that language were not provided with the original dataset release.

Methods To see how our fully-unsupervised method compares with methods that require (some) cross-lingual supervision, we follow [Conneau et al., 2018] and consider a simple but strong baseline consisting of solving a Procrustes problem directly using the available cross-lingual embedding pairs. We refer to this method simply as Procrustes. In addition, we compare against the fully-unsupervised methods of Zhang et al. [2017a], Artetxe et al. [2018a] and Conneau et al. [2018]. Whenever nearest neighbor search is required, we use the Cross-domain Similarity Local Scaling (Csls) step proposed by the latter, which has been shown to improve upon naive nearest-neighbor retrieval in all

⁶Despite its relevance, we do not include the OT-based method of Zhang et al. [2017b] in the comparison because their implementation required use of proprietary software.

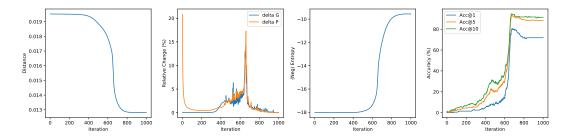


Figure 1: Results on procrustes OT for English to Italian word translation. Vocabulary is 5000 words on each side. From left to right: (1) objective, (2) relative change in variables P and γ from iteration to iteration, (3) Negative entropy of γ_t , (4) Translation accuracy in validation dictionary at different precision levels (e.g. @10 means true translation is among top 10 most similar predicted).

			En-Es		En-Fr		En-De		En-It		En-Ru	
	Seeds	Time	\rightarrow	\leftarrow								
Weakly Supervised Methods:												
PROCRUSTES	5K words	3	77.6	77.2	74.9	75.9	68.4	67.7	73.9	73.8	47.2	58.2
Procrustes + CSLS	5K words	3	81.2	82.3	81.2	82.2	73.6	71.9	76.3	75.5	51.7	63.7
From [Conneau et al., 2018]:												
Adv + Csls	None	643	75.7	79.7	77.8	71.2	70.1	66.4	72.4	71.2	37.1	48.1
Adv + Csls + Refine	None	957	81.7	83.3	82.3	82.1	74.0	72.2	77.4	76.1	44.0	59.1
ℓ_{∞} -InvarOt + Csls	None	70	81.3	81.8	80.7	80.5	73.7	67.1	77.3	75.0	41.7	55.4

Table 1: Results of unsupervised and minimally-supervised methods on the dataset of Conneau et al. [2018]. The time columns shows the average runtime in minutes of an instance (i.e., one language pair) of the method in this task on the same quad-core CPU machine. Note that we show results for our method without relying on the iterative refinement step of Conneau et al. [2018], so it is more appropriately compared to their corresponding method ADV + CSLS.

such methods. At the time of writing, the implementation of Grave et al. [2018] was not available, and thus we do not compare against their method in our experiments.

6 Results

As is common practice in this task, for each word in the test dictionary we compute translation accuracy at different precision levels: A@K, where K denotes the top-K highest scored translations. We show in Figure 1 the optimization dynamics of our ℓ_{∞} -invariant formulation on an instance of the word embedding alignment task. This behavior closely resembles what we observed across datasets and parameter configurations. There is little progress at the beginning (during which **P** is being aggressively adjusted), followed by a steep decline in the objective (during which both **P** and Γ are increasingly modified in

each step, after which convergence is reached. Note how the value of the optimization objective (left) and the accuracy in the translation task (right) are strongly correlated, particularly when compared against adversarial objectives Conneau et al. [2018]. This is important because while we show validation accuracies here for analysis purposes, for the final task we do not use use any supervision during training, and do model selection and early stopping based purely on the unsupervised objective. In addition, note that except for a small adjustment at the end of training, our method does not risk degradation by over-training, as is often the case for adversarial training alternatives.

In Table 1 we show the complete set of results on 5 pairs of languages from the dataset of Conneau et al. [2018]. Following them, we compare against a strong minimally-supervised baseline, consisting of solving a single Procrustes problem with a seed vocabulary of the the 5 thousand most frequent words for the source language and their gold translations. In addition, we compare against two versions of the adversarial approach of Conneau et al. [2018], with and without a heuristic refinement step that alternatively builds nearest neighbors with Csls and solves the Procrustes problem for these pseudo-translations. These results show that our general framework performs on par with state-of-the-art approaches tailored this task, at a fraction of the computational cost, and with a optimization objective more faithful to the true evaluation metric of interest.

7 Discussion and future work

We have proposed a formulation of optimal transport that accounts for global invariances in the underlying feature spaces. This formulation unifies various approaches to deal with such invariances in one general class of optimal transport distances. Rather than a single problem, what we propose here is a general recipe for injecting such invariances into OT. The nature of the resulting optimization problem naturally depends on the class of invariances of interest, and solving it efficiently requires algorithms tailored to it. Here we focused on the rigid transformation case due to its prevalence, providing detailed analysis, proposing efficient optimization algorithms and empirically validating its use in practice. Exploring other types of invariances offers a rich avenue of future work.

In terms of applications, we showed how an orthogonally-invariant version of the problem leads to a lean, compact objective that yields state of the art results at a fraction of the computational cost. These promising results suggest that optimal transport distances are a viable alternative to methods that learn correspondences by complex, often underdetermined, adversarially learnt maps.

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A Proofs

Lemma A.1. Let **M** be a matrix with SVD decomposition $\mathbf{M} = \mathbf{U}\Sigma\mathbf{V}'$ and let $\Sigma = \operatorname{diag}(\boldsymbol{\sigma})$, then

$$\underset{P:\|P\|_{p} \leq k}{\operatorname{argmax}} \langle P, M \rangle = U \operatorname{diag}(s) V'$$
 (22)

where **s** is such that $\|\mathbf{s}\|_p \leq k$ and attains $\mathbf{s}'\boldsymbol{\sigma} = k\|\boldsymbol{\sigma}\|_q$, for $\|\cdot\|_q$ the dual norm of $\|\cdot\|_p$.

Proof. Suppose **P** is such that $\|\mathbf{P}\|_p \leq k$, and let $\mathbf{U}_{\mathbf{P}} \operatorname{diag}(\mathbf{s}) \mathbf{V}'_{\mathbf{P}}$ be its singular value decomposition. This implies that $\|\mathbf{s}\|_p = \|\mathbf{P}\| \leq k$. In addition,

$$\langle \mathbf{P}, \mathbf{M} \rangle = \langle \mathbf{P}, \mathbf{U} \Sigma \mathbf{V}' \rangle = \langle \mathbf{U}' \mathbf{P} \mathbf{V}, \Sigma \rangle = \sum_{i=1}^{d} [\mathbf{U}' \mathbf{P} \mathbf{V}]_{ii} \sigma_i(\mathbf{M})$$
 (23)

$$=\sum_{i=1}^{d}\mathbf{u}_{i}\mathbf{P}\mathbf{v}_{i}\sigma_{i}(\mathbf{M})\leq\sum_{i=1}^{d}s_{i}\sigma_{i}(\mathbf{M})=\langle\mathbf{s},\boldsymbol{\sigma}\rangle$$
 (24)

Here, the inequality holds because, by definition of the SVD decomposition, $\|\mathbf{u}_i\|_2 = \|\mathbf{v}_i\|_2 = 1$ for every i and

$$\mathbf{u}_{i} \mathbf{P} \mathbf{v}_{i} \leq \sup_{\substack{\mathbf{u} \perp \text{span}\{\mathbf{u}_{1}, \dots, \mathbf{u}_{i-1}\}\\ \mathbf{v} \perp \text{span}\{\mathbf{v}_{1}, \dots, \mathbf{v}_{i-1}\}}} \frac{\mathbf{u}' \mathbf{P} \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|} \leq \sigma_{i}(\mathbf{P}) = s_{i} \quad \forall i$$
(25)

Therefore:

$$\sup_{\mathbf{P}:\|\mathbf{P}\|_p \le k} \langle \mathbf{P}, \mathbf{M} \rangle \le \sup_{\mathbf{s}:\|\mathbf{s}\|_p \le k} \langle \mathbf{s}, \boldsymbol{\sigma} \rangle = k \sup_{\mathbf{s}:\|\mathbf{s}\|_p \le 1} \langle \mathbf{s}, \boldsymbol{\sigma} \rangle = k \|\boldsymbol{\sigma}\|_q$$

where the last equality follows from the definition of dual norm for vectors. Conversely, take any vector \mathbf{s} with $\|\mathbf{s}\|_p = k$, and define $\tilde{\mathbf{P}}(\mathbf{s}) = \mathbf{U} \operatorname{diag}(\mathbf{s}) \mathbf{V}'$. Clearly, $\|\tilde{\mathbf{P}}(\mathbf{s})\|_p = k$, so the supremum must satisfy:

$$\sup_{\mathbf{P}} \langle \mathbf{P}, \mathbf{M} \rangle \geq \sup_{\mathbf{s}: \|\mathbf{s}\|_p \leq k} \langle \tilde{\mathbf{P}}(\mathbf{s}), \mathbf{M} \rangle = \sup_{\mathbf{s}: \|\mathbf{s}\|_p \leq k} \langle \mathbf{U} \operatorname{diag}(\mathbf{s}) \mathbf{V}', \mathbf{U} \Sigma \mathbf{V}' \rangle = \sup_{\mathbf{s}: \|\mathbf{s}\|_p \leq k} \langle \operatorname{diag}(\mathbf{s}), \Sigma \rangle = k \|\boldsymbol{\sigma}\|_q$$

Therefore, we conclude that the optimal value of (22) is exactly $k\|\boldsymbol{\sigma}\|_q$. Furthermore, (25) holds with equality if and only if $(\mathbf{u}_i, \mathbf{v}_i)$ coincide with the left and right singular vectors of \mathbf{P} . Thus, any \mathbf{P} maximizing (22) must have the form $\mathbf{P} = \mathbf{U} \operatorname{diag}(\mathbf{s}) \mathbf{V}'$, with $\|\mathbf{s}\|_p \leq k$ and $\langle \mathbf{s}, \boldsymbol{\sigma} \rangle = k\|\boldsymbol{\sigma}\|_q$, as stated.

Lemma A.2. If any of the following conditions holds;

- 1. $\forall P \in \mathcal{F}$, P is angle-preserving
- 2. $\exists k \geq 0 : \|\mathbf{P}\|_F = k \quad \forall \mathbf{P} \in \mathcal{F} \text{ and the matrix } \mathbf{Y} \text{ is } \nu\text{-whitened (i.e., } \mathbf{Y} \operatorname{diag}(\mathbf{q})^2 \mathbf{Y}' = \mathbf{I}_d$).

then problem (10) is equivalent to

$$\max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} \langle \Gamma, \mathbf{X}' \mathbf{P} \mathbf{Y} \rangle = \max_{\Gamma \in \Pi(\mu,\nu)} \max_{\mathbf{P} \in \mathcal{F}} \langle \mathbf{X} \Gamma \mathbf{Y}', \mathbf{P} \rangle$$
(26)

Proof. Suppose (1) holds, i.e., $\langle \mathbf{Px}, \mathbf{Py} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$ for every $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$. Then, in particular $\|\mathbf{Py}\|_2 = \|\mathbf{y}\|_2$ for every $\mathbf{y}^{(j)}$, and therefore:

$$\langle \mathbf{v}, \nu \rangle = \sum_{j=1}^{m} \| \mathbf{P} \mathbf{y}^{(j)} \|_2 = \| \mathbf{y}^{(j)} \|_2$$

and therefore only the first term in (11) depends on P or Γ , from which the conclusion follows. On the other hand, suppose (2) holds, and let $\tilde{Y} = Y \operatorname{diag}(q)$, so that $\tilde{Y}\tilde{Y}' = I_d$. We have:

$$\langle \mathbf{v}, \nu \rangle = \sum_{i=1}^m q_i \|\mathbf{P}\mathbf{y}^{(i)}\|_2^2 = \sum_{j=1}^m \|\mathbf{P}\mathbf{y}^{(j)}q_j\|_2^2 = \|\mathbf{P}\tilde{\mathbf{Y}}\|_2^2 = \langle \mathbf{P}\tilde{\mathbf{Y}}, \mathbf{P}\tilde{\mathbf{Y}}\rangle = \langle \mathbf{P}, \mathbf{P}\tilde{\mathbf{Y}}\tilde{\mathbf{Y}}'\rangle = \|\mathbf{P}\|_F^2 = k^2,$$

that is, $\langle \mathbf{v}, \nu \rangle$ again does not depend on **P**. This concludes the proof.

Lemma A.3. Problem (18) is a lower bound on the Gromov-Wasserstein problem between the matrices X and Y with intra-space cosine metric and ℓ_2 cost between similarity matrices.

Proof. The discrete Gromov-Wasserstein problem [Peyré et al., 2016] reads:

$$\min_{\Gamma \in \Pi(\mu,\nu)} \sum_{i,j,k,l} L(\mathbf{C}_{ik}^{x}, \mathbf{C}_{jl}^{y}) \Gamma_{ij} \Gamma_{kl} := \mathcal{L}(\Gamma)$$
(27)

where \mathbf{C}^x and \mathbf{C}^y are intra-space similarity matrices, i.e., \mathbf{C}^x_{ik} corresponds to the similarity between $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(j)}$, and analogously for \mathbf{C}^y . For the choice of cosine metric, and assuming without loss of generality that the columns of \mathbf{X} and \mathbf{Y} are normalized, these are given by $\mathbf{C}^x = \mathbf{X}'\mathbf{X}$ and $\mathbf{C}^y = \mathbf{Y}'\mathbf{Y}$. In addition, let L be the ℓ_2 loss, i.e., $L(a,b) = |a-b|^2$. Then the objective in problem (27) becomes:

$$\mathcal{L}(\Gamma) = \sum_{i,j,k,l} (\mathbf{C}_{ik}^{x} - \mathbf{C}_{jl}^{y})^{2} \Gamma_{ij} \Gamma_{kl} = \frac{1}{2} \sum_{i,j,k,l} (\mathbf{C}_{ik}^{x})^{2} \Gamma_{ij} \Gamma_{kl} - \sum_{i,j,k,l} (\mathbf{C}_{ik}^{x} \mathbf{C}_{jl}^{y}) \Gamma_{ij} \Gamma_{kl} + \frac{1}{2} \sum_{i,j,k,l} (\mathbf{C}_{jl}^{y})^{2} \Gamma_{ij} \Gamma_{kl}$$

But note that for the first of these terms, we have that for every $\Gamma \in \Pi(\mu, \nu)$,

$$\frac{1}{2} \sum_{i,k} (\mathbf{C}_{ik}^{x})^{2} \sum_{j,l} \Gamma_{ij} \Gamma_{jl} = \frac{1}{2} \sum_{i,k} (\mathbf{C}_{ik}^{x})^{2} \mathbf{p}_{i} \mathbf{p}_{k} = \frac{1}{2} \mathbf{p}' (\mathbf{C}^{x})^{2} \mathbf{p}_{i}$$

where \mathbf{p} is the vector of probabilities in empirical distribution μ , and the last equation follows from the definition of the transportation polytope. Crucially, this term does not depend on Γ anymore. Analogously, the last term in $\mathcal{L}(\Gamma)$ does not depend on Γ either, so we have

$$\underset{\Gamma \in \Pi(\mu,\nu)}{\operatorname{argmin}} \mathcal{L}(\Gamma) = \underset{\Gamma \in \Pi(\mu,\nu)}{\operatorname{argmax}} \sum_{i,j,k,l} (\mathbf{C}_{ik}^{x} \mathbf{C}_{jl}^{y}) \Gamma_{ij} \Gamma_{kl}$$
(28)

On the other hand, consider problem (18). The objective it seeks to maximize is

$$\begin{split} \|\mathbf{X}\Gamma\mathbf{Y}'\|_F &= \langle \mathbf{X}\Gamma\mathbf{Y}', \mathbf{X}\Gamma\mathbf{Y}' \rangle = \langle \mathbf{X}'\mathbf{X}\Gamma, \Gamma\mathbf{Y}\mathbf{Y}' \rangle = \sum_{i=1}^n \sum_{j=1}^m [\mathbf{X}'\mathbf{X}\Gamma]_{ij} [\Gamma\mathbf{Y}'\mathbf{Y}]_{ij} \\ &= \sum_{i=1}^n \sum_{j=1}^m [\mathbf{C}^x \Gamma]_{ij} [\Gamma\mathbf{C}^y]_{ij} \\ &= \sum_{i=1}^n \sum_{j=1}^m (\sum_{k=1}^n \mathbf{C}^x_{ik} \Gamma_{kj}) (\sum_{l=1}^m \Gamma_{il} \mathbf{C}^y_{lj}) \end{split}$$

which is a lower bound on (28), concluding the proof.