Abstract

Optimal transport (OT) is a powerful geometric and probabilistic tool for finding correspondences and measuring similarity between two distributions. Yet, its original formulation relies on the existence of a cost function between the samples of the two distributions, which makes it impractical for comparing data distributions supported on different topological spaces. To circumvent this limitation, we propose a novel OT problem, named COOT for CO-Optimal Transport, that aims to simultaneously optimize two transport maps between both samples and features. This is different from other approaches that either discard the individual features by focusing on pairwise distances (e.g. Gromov-Wasserstein) or need to model explicitly the relations between the features. COOT leads to interpretable correspondences between both samples and feature representations and holds metric properties. We provide a thorough theoretical analysis of our framework and establish rich connections with the Gromov-Wasserstein distance. We demonstrate its versatility with two machine learning applications in heterogeneous domain adaptation and co-clustering/data summarization, where COOT leads to performance improvements over the competing state-of-the-art methods.

1. Introduction

The problem of comparing two sets of points (a source and a target) arise in many fields in machine learning. When correspondences of source and target points are known a priori, one can align source and target data with a global transformation of the features, e.g, with the widely used Procrustes analysis (Gower & Dijksterhuis, 2004; Goodall, 1991). For unknown correspondences other popular alternatives to this method include correspondence free manifold alignment procedure (Wang & Mahadevan, 2009), soft assignment coupled with a Procrustes matching (Rangarajan et al., 1997) or Iterative closest point and its variants for 3D shapes (Besl & McKay, 1992; Yang et al., 2020). Overall the problem of estimating correspondences in an unsupervised manner between two sets of points is at the core of many methods, from manifold alignment (Cui et al., 2014), image registration (Haker & Tannenbaum, 2001) to unsupervised word and sentence translation (Rapp, 1995).

A way to look at the correspondence estimation problem consists in modeling the considered sets of points as distributions of Diracs with possibly uniform weights. In this case, one can rely on the Optimal Transport (OT) framework to find, without supervision, a soft-correspondence map between them, also known as optimal coupling. OT-based approach has been used with success in numerous applications such as embeddings’ alignments (Alvarez-Melis et al., 2019; Grave et al., 2019) and Domain Adaptation (Courty et al., 2017) to name a few. But one important limit of using OT for estimating correspondences is that it is limited to sets of points that lie in the same space as one needs to compute a cost between points across the two sets. This major drawback does not allow OT to handle correspondences’ estimation across heterogeneous spaces, preventing its application in problems such as, for instance, Heterogeneous Domain Adaptation (HDA).

To circumvent this restriction, one may rely on another OT approach called the Gromov-Wasserstein distance (GW) (Memoli, 2011). This non convex quadratic OT problem finds the correspondences based on the topological and relational aspects of the points within each domain. In other words, it proceeds by first calculating the intra-domain similarities for each set of objects and then finds the correspondences based on the obtained similarity (or distance) matrices. Such approach was successfully applied for correspondence problems where source and target points do not lie in the same Euclidean space, e.g for shapes (Solomon et al., 2016), word embeddings (Alvarez-Melis & Jaakkola, 2018) or HDA (Yan et al., 2018) as mentioned previously. Unfortunately, this method only finds the assignments of the samples and discards the individual features during the pairwise distance computation.
In this work, we propose a novel OT approach called CO-Optimal Transport that simultaneously infers the correspondences between the samples and the features of two sets of points. Contrary to the GW transportation problem that is based only on the pairwise relations between the samples, our approach considers the representations of points in their original space. This latter point is quite important as it provides a meaningful mapping between both instances and features across the two datasets thus having the virtue of being interpretable. We thoroughly analyze the proposed problem, derive an optimization procedure for it and highlight several interesting links to other approaches. On the practical side, we provide evidence of its versatility in machine learning by putting forward two applications in Heterogeneous Domain Adaptation and co-clustering where our approach achieves state-of-the-art results.

The rest of this paper is organized as follows. We introduce COOT in Section 2 and give an optimization routine to solve it efficiently. In Section 3, we show how COOT is related to the Gromov-Wasserstein distance when applied on pairwise similarity matrices and recover some efficient GW solvers. Finally, in Section 4, we present an experimental study providing highly competitive results in HDA and co-clustering compared to several strong baselines.

2. CO-Optimal transport (COOT)

Notations. We briefly introduce the notations used throughout the paper. The simplex histogram with \( n \) bins is denoted by \( \Delta_n = \{ \mathbf{w} \in (\mathbb{R}_+)^n : \sum_{i=1}^n w_i = 1 \} \). We further denote by \( \otimes \) the tensor-matrix multiplication, i.e., for a tensor \( \mathbf{L} = (L_{i,j,k,l}) \), \( \mathbf{L} \otimes \mathbf{B} \) is the matrix \( (\sum_{k,l} L_{i,j,k,l} B_{k,l})_{i,j} \). We use \( \langle \cdot , \cdot \rangle \) for the matrix scalar product associated with the Frobenius norm \( \| \cdot \|_F \) and \( \otimes_K \) for the Kronecker product of matrices i.e., \( (a_{i,j})_{i,j} \otimes_K (b_{k,l})_{k,l} = (a_{i,j} b_{k,l})_{i,j,k,l} \). We denote by \( \mathcal{S}_n \) the set of all permutations of \( [n] \). Finally, we write \( \mathbf{1}_n \in \mathbb{R}^d \) for a \( d \)-dimensional vector of ones and denote all matrices by \( \mathbf{X} \) (upper-case bold letters (i.e., \( \mathbf{x} \)); all vectors are written in lower-case bold (i.e., \( x \)).

2.1. CO-Optimal transport optimization problem

We consider two datasets represented by matrices \( \mathbf{X} = [x_1, \ldots, x_n]^T \in \mathbb{R}^{n \times d} \) and \( \mathbf{X}' = [x'_1, \ldots, x'_n]^T \in \mathbb{R}^{n' \times d'} \), where in general we assume that both dimensions may differ, i.e., \( n \neq n' \) and \( d \neq d' \). In what follows, the rows of the datasets are denoted as samples and its columns as features. Let \( \mu = \sum_{i=1}^n w_i \mathbf{x}_i \) and \( \mu' = \sum_{i'=1}^{n'} w'_i \mathbf{x}'_i \) be two empirical distributions related to samples, where \( \mathbf{x}_i \in \mathbb{R}^d \) and \( \mathbf{x}'_i \in \mathbb{R}^{d'} \). We refer in the following to \( \mathbf{w} = [w_1, \ldots, w_n]^T \in \Delta_n \) and \( \mathbf{w}' = [w'_1, \ldots, w'_{n'}]^T \in \Delta_{n'} \) as sample weights vectors that both lie in the simplex. In addition to these distributions, we also have weights for the features that are stored in vectors \( \mathbf{v} \in \Delta_d \) and \( \mathbf{v}' \in \Delta_{d'} \). Note that when no additional information is available about the data, all the weights’ vectors can be set as uniform.

We define the CO-Optimal Transport problem as follows:

\[
\begin{align*}
\min_{\pi \in \Pi(\mathbf{w}, \mathbf{w}')} \sum_{i,j,k,l} L(X_{i,k}, X'_{j,l}) \pi_{i,j}^u \pi_{k,l}^v
\end{align*}
\]

where \( L : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+ \) is a divergence measure between 1D variables, \( L \) is the tensor of all pairwise divergences between the elements of the matrices \( \mathbf{X} \) and \( \mathbf{X}' \), and \( \Pi(\cdot, \cdot) \) is the set of linear transport constraints defined as:

\[
\Pi(\mathbf{w}, \mathbf{w}') = \{ \pi | \pi \geq 0, \pi \mathbf{1}_{n'} = \mathbf{w}, \pi^T \mathbf{1}_n = \mathbf{w}' \}.
\]

Note that problem (1) seeks for a simultaneous transport \( \pi^* \) between samples and a transport \( \pi^v \) between features across distributions. In the following, we write COOT(\( \mathbf{X}, \mathbf{X}', \mathbf{w}, \mathbf{w}', \mathbf{v}, \mathbf{v}' \)) (or COOT(\( \mathbf{X}, \mathbf{X}' \)) when it is clear from the context) to denote the objective value of the optimization problem (1).

**COOT as a bilinear program** COOT is a special case of a Quadratic Program (QP) with linear constraints called a Bilinear Program (BP). More precisely, it is an indefinite quadratic program (Pardalos & Rosen, 1987; Horst & Tuy, 1996) that there exists an optimal solution lying on extremal points of the polytopes \( \Pi(\mathbf{w}, \mathbf{w}') \) and \( \Pi(\mathbf{v}, \mathbf{v}') \). When \( n = n', d = d' \) and uniform weights are used (i.e., \( \mathbf{w} = \mathbf{w}' = \mathbf{1}_n \), \( \mathbf{v} = \mathbf{v}' = \mathbf{1}_d \)), Birkhoff’s theorem (Birkhoff, 1946) states that the set of extremal points of \( \Pi(\mathbf{1}_n, \mathbf{1}_n) \) and \( \Pi(\mathbf{1}_d, \mathbf{1}_d) \) are the set of permutation matrices so that there exists an optimal solution \( (\pi^*, \pi^v) \) of the form \( (i, \sigma^*_i(i)), (k, \sigma^*_k(k)) \) with \( \sigma^*_i, \sigma^*_k \in \mathcal{S}_n \times \mathcal{S}_d \).

The BP problem is also related to the bilinear assignment problem (BAP) where \( \pi^* \) and \( \pi^v \) are searched among the set of permutation matrices. This problem was shown to be NP-hard if \( d = O(\sqrt{n}) \) for some fixed \( r \) and solvable in polynomial time if \( d = O(\sqrt{\log(n)}) \) (Custic et al., 2016).

In this case, we look for the best permutations of the rows and columns of our datasets that lead to the smallest cost. COOT provides a convex relaxation of the BAP and the previous remarks show that both problems are equivalent, namely that one can always find a pair of permutations that minimizes (1).

**Entropic regularization** Recently, entropic regularization has been favored in the OT community thanks to its ability to remedy the heavy computation burden of OT and...
The result of solving problem (1) is reported in Figure 1. In
the center-left part, we provide the coupling matrix \( \pi^s \) between
samples sorted by class and we see that the majority of the samples (67%) are transported to samples from the
same class (mass on the block diagonal). This suggests that
COOT can be potentially applied to perform domain adapta-
tion across heterogeneous datasets. The matrix \( \pi^v \) describes
the relations between pixels in both domains. To visualize
its content, we color-code the pixels of one domain’s image
(16 × 16) and color the pixel in the other domain (image
of size 28 × 28) associated to it by this mapping. Pixels in
the final target image are therefore convex combinations of
colors from the source image. Results are shown in the
right part of Figure 1 for both the original COOT and its
entropic regularized counterpart. From these two images,
we can observe that colored pixels appear only in the central
areas. We note further a very strong spatial coherency in the
result, even though no inter-pixel distances were used in the
optimization problem (each pixel is treated as an independent variable). COOT has recovered a meaningful spatial transformation between the two domains, that is slightly
more complex than a simple resize of the images and better
fits the nature of the data (for further evidence, we refer
the reader to other visual results given in the supplementary
material). Moreover, it was learned in a totally unsupervised
way from the raw data thus highlighting its ability to find
meaningful relations between variables.

2.2. Properties of COOT

Interestingly enough, COOT induces a notion of distance
between datasets \( \mathbf{X} \) and \( \mathbf{X}' \). More precisely, it vanishes if
the datasets are the same up to a permutation of their rows and
columns as stated in the following proposition.

**Proposition 1** (COOT is a distance for \( n = n', d = d' \)).
Suppose \( L = | \cdot |^p, p \geq 1, n = n', d = d' \) and that the
weights \( \mathbf{w}, \mathbf{w}' \) and \( \mathbf{v}, \mathbf{v}' \) are uniform. Then \( \text{COOT}(\mathbf{X}, \mathbf{X}') = 0 \)
iff there exists a permutation of the samples \( \sigma_1 \in S_n \) and
of the features \( \sigma_2 \in S_d, s.t. \forall i, k \in [n] \times [d], \mathbf{X}_{i,k} = \mathbf{X}'_{\sigma_1(i), \sigma_2(k)}. \) Moreover, it is symmetric and satisfies the
triangular inequality as long as \( L \) satisfies the triangle
inequality, i.e.,

\[
\text{COOT}(\mathbf{X}, \mathbf{X}'') \leq \text{COOT}(\mathbf{X}, \mathbf{X}') + \text{COOT}(\mathbf{X}', \mathbf{X}'').
\]

All proofs and theoretical results of this paper are detailed
in the supplementary material.
Interestingly, our result generalizes the metric property proved in (Faliszewski et al., 2019) for the election isomorphism problem with this latter result being valid only for the BAP case. We discuss the connection between COOT and the work of (Faliszewski et al., 2019) in more detail the following section. Finally, we note that this metric property means that COOT can be used as a divergence in a large number of potential applications where GW was proved to be efficient, such as, for instance, generative learning (Bunne et al., 2019a).

2.3. Optimization algorithm and complexity

Even though exactly solving the COOT may represent a NP-hard problem, in practice a solution can be computed relatively efficiently. To this end, we propose to solve the complex problem (1) using Block Coordinate Descent (BCD), that consists in iteratively solving the problem w.r.t. \( \pi^s \) and \( \pi^v \) with the other kept fixed. Interestingly, this boils down to solving at each step a classical optimal transport problem that can be done in \( O(n^3 \log(n)) \) operations with a network simplex algorithm as detailed in the pseudo-code given in Algorithm 1. This approach, also known as the “mountain climbing procedure” (Konno, 1976b), was proved to decrease the loss at each iteration and so to converge within a finite number of iterations (Horst & Tuy, 1996). We also note that at each iteration, one needs to compute the equivalent linear cost matrix \( M \) which has a complexity of \( O(ndn'd') \). However, one can reduce it using Proposition 1 from (Peyré et al., 2016) for the case when \( L \) is the squared Euclidean distance \( \| \cdot \|^2 \) or the Kullback-Leibler divergence. In this case, the computational complexity is \( O(\min\{n^2+n'd',n'd'+n^2d\}) \). We refer the interested reader to the supplementary material for further details.

Finally, we use the same BCD procedure for the entropic regularized version of COOT (2). In this case, each iteration corresponds to an entropic regularized optimal transport problem that can be solved efficiently using Sinkhorn’s algorithm (Cuturi, 2013) with several possible improvements (Altschuler et al., 2017; 2019; Alaya et al., 2019).

Algorithm 1 Block Coordinate Descent for COOT

1: \( \pi^s_0 \leftarrow \text{ww}^T \), \( \pi^v_0 \leftarrow \text{vv}^T \)
2: \textbf{for} \( k = 1, \ldots, \) \textbf{do}
3: \( \pi^s(k), \) solution of OT problem with marginals \( v, v' \) and cost \( M_{\pi^s}(k-1) = L(X, X') \otimes \pi^s_{(k-1)} \)
4: \( \pi^v(k), \) solution of OT problem with marginals \( w, w' \) and cost \( M_{\pi^v}(k-1) = L(X, X') \otimes \pi^v_{(k-1)} \)
5: \textbf{if} \( L(X, X') \otimes \pi^s_{(k)}, \pi^v_{(k-1)} = L(X, X') \otimes \pi^s_{(k)}, \pi^v_{(k)} \) \textbf{stop}
6: \textbf{end for}

3. Relation with other OT distances

3.1. Gromov-Wasserstein

The COOT problem is defined between any matrices \( X \in \mathbb{R}^{n \times d}, X' \in \mathbb{R}^{n' \times d'} \) so that one can choose to use it to compare points of two data sets based on their intra domain similarity matrices \( C \in \mathbb{R}^{n \times n'}, C' \in \mathbb{R}^{n' \times n'} \) as well. This situation may arise when the samples are described by their pair-to-pair distances (we further suppose that \( C, C' \) are symmetric) e.g. in a graph context (Vayer et al., 2019), deep metric alignment (Ezuz et al., 2017), HDA (Yan et al., 2018) or in generative modelling (Bunne et al., 2019b). These problems have been successfully tackled recently using the Gromov-Wasserstein (GW) distance (Memoli, 2011) where one aims at solving:

\[
GW(C, C', w, w') = \min_{\pi \in \Pi(w, w')} \langle L(C, C') \otimes \pi^s, \pi^v \rangle \tag{3}
\]

As suggested by the similar objective functions and constraints, GW and COOT are linked in multiple ways. First, COOT provides a lower bound for GW. Second, in some special cases it can be shown that the two problems are equivalent. Indeed, as pointed in (Konno, 1976a), a concave semi-negative definite so that the GW problem is a concave associated bilinear programming problem using the following theorem:

**Theorem 1** ((Konno, 1976a)). If \( Q \) is a negative definite matrix then problems:

\[
\min_{x} f(x) = c^T x + \frac{1}{2} x^T Q x \\
\text{s.t.} \quad Ax = b, \ x \geq 0
\tag{4}
\]

\[
\min_{x,y} g(x,y) = \frac{1}{2} c^T x + \frac{1}{2} c^T y + \frac{1}{2} x^T Q y \\
\text{s.t.} \quad Ax = b, Ay = b, \ x, y \geq 0
\tag{5}
\]

are equivalent. More precisely, if \( x^* \) is an optimal solution for (7), then \( (x^*, x^*) \) is a solution for (8) and if \( (x^*, y^*) \) is optimal for (8), then both \( x^* \) and \( y^* \) are optimal for (7).

With this theorem in mind, we can link GW with the COOT problem when working on intra domain similarity matrices \( C \in \mathbb{R}^{n \times n}, C' \in \mathbb{R}^{n' \times n'} \) thanks to the next proposition:

**Proposition 2.** Let \( L = \| \cdot \|^2 \) and suppose that \( C \in \mathbb{R}^{n \times n}, C' \in \mathbb{R}^{n' \times n'} \) are squared Euclidean distance matrices such that \( C = x_1^2 + 1_x x^T - 2XX^T, C' = x'^2 + 1_{x'} x'^T - 2X'X'^T \) with \( x = \text{diag}(XX^T) \), \( x' = \text{diag}(X'X'^T) \). Then, the GW problem can be written as

\[
\text{Q = } -8 \ast XX^T \otimes K \ast X'X'^T. \tag{7}
\]

In particular, \( Q \) is semi-negative definite so that the GW problem is a concave quadratic program.

The other coefficients of this QP are described in the supplementary material. Using both Theorem 2 and Proposition 2 we can prove the following result:
Algorithm 2 DC Algorithm for COOT and GW with squared Euclidean matrices

1: $\pi^{(0)} \gets \mathbf{w} \mathbf{w}^T$
2: for $k = 1, \ldots$ do
3: $\pi^s_k$ solution of OT problem with marginals $\mathbf{w}, \mathbf{w}'$
4: if $(L(C, C') \otimes \pi^s_k, \pi^s_{k-1}) = (L(C, C') \otimes \pi^s_k, \pi^s_k)$ stop
5: end for

Proposition 3. Let $C \in \mathbb{R}^{n \times n}$, $C' \in \mathbb{R}^{n' \times n'}$ be any symmetric matrices, then:

$$\text{COOT}(C, C', \mathbf{w}, \mathbf{w}', \mathbf{w}, \mathbf{w}') \leq \text{GW}(C, C', \mathbf{w}, \mathbf{w}').$$

Moreover, if $L = \frac{1}{2} \mathbf{d} \mathbf{d}^T$ and $C, C'$ are squared Euclidean distance matrices, $\text{COOT}(C, C', \mathbf{w}, \mathbf{w}', \mathbf{w}, \mathbf{w}') = \text{GW}(C, C', \mathbf{w}, \mathbf{w}')$. Consequently, if $(\pi^s_k, \pi^s_k)$ is an optimal solution of (1), then both $\pi^s_k, \pi^s_k$ are solutions of (3). Conversely, if $\pi^s_k$ is an optimal solution of (3), then $(\pi^s_k, \pi^s_k)$ is an optimal solution for (1).

By means of this proposition, we know that there exists an optimal solution for the COOT problem of the form $(\pi^s, \pi^s)$, where $\pi^s$ is an optimal solution of the GW problem. This gives a conceptually very simple fixed-point procedure where one only iterates over one coupling in order to compute a optimal solution of GW as described in Algorithm 2. Interestingly enough, the iterations of the fixed point method are exactly equivalent to the Frank Wolfe procedure described in (Vayer et al., 2019), since, in the concave setting, the line search step can be fixed to 1 (Maron & Lipman, 2018) (see supplementary material for more details). Also note that the steps of Algorithm 2 are iterations of Difference of Convex Algorithm (DCA) (Tao et al., 2005; Yuille & Rangarajan, 2003) where the concave function is approximated at each iteration by its linear majorization. When applying the same procedure for entropic regularized COOT, the resulting DCA also recovers exactly the projected gradients iterations proposed in (Peyré et al., 2016) for solving the entropic regularized version of GW.

3.2. Invariant OT

In (Alvarez-Melis et al., 2019), authors consider a scenario where the OT problem is used to align measures supported on sets of points for which meaningful pairwise distances are hard or impossible to calculate. This may happen, for instance, due to some latent transformation that have been applied to the features. The main underlying idea of their approach is to find an assignment of the points and to calculate a transformation to match the features. More precisely, for two measures $\mu, \mu'$, supported on the same Euclidean space $\mathbb{R}^d$, the corresponding objective function is:

$$\text{InvOT}^L_p(\mathbf{X}, \mathbf{X}') := \min_{\pi \in \Pi} \min_{f \in \mathcal{F}_p} \langle M_f, \pi \rangle,$$

where $(M_f)_{ij} = L(x_i, f(x'_j))$ and $\mathcal{F}_p$ is a space of matrices with bounded Shatten $p$-norm, i.e., $\mathcal{F}_p = \{P \in \mathbb{R}^{d \times d} : \|P\|_F \leq k_p\}$. As noted by the authors in Lemma 4.3, (16) can be related to the GW problem when $C, C'$ are calculated using the cosine similarity for $p = 2$. In this case, author show that GW and InvOT are equivalent, namely a solution of GW is a solution of InvOT and conversely. We can further show that the GW problem with cosine similarities is actually concave so that COOT and GW are also equivalent in this case. Overall, we have the following result:

**Proposition 4.** Using previous notations, $L = \|\cdot\|_2^2$, $p = 2$ (i.e. $\mathcal{F}_2 = \{P \in \mathbb{R}^{d \times d} : \|P\|_F = \sqrt{d}\}$) and cosine similarities $C = XX^T, C' = XX'^T$ (columns are normalized without loss of generality). Then problems of computing $\text{InvOT}^2(\|\cdot\|_2^2, \mathbf{X}, \mathbf{X}')$, COOT($C, C'$) and GW($C, C'$) are equivalent, namely any solution of one of these problems is a solution for others problems.

3.3. Election isomorphism

The election isomorphism problem mentioned earlier has recently been introduced in (Faliszewski et al., 2019) to compare two elections given by preference orders for candidates of voters. The authors express their problem quite similarly to COOT and also seek for correspondences between voters and candidates across two elections where the preferences of each voter are known (which is unrealistic in modern democracies). They focus on the setting where both elections have exactly the same number of voters $n = n'$ and candidates $d = d'$ and search for an optimal permutation via a Linear Integer Program. It is interesting to see that their problem consisting in aligning voters using the Spearman distance is actually equivalent to solving COOT with $L = \|\cdot\|_2$ on voters preferences. To that extent, COOT is a more general approach as it is applicable for general loss functions $L$, contrary to the Spearman distance used in (Faliszewski et al., 2019), and generalizes to the cases where $n \neq n'$ and $m \neq m'$. A more detailed comparison is given in supplementary.

4. Numerical experiments

In this section, we highlight two potential applications of COOT in a machine learning context: heterogeneous domain adaptation and co-clustering.

4.1. Heterogeneous domain adaptation

In a classification context, the problem of domain adaptation (DA) arises whenever one has to perform classification on a
set of data $X_t = \{x_t^i\}_{i=1}^{N_t}$ (usually called the target domain) but has only few or no labelled data associated. Given a second (source) domain $X_s = \{x_s^i\}_{i=1}^{N_s}$ with associated labels $Y_s = \{y_s^i\}_{i=1}^{N_s}$, one would like to leverage on this knowledge to train a classifier in the target domain. Unfortunately, direct use of the source information usually leads to poor results because of the discrepancy between source and target distributions. Among others, several works, e.g. (Courty et al., 2017), use OT to perform this adaptation. However, in the case where the data do not belong to the same metric space ($X_s \in \mathbb{R}^{N_s \times d}$ and $X_t \in \mathbb{R}^{N_t \times d'}$ with $d \neq d'$), the problem is getting harder as domains probability distributions cannot be anymore compared or aligned in a straightforward way. This instance of the DA problem, known as heterogeneous domain adaptation (HDA), has received less attention in the literature, partly due to the lack of appropriate divergence measures that can be used in such context. State-of-the-art HDA methods include Canonical Correlation Analysis (Yeh et al., 2014) and its kernelized version and a more recent approach based on the Gromov-Wasserstein discrepancy (Yan et al., 2018). Usually, one considers a semi-supervised variant of the problem, where one has access to a small number $n_t$ of labelled samples per class in the target domain, because the unsupervised problem ($n_t = 0$) is much more difficult. Our goal is to show that COOT can achieve good results in both settings.

Solving HDA with COOT In order to perform adaptation of the two domains, we solve COOT($X_s, X_t$) between the samples from the two domains. Once solved, the $\pi^*$ matrix provides a transport/correspondence between samples (as illustrated in Figure 1) that can be used to estimate the labels of the target samples using label propagation (Redko et al., 2019). Assuming uniform sample weights and one-hot encoded labels, a class prediction $\hat{Y}_t$ on the target domain samples can be achieved by computing $\hat{Y}_t = N_t \pi^* Y_s$. When available, existing labelled target samples can be used to obtain a better mapping by using the semi-supervised strategy from (Courty et al., 2017, Sec. 4.2). We prevents samples from source domain to domain to connect to samples in the target domain when the two belong to different classes by adding a very high cost in the cost matrix for every such source sample.

Datasets We choose to test our method on the classical Caltech-Office dataset (Saenko et al., 2010), which is dedicated to object recognition in images from several domains. Those domains exhibit variability in term of presence/absence of background, lightning conditions, image quality, that as such induce distribution shifts between the domains. Among the available domains, we select the following three: Amazon (A), the Caltech-256 image collection (C) and Webcam (W). Ten overlapping classes between the domains are used and two different deep feature representations of image in each domain are obtained using the Decaf (Donahue et al., 2014) and GoogleNet (Szegedy et al., 2015) neural network architectures. In both cases, we extract the image representations as the activations of the last fully-connected layer, yielding respectively sparse 4096 and 1024 dimensional vectors. The heterogeneity comes from these two very different representations.

Competing methods and experimental settings We compare COOT with four other methods. First two baselines, CCA and KCCA (Yeh et al., 2014), based on canonical correlation analysis and its kernelized version for which we use a Gaussian kernel with width parameter set as the inverse of the dimension of the input vector. Other two baselines, EGW and SGW (Yan et al., 2018) are two methods based on the Gromov-Wasserstein distance. The first one is an entropic version of GW, while the second leverages on the availability of labelled target data through two regularization terms. In both cases, the entropic regularization term was set to .1, and the two other regularization hyperparameters for the semi-supervised case to $\lambda = 1e-5$ and $\gamma = 1e-2$ following authors recommendations. We use COOT with entropic regularization on the feature mapping, with parameter 1 in all experiments. For each OT method, label propagation was used for classifying target samples, and the final class is determined as the maximum entry of $\hat{Y}_t$ per column. Classification was conducted with a knn classifier, with $k = 3$, for all non-OT methods. We run the experiment in a semi-supervised setting with $n_t = 3$, i.e., 3 samples per class were labelled in the target domain. The baseline score is the result of classification by only considering labelled samples in the target domain as the training set. For each pair of domains, we selected 20 samples per class to form the learning sets. We run this random selection process 10 times and consider the mean accuracy of the different runs as a performance measure. In the presented results, we perform adaptation from Decaf to GoogleNet features, but we also report the results for $n_t \in \{0, 1, 3, 5\}$ in the opposite direction in the supplemental material.

Results We first provide in Table 1 the results for the semi-supervised case. From it, we see that COOT surpasses all the other state-of-the-art methods in terms of mean accuracy. This result is confirmed by a p-value lower than 0.001 on a pairwise method comparison with COOT in a Wilcoxon signed rank test. SGW provides the second best result, while CCA and EGW give less than average results. A possible explanation for this is the fact that the considered problem is high-dimensional with only a low number of samples. Consequently, both methods seem to struggle in finding meaningful relations between the domains. Finally, KCCA performs better, but still fails most of the time to surpass the baseline score.
Table 1. Semi-supervised Heterogeneous Domain Adaptation results. In this table we perform adaptation from Decaf to GoogleNet representation. $n_u = 3$ labelled samples per class are used in the target domain to help the adaptation process.

| Domains | baseline | CCA | KCNA | EGW | SGW | COOT |
|---------|----------|-----|------|-----|-----|------|
| C→W    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| W→C    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| W→W    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| A→C    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| A→W    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| C→A    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| A→A    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| Mean    | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 | 84.10±1.44 |
| p-value | .001      | .001  | .001  | .001  | .001  | .001  |

Table 2. Unsupervised Heterogeneous Domain Adaptation results. In this table we perform adaptation from Decaf to GoogleNet representation.

Results for the unsupervised case can be found in Table 2. This setting is rarely considered in the literature as unsupervised HDA is a very difficult problem. In this table, we do not provide scores for the no-adaptation baseline and SGW, as they require labelled data. As one can expect, most of the methods fail in obtaining good classification accuracies in this setting, despite the high discriminative quality of the deep feature representations. Yet, COOT succeeds in providing a meaningful mapping in some cases. This illustrates the capacity our method to reveal relationships between very different, high-dimensional data even in the absence of any known pairwise relations.

4.2. Co-clustering and data summarization

While clustering methods present an important discovery tool for data analysis, one of their main limitations is to completely discard the potential relationships that may exist between the features that describe the data samples. For instance, in recommendation systems, where each user is described in terms of his or her preferences for some product, clustering algorithms may benefit from the knowledge about the correlation between different products revealing their probability of being recommended to the same users. This idea is the cornerstone of co-clustering (Hartigan, 1972)

where the goal is to perform clustering of both data points and features simultaneously. The obtained latent structure of data is composed of blocks usually called co-clusters. Below, we consider a co-clustering task that consists in finding $g$ and $m$ homogeneous clusters of both samples (rows) and features (columns) of a given data matrix $X \in \mathbb{R}^{n \times d}$ where $g \leq n$ and $m \leq d$.

**COOT-clustering** In the context of our algorithm, we propose to solve the following optimization problem:

$$\min_{\pi, \pi'} \text{COOT}(X, X_c)$$

where $X_c \in \mathbb{R}^{g \times m}$ contains the average values representing the clusters. Note that in practice, we propose again to perform a BCD algorithm by optimizing iteratively over $(\pi, \pi')$ and $X_c$. This boils down to alternating the following steps with $X_c$ initialized with random values and supposing uniform weights: 1) obtain $\pi$ and $\pi'$ by solving $\text{COOT}(X, X_c)$; 2) set $X_c$ to $\text{gnrm}^+ \left( X \pi \right)$. The second step of the procedure is a least-square estimation when $L = \| \cdot \|_2^2$ and corresponds to minimizing the COOT objective w.r.t. $X_c$. It is reminiscent of the updates used in the calculation of Gromov-Wasserstein barycenter as mentioned in (Peyr et al., 2016, Proposition 3) and to the use of barycentric mapping in domain adaptation as described in (Courty et al., 2017). In practice, we observed that few iterations of this procedure are enough to ensure a convergence in objective value and iterations.

**Simulated data** We simulate data following the generative process of (Laclau et al., 2017) where four scenarios with different number of co-clusters, degrees of separation and sizes were considered (the details on the characteristics of each dataset are given in the supplementary materials). As in (Laclau et al., 2017), we use the same co-clustering baselines including ITCC (Dhillon et al., 2003), Double K-Means (DKM) (Rocci & Vichi, 2008), Orthogonal Non-negative Matrix Tri-Factorizations (ONTFM) (Ding et al., 2006), the Gaussian Latent Block Models (GLBM) (Nadif & Govaert, 2008) and Residual Bayesian Co-Clustering (RBC) (Shan & Banerjee, 2010) as well as the K-means and NMF run on both modes of the data matrix, as clustering baseline. The performance of all methods is measured using the co-clustering error (CCE) (Patrikainen & Meila, 2006). For all configurations, we generate 100 data sets and present the mean and standard deviation of the CCE over all sets for all baselines in Table 2. Based on these results, we see that our algorithm outperforms all the other baselines on D1, D2 and D4 data sets while being behind COOT–GW proposed by (Laclau et al., 2017) on D3. This result is rather strong as our method relies on the original data matrix while the method of (Laclau et al., 2017) relies on its kernel representations and thus benefits from the non-linear information captured by it.
Table 2. Mean (± standard-deviation) of the co-clustering error (CCE) obtained for all configurations. “-” indicates that the algorithm cannot find a partition with the requested number of co-clusters. All the baselines results (first 9 columns) are from (Laclau et al., 2017).

| Data set | K-means | NMF | DKM | Tri-NMF | GLBM | FTCC | RBC | COOT | COOT–GW | COOT |
|----------|---------|-----|-----|---------|------|------|-----|------|---------|------|
| D1       | 0.018 ± 0.003 | 0.042 ± 0.037 | 0.025 ± 0.048 | 0.082 ± 0.063 | 0.021 ± 0.011 | 0.021 ± 0.001 | 0.017 ± 0.045 | 0.018 ± 0.013 | 0.004 ± 0.002 | 0     |
| D2       | 0.072 ± 0.044 | 0.083 ± 0.063 | 0.038 ± 0.000 | 0.052 ± 0.065 | 0.032 ± 0.041 | 0.047 ± 0.042 | 0.039 ± 0.052 | 0.023 ± 0.036 | 0.011 ± 0.056 | 0.009 ± 0.04  |
| D3       | -        | -   | 0.310 ± 0.000 | -        | 0.262 ± 0.022 | 0.241 ± 0.031 | -        | 0.031 ± 0.027 | 0.008 ± 0.001 | 0.04 ± 0.05  |
| D4       | 0.126 ± 0.038 | -   | 0.145 ± 0.082 | -        | 0.115 ± 0.047 | 0.121 ± 0.075 | 0.102 ± 0.071 | 0.093 ± 0.032 | 0.079 ± 0.001 | 0.068 ± 0.04  |

Table 3. Top 5 of movies in clusters M1 and M20. Average rating of the top 5 rated movies in M1 is 4.42, while for the M20 it is 1.

| M1       | M20       |
|----------|-----------|
| Shawshank Redemption (1994) | Police Story 4: Project S (Chao ji ji hua) (1993) |
| Schindler’s List (1993) | Eye of Vichy, The (Oeil de Vichy, L) (1993) |
| Casablanca (1942) | Promise, The (Versprechen, Das) (1994) |
| Rear Window (1954) | To Cross the Rubicon (1991) |
| Usual Suspects, The (1995) | Daens (1992) |

5. Discussion and conclusion

In this paper, we presented a novel variant of the optimal transport problem which aims at comparing distributions supported in different spaces. To this end, two optimal transport maps, one acting on the sample space, and the other on the feature space, are optimized to connect the two heterogeneous distributions. We show that this novel problem has connections with bilinear assignment and provide algorithms to solve it. We demonstrate its usefulness and versatility on two difficult machine learning problems: heterogeneous domain adaptation and co-clustering/data summarization, where promising results were obtained.

Figure 2. Co-clustering with COOT on the Olivetti faces dataset. (left) Example images from the dataset (center) centroids estimated by COOT; (right) clustering of the pixels estimated by COOT where each color represents a cluster.

Figure 3. (left) MOVIELENS matrix; (right) the summarized matrix $X_s$ obtained with COOT. Darker blue indicate higher values.

Figure 4. Heatmap for the top 5 rated movies in clusters M1 and M20.

Table 4. Top 5 of movies in clusters M1 and M20. Average rating of the top 5 rated movies in M1 is 4.42, while for the M20 it is 1.

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Footnote: 1https://grouplens.org/datasets/movielens/100k/
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6. Supplementary material

6.1. Metric properties

**Proposition 5** (COOT is a distance between same sized datasets). Suppose $L = | \cdot |^p$, $p \geq 1$, $n = n'$, $d = d'$ and that the weights $w, w', v, v'$ are uniform.

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Then \( \text{COOT}(X, X') = 0 \) iff there exists a permutation of the samples \( \sigma_1 \in \mathbb{S}_n \) and of the features \( \sigma_2 \in \mathbb{S}_d \), s.t. \( \forall i, k \in [n] \times [d], X_{i,k} = X'_{\sigma_1(i), \sigma_2(k)} \).

Moreover, it is symmetric and satisfies the triangular inequality as long as \( L \) satisfies the triangle inequality \( \text{COOT}(X, X') \leq \text{COOT}(X, X') + \text{COOT}(X', X'') \).

**Proof.** The symmetry is obvious. To prove the triangle inequality of COOT for arbitrary measures we will use the gluing lemma (see (Villani, 2008)) which stresses the existence of couplings with a prescribed structure. Let \( X \in \mathbb{R}_n \times d, X' \in \mathbb{R}_n \times d' \), \( X'' \in \mathbb{R}_n \times d'' \) associated with \( w \in \Delta_n, v \in \Delta_d, w' \in \Delta'_n, v' \in \Delta'_d, w'' \in \Delta''_n, v'' \in \Delta''_d \). Without loss of generality for our proof we can suppose that all weights are different from zeros (otherwise we can consider \( \tilde{w}_i = w_i \) if \( w_i > 0 \) and \( \tilde{w}_i = 1 \) if \( w_i = 0 \) see proof of Proposition 2.2 in (Peyré & Cuturi, 2019)).

Let \( \pi_1^v, \pi_1^w \) and \( \pi_2^v, \pi_2^w \) be two couple of optimal solutions for the COOT problems associated with \( \text{COOT}(X, X', w, w', v, v') \) and \( \text{COOT}(X', X'', w', w'', v', v'') \) respectively.

We define:

\[
S_1 = \pi_1^v \text{diag}(\frac{1}{w}) \pi_2^w \\
S_2 = \pi_1^v \text{diag}(\frac{1}{v'}) \pi_2^w
\]

Then it is easy to check that \( S_1 \in \Pi(w, w') \) and \( S_2 \in \Pi(v, v'') \)

\[
\begin{align*}
\text{COOT}(X, X'', w, w'', v, v'') & \leq \langle L(X, X'') \rangle \circ S_1 \circ S_2 \\
& = \langle L(X, X'') \rangle \circ [\pi_1^v \text{diag}(\frac{1}{w}) \pi_2^w, \pi_1^v \text{diag}(\frac{1}{v'}) \pi_2^w]
\end{align*}
\]

Where in (*) we used the suboptimality of \( S_1 \), \( S_2 \) and in (**) the fact that \( L \) satisfies the triangular inequality.

Now note that:

\[
\begin{align*}
& \langle L(X, X') \rangle \otimes [\pi_1^v \text{diag}(\frac{1}{w'}) \pi_2^w, \pi_1^v \text{diag}(\frac{1}{v'}) \pi_2^w] \\
& \leq \langle L(X, X') \rangle + \langle L(X', X'') \rangle \\
& = \langle L(X, X') \rangle + [\pi_1^v \text{diag}(\frac{1}{w'}) \pi_2^w, \pi_1^v \text{diag}(\frac{1}{v'}) \pi_2^w]
\end{align*}
\]

6.2. Equivalence bilinear assignment and QAP

**Theorem 2.** If \( Q \) is a negative definite matrix then problems:

\[
\begin{align*}
\min_{x} f(x) & = c^T x + \frac{1}{2} x^T Q x \\
s.t. & \quad Ax = b, \quad x \geq 0
\end{align*}
\]

\[
\begin{align*}
\min_{x, y} g(x, y) & = \frac{1}{2} c^T x + \frac{1}{2} c^T y + \frac{1}{2} x^T Q y \\
s.t. & \quad Ax = b, Ay = b, \quad x, y \geq 0
\end{align*}
\]

are equivalent. More precisely if \( x^* \) is an optimal solution for (7) then \( (x^*, x^*) \) is a solution for (8) and if \( (x^*, y^*) \) is optimal for (8) then both \( x^* \) and \( y^* \) are optimal for (7).
are equivalent. More precisely if \( x^* \) is an optimal solution for (7) then \((x^*, x^*)\) is a solution for (8) and if \((x^*, y^*)\) is optimal for (8) then both \(x^*\) and \(y^*\) are optimal for (7).

**Proof.** This proof is mostly a rewriting of proof of theorem 2.2 in (Konno, 1976a). First note than both (7) and (8) are equivalent to:

\[
\begin{align*}
\max_x f(x) &= c^Tx + \frac{1}{2}x^T Q x \\
\text{s.t.} \quad Ax &= b, \quad x \geq 0
\end{align*}
\]

(9)

\[
\begin{align*}
\max_{x,y} g(x, y) &= \frac{1}{2}c^T x + \frac{1}{2}y^T y + \frac{1}{2}x^T Q y \\
\text{s.t.} \quad Ax &= b, \quad A^T y = b, \quad x, y \geq 0
\end{align*}
\]

(10)

with \(Q\) being semi positive definite. Let \(z^*\) be optimal for (9) and \((x^*, y^*)\) be optimal for (10). Then by definition for all \(x\) satisfying the restricts of (9) \(f(z^*) \geq f(x)\). In particular \(f(z^*) \geq f(x^*) = g(x^*, x^*)\) and \(f(z^*) \geq f(y^*) = g(x^*, y^*)\). Also \(g(x^*, y^*) \geq \max_{x \geq 0, x \geq 0} g(x, x) = f(z^*)\).

To prove the theorem it suffices to prove that

\[
f(y^*) = f(x^*) = g(x^*, y^*)
\]

(11)

since in this case \(g(x^*, y^*) = f(x^*) \geq f(z^*)\) and \(g(x^*, y^*) = f(y^*) \geq f(z^*)\).

Let us prove (11). Since \((x^*, y^*)\) is optimal we have:

\[
0 \leq g(x^*, y^*) - g(x^*, x^*) = \frac{1}{2}c^T (y^* - x^*) \\
+ \frac{1}{2}x^T Q (y^* - x^*)
\]

(12)

\[
0 \leq g(x^*, y^*) - g(y^*, y^*) = \frac{1}{2}c^T (x^* - y^*) \\
+ \frac{1}{2}y^T Q (x^* - y^*)
\]

(13)

By adding these inequalities we obtain:

\[
(x^* - y^*)^T Q (x^* - y^*) \leq 0
\]

(14)

Since \(Q\) is positive definite this implies that \(Q(x^* - y^*) = 0\). So using previous inequalities \(c^T (x^* - y^*) = 0\) hence \(g(x^*, y^*) = g(x^*, x^*) = g(y^*, y^*)\) as required.

Note also that this result holds when we add a constant term in the costs.

6.3. Relation with GW distance

This section aim at proving all the theorems of Section 3.1 of the main paper. We first recall the GW problem:

\[
GW(C, C', w, w') = \min_{\pi \in \Pi(w, w')} \langle L(C, C') \otimes \pi, \pi^* \rangle
\]

(15)

6.3.1. Concavity of the Gromov-Wasserstein problem

We will now prove the proposition 2 in the main paper which is the following:

**Proposition 6.** Let \(L = || \cdot ||^2\) and suppose that \(C \in \mathbb{R}^{n \times n}, C' \in \mathbb{R}^{n' \times n'}\) are squared Euclidean distance matrices such that \(C = x1_n^T + x^T X X^T\), \(C' = y1_{n'}^T + y^T X' X'^T\) with \(x = \text{diag}(XX^T), x' = \text{diag}(X'X'^T)\). Then, the GW problem can be written as (7) with \(Q = -8 * XX^T \otimes X'X'^T\). In particular, \(Q\) is semi-negative definite so that the GW problem is a concave quadratic program.

This result is actually a consequence of the following proposition which is a more detailed version:

**Proposition 7.** With previous notations and hypothesis the Gromov-Wasserstein problem can be formulated as:

\[
GW(C, C', w, w') = \min_{\pi \in \Pi(w, w')} -4\text{vec}(M)^T \text{vec}(\pi^*) \\
- 8\text{vec}(\pi^*)^T \text{Qvec}(\pi^*) + Cte
\]

with:

\[
M = xx^T - 2xw'^T X X' T - 2XX^Twx'^T \\
Q = XX^T \otimes \pi X'X'^T \\
Cte = 2w^T x + 2w'^T x' - 2\|X^T w\|_2^2 - 2\|X'^T w'\|_2^2 \\
- 4(w^T x)(w'^T x')
\]

In particular, \(Q\) is semi-positive definite so that the GW problem is a concave quadratic program.

**Proof.** Using the results in (Peyré et al., 2016) for \(L = || \cdot ||^2\) we have \(L(C, C') \otimes \pi^* = c_{C, C'} - 2C \pi^* C'\) with \(c_{C, C'} = Cw1_{n'}^T + w'^T C'\). With the definition of \(C, C'\) we then have:

\[
c_{C, C'} = Cw1_{n'}^T + w'^T C' \\
= (x1_n^T + x^T X X^T)w1_{n'}^T \\
+ 1_n^T w'^T (x1_n^T + x^T X X^T) \\
= (x1_n^T w1_{n'}^T + 1_n^T x^T X X'^T) \\
+ 1_n^T w'^T x1_n^T + 1_n^T x^T (x'1_{n'}^T - 21_n^T w'^T X X'^T) \\
= 2(x1_n^T - XX^T w1_{n'}^T) + 2(1_n^T x^T - 1_n^T w'^T X X'^T) \\
\]
where in the last equality we used $1^T_n w = w^T 1_n = 1^T_n w' = w'^T 1_n = 1$ and that $x^T w = w^T x \in \mathbb{R}$ (same argument for $x'$).

Moreover:

$$
\langle C\pi^* C', \pi^* \rangle = \text{tr}[\pi^T (x 1^T_n + 1_n x^T - 2XX^T) \pi^*]
$$

$$
\langle x^T 1^T_n + 1_n x^T - 2X' X'^T \rangle
$$

$$
\text{tr}[\pi^T x^T (\pi^* 1^T_n + w^T x^T - 2\pi^T XX^T + \pi^T X X^T - 2\pi^T X X^T w x^T - 2\pi^T X X^T w x^T + 4\pi^T XX^T \pi^* X X^T)]
$$

where in (*) we used:

$$
\text{tr}(w x^T \pi^* x') = \langle x^T 1^T_n, w x^T \pi^* \rangle = \langle \pi^* x^T w, x_n \rangle
$$

and therefore:

$$
\langle C\pi^* C', \pi^* \rangle = \text{tr}(\pi^T x^T XX^T \pi^* x')
$$

so that:

$$
\langle c_{C, C'} - 2C\pi^* C', \pi^* \rangle = C te - 4\langle x x^T - 2wx' X X^T - 2X^T X wx^T, \pi^* \rangle - 8\text{tr}(\pi^T XX^T \pi^* X X^T)
$$

with $Cte = 2w^T x + 2w^T x - 2\|X^T w\|^2 - 2\|X^T w\|^2 - 2\|X^T w\|^2 - 2\|X^T w\|^2$. Finally it is clear that $Q$ is negative semi-definite since as the opposite of a Kronecker product of positive semi-definite matrices.

Using previous theorems we are able to prove the proposition 3 of the paper:

**Proposition 8.** Let $C \in \mathbb{R}^{n \times n}$, $C' \in \mathbb{R}^{n' \times n'}$ be any matrices, then:

$$
\text{COOT}(C, C', w, w', w, w') \leq GW(C, C', w, w')
$$

Moreover, if $L = \| \cdot \|^2$ and $C, C'$ are squared Euclidean distance matrices, $\text{COOT}(C, C', w, w', w, w') = GW(C, C', w, w')$. Moreover, if one finds an optimal solution $(\pi^*_t, \pi^*_w)$ of COOT, then both $\pi^*_t, \pi^*_w$ are solutions of (15). Conversely, if $\pi^*_t$ is an optimal solution of (15), then $(\pi^*_t, \pi^*_w)$ is an optimal solution for COOT.

**Proof.** The first inequality is obvious, since any optimal solution of the GW problem is an admissible solution for the COOT problem, hence the inequality is true by suboptimality of this optimal solution.

For the equality part, by following the same calculus of the proof of proposition 7 we can check that:

$$
\text{COOT}(C, C', w, w', w, w') = \min_{\pi^* \in (\mathbb{R}^n, w')^T} -2\text{vec}(M)^T \text{vec}(\pi^*) - 2\text{vec}(M)^T \text{vec}(\pi^*) - 8\text{vec}(\pi^*)^T \text{Qvec}(\pi^*) + C te
$$

with $M, Q, Cte$ defined in proposition 7.

Since $Q$ is negative semi-definite we can apply theorem 2 to prove that both problems are equivalent and lead to the same cost (as the theorem is valid if we add a constant term to the costs).

**6.3.2. EQUIVALENCE OF DC ALGORITHM AND FRANK-WOLFE ALGORITHM FOR GW**

In this section we prove that the DC algorithm for solving GW problems presented in the paper, when $L = \| \cdot \|^2$ and for squared euclidean distance matrices, is equivalent to the Frank-Wolfe (FW) based algorithm presented in (Vayer et al., 2019).

Both algorithms to solve (15) are presented in Algorithm.3 and Algorithm.4.
The case when $L = \| \cdot \|^2$ and $C, C'$ are squared euclidean distance matrices has interested implications since the resulting GW problem is a concave QP (as explained in the paper and shown in Section 6.3.1 of this supplementary). In (Maron & Lipman, 2018) authors were interested in solving QP with conditionally concave energies using a FW algorithm. They showed that in this case the line-search step of the FW is always 1. Moreover as shown in Prop.7 the GW problem can be written as a concave QP with concave energy and is minimizing a fortiori a conditionally concave energy. As a matter of consequence, the line-search step of the FW algorithm proposed in (Vayer et al., 2019) and described in Algorithm.4 always leads to an optimal line-search step of 1. In this case the Algorithm.4 is equivalent to Algorithm.5 since $\tau(k) = 1$ for all $k$.

Finally by noticing that in the step 3 of Algorithm.5 the gradient of Eq. (15) w.r.t $\pi^*_k(k-1)$ is $2L(C, C') \otimes \pi^*_k(k-1)$, which gives the same OT solution as for the OT problem in step 3 of Algorithm.3, we can conclude that the iterations of both algorithms are equivalent.

6.4. Relation with InvariantOT

The objective of this part is to prove the connections between GW, COOT and InvOT as recalled below:

Proof. For GW see eq.6 in (Vayer et al., 2019). For COOT
we have:

\[
\text{COOT}(C, C', w, w') = \min_{\pi^i \in \Pi(w, w'), \pi^v \in \Pi(w, w')} \langle L(C, C') \otimes \pi^i, \pi^v \rangle \\
= \min_{\pi^i \in \Pi(w, w'), \pi^v \in \Pi(w, w')} \frac{1}{2} \langle L(C, C') \otimes \pi^i, \pi^v \rangle \\
+ \frac{1}{2} \langle L(C, C') \otimes \pi^i, \pi^v \rangle \\
= \min_{\pi^i \in \Pi(w, w'), \pi^v \in \Pi(w, w')} \frac{1}{2} \langle Cw_{1,v} + 1_n w'C', \pi^v \rangle \\
+ \frac{1}{2} \langle Cw_{1,v} + 1_n w'C', \pi^v \rangle - 2 \langle C\pi^i C', \pi^v \rangle
\]

Last equality gives the result. □

Proof. Of proposition 9

Let \( C = XX^T, C' = X'X'^T \) be the two cosine similarities (we can suppose without loss of generality that the column are normalized). We know from (Alvarez-Melis et al., 2019) that \( GW(C, C') \) and \( \text{InvOT}_{\frac{1}{2}}(X, X') \) are equivalent (see Lemma 4.3 of the paper). It sufficies to show that \( GW(C, C') \) and \( \text{COOT}(C, C') \) are equivalent. By virtue of proposition 10 the Q associated with the QP and BP problems of GW and COOT is \( Q = -4XX^T \otimes \gamma X'X'^T \) which is a negative semi-definite matrix. In this way we have all the hypothesis to apply theorem 2 which prove that \( GW(C, C') \) and \( \text{COOT}(C, C') \) are equivalent.

6.5. Relation with election isomorphism

This section aims at showing that our COOT approach can be used to solve the election isomorphism problem defined in (Faliszewski et al., 2019). The problem is the following: let \( E = (C, V) \) and \( E' = (C', V') \), where \( C = \{c_1, \ldots, c_m\} \) (resp. \( C' \)) is a set of candidates and \( V = \{v_1, \ldots, v_n\} \) (resp. \( V' \)) is a set of voters, where each voter \( v_i \) has a preference order, also denoted by \( v_i \). The two elections \( E = (C, V) \) and \( E' = (C', V') \), where \( |C| = |C'|, V = \{v_1, \ldots, v_n\} \), and \( V' = \{v'_1, \ldots, v'_n\} \), are said to be isomorphic if there is a bijection \( \sigma : C \rightarrow C' \) and a permutation \( \nu \in S_n \) such that \( \sigma(v_i) = v'_\nu(i) \) for all \( i \in [n] \). The authors further propose a distance underlying this problem defined as follows:

\[
d-\text{ID}(E, E') = \min_{\nu \in S_n} \min_{\sigma \in \Pi(C, C')} \sum_{i=1}^{n} d\left(\sigma(v_i), v'_\nu(i)\right)
\]

where \( S_n \) denotes the set of all permutations over \( \{1, \ldots, n\} \), \( \Pi(C, C') \) is a set of bijections and \( d \) is an arbitrary distance between preference orders. The authors of (Faliszewski et al., 2019) compute d-ID\((E, E')\) in practice by expressing it as the following Integer Linear Programming problem over the tensor \( P_{ijkl} = M_{ij}N_{kl} \) where \( M \in \mathbb{R}^{m \times m}, N \in \mathbb{R}^{n \times n} \)

\[
\min_{P,N,M} \sum_{i,j,k,l} P_{ijkl} |\text{pos}_{v_i}(c_k) - \text{pos}_{v'_j}(c'_l)|
\]

s.t. \( (N1_i)_k = 1, \forall k, (N^T1)_n = 1, \forall l \) (17)

\( (M1_m)_i = 1, \forall i, (M^T1_m)_l = 1, \forall l \)

\( P \leq N_{k,l}, P_{i,j,k,l} \leq M_{i,j}, \forall i, j, k, l \)

\( \sum_{i,k} P_{i,j,k,l} = 1, \forall j, l \) (18)

\[
\min_{N,M} \sum_{i,j,k,l} M_{ij}N_{kl} |\text{pos}_{v_i}(c_k) - \text{pos}_{v'_j}(c'_l)|
\]

s.t. \( N1_i = 1, M^T1_m = 1 \) (19)

where \( \text{pos}_{v_i}(c_k) \) denotes the position of candidate \( c_k \) in the preference order of voter \( v_i \). Let us now define two matrices \( X \) and \( X' \) such that \( X_{i,k} = \text{pos}_{v_i}(c_k) \) and \( X'_{j,l} = \text{pos}_{v'_j}(c'_l) \) and denote by \( \pi^i, \pi'^v \) a minimizer of COOT\((X, X'), 1_n/n, 1_n/n, 1_m/m, 1_m/m \) with \( L = |\cdot| \) and by \( N^*, M^* \) the minimizers of problem (18), respectively.

As shown in the paper there exists an optimal solution for COOT\((X, X')\) given by permutation matrices as solutions of the Monge-Kantorovich problems for uniform distributions supported on the same number of elements. Then, one may show that the solution of the two problems coincide modulo a multiplicative factor, i.e., \( \pi^i = \frac{1}{|C|} N^* \) and \( \pi'^v = \frac{1}{|C'|} M^* \) are optimal since \( |C| = |C'| \) and \( |V| = |V'| \). For \( \pi^i \) (the same reasoning holds for \( \pi'^v \) as well), we have that

\[
(\pi^i)_{ij} = \begin{cases} 
\frac{1}{n}, & j = v^i_l \\
0, & \text{otherwise.}
\end{cases}
\]

where \( v^i_l \) is a permutation of voters in the two sets. The only difference between the two solutions \( \pi^i \) and \( N^* \) thus stems from marginal constraints (19). To conclude, we note that COOT is a more general approach as it is applicable for general loss functions \( L \), contrary to the Spearman distance used in (Faliszewski et al., 2019), and generalizes to the cases where \( n \neq n' \) and \( m \neq m' \).

6.6. Complementary results for the HDA experiment

Here we propose the full results for the heterogeneous domain adaptation experiment. Table 5 follows the same experimental protocol as in the paper but shows the two cases where \( n_t = 1 \) and \( n_t = 5 \). Table 6 and Table 7 deal with
the adaptation from GoogleNet to Decaf features, in a semi-supervised and resp. unsupervised adaptation. Overall, the results are coherent with the analysis proposed in the paper. In both settings, when $n_t = 5$, one can see that the performance differences between SW and COOT is diminishing.

| Table 5. Semi-supervised Heterogeneous Domain Adaptation results. In this table we adapt from Decaf to GoogleNet for different values of $n_t$. |
|-------------------------------------------------------------|
| Domainsc | baseline | CCA | KCKA | EGW | SW | COOT |
| C→A | 3.2 | 3.0 | 2.7 | 2.3 | 1.8 | 1.0 |
| C→B | 2.9 | 2.6 | 2.3 | 2.0 | 1.5 | 0.8 |
| C→C | 2.6 | 2.3 | 2.1 | 1.8 | 1.4 | 0.7 |
| C→D | 2.3 | 2.0 | 1.8 | 1.5 | 1.1 | 0.5 |
| C→E | 2.0 | 1.8 | 1.6 | 1.4 | 1.0 | 0.4 |

| Table 6. Semi-supervised Heterogeneous Domain Adaptation results. In this table we adapt from GoogleNet to Decaf representations for different values of $n_t$. |
|-------------------------------------------------------------|
| Domains | baseline | CCA | KCKA | EGW | SW | COOT |
| C→A | 3.2 | 3.0 | 2.7 | 2.3 | 1.8 | 1.0 |
| C→B | 2.9 | 2.6 | 2.3 | 2.0 | 1.5 | 0.8 |
| C→C | 2.6 | 2.3 | 2.1 | 1.8 | 1.4 | 0.7 |
| C→D | 2.3 | 2.0 | 1.8 | 1.5 | 1.1 | 0.5 |
| C→E | 2.0 | 1.8 | 1.6 | 1.4 | 1.0 | 0.4 |

| Table 7. Unsupervised Heterogeneous Domain Adaptation results. In this table we adapt from GoogleNet to Decaf representations. |
|-------------------------------------------------------------|
| Domainsc | baseline | CCA | KCKA | EGW | SW | COOT |
| C→A | 3.2 | 3.0 | 2.7 | 2.3 | 1.8 | 1.0 |
| C→B | 2.9 | 2.6 | 2.3 | 2.0 | 1.5 | 0.8 |
| C→C | 2.6 | 2.3 | 2.1 | 1.8 | 1.4 | 0.7 |
| C→D | 2.3 | 2.0 | 1.8 | 1.5 | 1.1 | 0.5 |
| C→E | 2.0 | 1.8 | 1.6 | 1.4 | 1.0 | 0.4 |

| Table 8. Size ($n \times d$), number of clusters ($g \times m$), degree of overlapping (+ for well-separated and ++ for ill-separated clusters) and the proportions of co-clusters for simulated data sets. |
|-------------------------------------------------------------|
| Data set | $n \times d$ | $g \times m$ | Overlapping | Proportions |
| D1 | 600 × 300 | 3 x 3 | + | 0.60 ± 0.26 | 0.24 ± 0.07 | 0.12 ± 0.04 | 0.05 ± 0.02 | 94.58 ± 1.17 |
| D2 | 600 × 300 | 3 x 3 | + | 0.60 ± 0.26 | 0.24 ± 0.07 | 0.12 ± 0.04 | 0.05 ± 0.02 | 94.58 ± 1.17 |
| D3 | 300 × 200 | 2 x 4 | ++ | 0.30 ± 0.10 | 0.15 ± 0.05 | 0.10 ± 0.03 | 0.05 ± 0.02 | 94.58 ± 1.17 |
| D4 | 300 × 200 | 2 x 4 | ++ | 0.30 ± 0.10 | 0.15 ± 0.05 | 0.10 ± 0.03 | 0.05 ± 0.02 | 94.58 ± 1.17 |
Figure 4. Linear mapping from USPS to MNIST using $\pi^v$. (top) USPS samples (middle top) Sample resized to target resolution (middle bottom) samples mapped using $\pi^v$ (bottom) samples mapped using $\pi^v$ with entropic regularization.

Figure 5. Linear mapping from MNIST to USPS using $\pi^v$. (top) MNIST samples (middle top) Sample resized to target resolution (middle bottom) samples mapped using $\pi^v$ (bottom) samples mapped using $\pi^v$ with entropic regularization.