INTEGRAL PROBABILITY METRIC BASED REGULARIZATION FOR OPTIMAL TRANSPORT

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ABSTRACT

Recently it has been shown that Maximum Mean Discrepancy (MMD) based regularization for Optimal Transport (OT) can improve the sample complexity of estimation. However, the metric and other important properties of such MMD-regularized OT formulations are not well-understood. In this work, we not only bridge this gap, but further study novel Integral Probability Metric (IPM) regularized p-Wasserstein style formulations. We present generic settings under which we prove that the proposed OT formulations induce novel metrics over measures. While some of these novel metrics can be interpreted as infimal convolutions of IPMs; interestingly, some others turn out to be IPM-analogues of the so-called generalized Wasserstein metrics and the Gaussian Hellinger-Kantorovich metrics. Finally, we present finite sample based simplified formulations for estimating the squared-MMD regularized metrics as well as the corresponding barycenter. We empirically validate our theoretical findings and show improvements in downstream applications.

1 Introduction

Recently optimal transport (OT) has witnessed a lot of success in machine learning applications. [Peyré & Cuturi] (2019) is an excellent manuscript on this subject. OT’s success is partly due to clever regularization, which seems to play a critical role in handling noisy marginals [Frogner et al., 2015], marginals of unequal masses [Chizat, 2017; Liero et al., 2018], in determining the computational complexity [Cuturi, 2013; Seguy et al., 2018], and in affecting the sample complexity [Mena & Niles-Weed, 2019; Genevay et al., 2019; Feydy et al., 2018; Nath & Jawanpuria, 2020].

Optimal transport with $\phi$-divergence based regularization for matching marginals is a very well-understood topic [Liero et al., 2016, 2018; Chizat et al., 2018a,b; Chizat, 2017]. Regularizers based on total variation [Piccoli & Rossi, 2014, 2016; Hanin (1992); Georgiou et al. (2009)] are also well-studied. On the other hand, Nath & Jawanpuria (2020) recently showed that MMD-based regularization may help alleviate the curse of dimensionality in OT estimation. Motivated by this result, we wish to study Integral Probability Metric (IPM) [Sriperumbudur et al., 2009] regularized optimal transport. Recall that the MMD is the IPM induced by the unit RKHS-norm ball of a characteristic kernel and is not a $\phi$-divergence. IPMs are a family of metrics that are complementary to $\phi$-divergences, with the total variation metric being the only common member.

We begin by proposing a novel family of p-Wasserstein style OT formulations that employ IPM-regularization for matching the marginals. This may be useful in ML applications as the marginals are typically noisy/estimated, or when the marginals have unequal masses (e.g., unbalanced OT). Also, the proposed family subsumes the generalizations
Figure 1: Level sets of distance function between a family of source distributions and a fixed target distribution (a) MMD (b) OT with no regularization (c) OT with TV regularization (d) OT with Proposed MMD regularization. The proposed formulation results in lesser number of non-optimal stationary points.

studied in [Piccoli & Rossi (2014, 2016) and Nath & Jawanpuria (2020)]. And, in the sense that we consider infimal convolutions involving $p$-Wasserstein ($p > 1$), the proposal is also more general than those considered in [Schmitzer & Wirth (2019)].

We then focus on two specific settings of the proposed family of OT formulations. The first setting leads to those that can be interpreted as $p$-degree infimal convolutions of 1-Wasserstein with general IPM metrics. We show that such settings induce novel norm-based metrics, with the $p = 1$ giving back IPMs.

In the second setting, the proposed formulations can be interpreted as $p$-Wasserstein metrics ($p > 1$) with IPM-regularization. Importantly, we present mild conditions under which these IPM-regularized $p$-Wasserstein metrics are indeed valid metrics. This key result is a non-trivial extension of that in [Piccoli & Rossi (2014), Georgiou et al. (2009)], where the IPM regularizer is restricted to be the total variation metric. Note that these novel metrics can be considered as MMD/IPM analogues of the Gaussian Hellinger-Kantorovich (GHK) metrics obtained with $\phi$-divergence-regularization.

Encouraged by the theoretical findings, we present a finite sample based simplified formulation for estimating the proposed metrics with squared-MMD regularization. We also present a simplified formulation for solving the corresponding barycenter problem in the finite sample case. These formulations turn out to be instances of convex quadratic programs with non-negative/simplex constraints, which can be solved using projected gradient descent or mirror descent based solvers.

We present experimental results on synthetic as well as real-world datasets. We perform an empirical study of the proposed IPM-regularized formulation with respect to the learned transport plan and distance between measures. We demonstrate that the proposed OT metric and it’s transport plan exhibit desirable properties (Figures 1 & 2). Results on downstream ML applications like domain adaptation and class-ratio estimation show that the proposed IPM-regularized formulation outperforms KL-divergence regularized unbalanced OT formulation. Our results on single cell RNA sequencing further validate the quality of Barycenter interpolation obtained by our approach.

The rest of the paper is organized as follows. Section 2 provides a summary of the IPM and OT literature. Section 3 is the main section where we present the novel family of OT formulations, and analyze their metric properties etc. Section 4 discusses the empirical results. We conclude the paper with a discussion in Section 5.

2 Preliminaries

In this section we summarize necessary basic results from IPM and OT literature. We begin with some notations.

Let $\mathcal{X}$ be a set (domain) that forms a compact Hausdorff space. Let $\mathcal{R}^+(\mathcal{X})$, $\mathcal{R}(\mathcal{X})$ denote the set of all non-negative, signed (finite) Radon measures defined over $\mathcal{X}$; while the set of all probability measures is denoted by $\mathcal{R}_1^+(\mathcal{X})$. For a measure on the product space, $\pi \in \mathcal{R}^+(\mathcal{X} \times \mathcal{X})$, let $\pi_1$, $\pi_2$ denote the first and second marginals respectively (i.e., they are the push-forwards under the canonical projection maps onto $\mathcal{X}$). Let $\mathcal{L}(\mathcal{X})$, $\mathcal{C}(\mathcal{X})$ denote the set of all real-valued measurable,continuous functions over $\mathcal{X}$.
2.1 Integral Probability Metrics

Given a set $G \subset \mathcal{L}(\mathcal{X})$, the Integral Probability Metric (IPM) (Muller, 1997; Sriperumbudur et al., 2009; Agrawal & Horel, 2020), or the dual norm, associated with $G$, is defined by:

$$\gamma_G(s_0, t_0) \equiv \max_{f \in G} \left| \int_{\mathcal{X}} f \, ds_0 - \int_{\mathcal{X}} f \, dt_0 \right| \forall \ s_0, t_0 \in \mathcal{R}^+(\mathcal{X}).$$  (1)

Classical examples of IPMs include:

**Kantorovich:** Let $d$ be a given (ground) metric over the domain $\mathcal{X}$. Let, $\|f\|_d \equiv \max_{x \neq y} \frac{|f(x) - f(y)|}{d(x, y)}$, denote the Lipschitz constant of $f$ with respect to the metric $d$. Kantorovich metric is the IPM associated with the generating set: $\mathcal{W}_d \equiv \{ f : \mathcal{X} \to \mathbb{R} | \|f\|_d \leq 1 \}$.

**MMD:** Let $k$ be a characteristic kernel (Sriperumbudur et al., 2011) over the domain $\mathcal{X}$. Let $\|f\|_k$ denote the norm of $f$ in the canonical RKHS, $\mathcal{H}_k$, corresponding to $k$. Maximum Mean Discrepancy (MMD) is the IPM associated with the generating set: $\mathcal{M}_k \equiv \{ f \in \mathcal{H}_k | \|f\|_k \leq 1 \}$.

**Total Variation:** This is the IPM associated with the generating set: $\mathcal{T} \equiv \{ f : \mathcal{X} \to \mathbb{R} | \|f\|_\infty \leq 1 \}$, where $\|f\|_\infty \equiv \max_{x \in \mathcal{X}} |f(x)|$.

**Dudley:** This is the IPM associated with the generating set: $\mathcal{D}_c \equiv \{ f : \mathcal{X} \to \mathbb{R} | \|f\|_\infty + \|f\|_d \leq 1 \}$, where $d$ is a ground metric over $\mathcal{X}$.

**Kolmogorov:** Let $\mathcal{X} = \mathbb{R}^n$. Then, Kolmogorov metric is the IPM associated with the generating set: $\mathcal{K} \equiv \{ 1_{(\infty, x)} | x \in \mathbb{R}^n \}$.

In order that the IPM metrizes weak convergence we assume that (Muller, 1997):

**Assumption 2.1.** $G$ is dense in $\mathcal{C}(\mathcal{X})$ and is compact.

Also, the IPM generated by $G$ and its absolute convex hull are the same. So without loss of generality we additionally assume that:

**Assumption 2.2.** $G$ is absolutely convex.

2.2 Optimal Transport

Given a cost function, $c : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and two probability measures $s_0 \in \mathcal{R}^+_1(\mathcal{X}), t_0 \in \mathcal{R}^+_1(\mathcal{X})$, the p-Wasserstein Kantorovich OT formulation is given by:

$$\bar{W}_p^c(s_0, t_0) \equiv \min_{\pi \in \mathcal{R}^+_1(\mathcal{X} \times \mathcal{X})} \int c^p \, d\pi \quad \text{s.t.} \quad \pi_1 = s_0, \pi_2 = t_0.$$  (2)

An optimal solution of (2) is called as a transport plan and has applications in domain adaptation (Courty et al., 2017) etc. Whenever the cost is a metric over $\mathcal{X}$ (ground metric), $W_p$ defines another metric, known as the p-Wasserstein metric, over $\mathcal{R}^+_1(\mathcal{X})$. This has many applications: as a loss function (Frogner et al., 2015), for measure interpolation (Gramfort et al., 2015), etc. The Kantorovich-Fenchel duality result shows that the 1-Wasserstein metric is same as the Kantorovich metric (when restricted to normalized measures).

In cases where the given measures are un-normalized and may be of unequal masses, known as the unbalanced optimal transport (UOT) setting, or when the measures are noisy, one employs a regularized version:

$$\min_{\pi \in \mathcal{R}^+_1(\mathcal{X} \times \mathcal{X})} \int c \, d\pi + \lambda D_\phi(\pi_1, s_0) + \lambda D_\phi(\pi_2, t_0),$$  (3)

where $D_\phi$ is the divergence generated by $\phi$. For example, in the special case $D_\phi$ is KL divergence and the ground cost $c$ is squared-euclidean, the optimal objective of (3) is square of the so-called Gaussian Hellinger-Kantorovich metric between the marginals $s_0, t_0$ (Liero et al., 2018).

An alternate formulation based on total variation metric (denoted by $\cdot|_{TV}$) is studied in (Piccoli & Rossi, 2016):

$$\min_{\pi \in \mathcal{R}^+_1(\mathcal{X} \times \mathcal{X})} |\pi|^p \int c^p \, d\pi + \lambda |\pi_1 - s_0|_{TV}^p + \lambda |\pi_2 - t_0|_{TV}^p,$$  (4)

where $|\pi|$ is the mass of measure $\pi$. The $p^{th}$-root of the optimal objective of (4) is the so-called generalized Wasserstein metric between $s_0, t_0$. 

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3
3 Proposed IPM-regularized OT

In this section, we study generic IPM-regularized OT formulations. To this end, we propose the following family of OT formulations:

\[
(U_{G,c,\lambda,p,q}(s_0, t_0))^q \equiv \min_{\pi \in \mathcal{P}(X \times X)} \left( |\pi|^{p-1} \int c^p \, d\pi \right)^{\frac{q}{p}} + \lambda \gamma_G^q(\pi_1, s_0) + \lambda \gamma_G^q(\pi_2, t_0),
\]

(5)

where \( \gamma_G \) is the IPM associated with the generating set \( G \), \( \lambda \geq 0 \) is the regularization hyperparameter, and \( p \geq 1, q \geq 1 \). The above can be equivalently re-written as:

\[
(U_{G,c,\lambda,p,q}(s_0, t_0))^q = \min_{s,t\in \mathbb{R}^+(X)} |s|^q \left( W_p(s, t) \right)^q + \lambda \gamma_G^q(s, s_0) + \lambda \gamma_G^q(t, t_0),
\]

(6)

where \( W_p(s, t) \equiv \left\{ \begin{array}{ll}
W_p(\frac{s}{|s|}, \frac{t}{|t|}) & \text{if } |s| = |t|, \\
\infty & \text{otherwise}.
\end{array} \right. \)

In the special case \( p = q = 1 \), and \( G \) is the unit \( \infty \)-norm ball, \( U \) recovers the generalized Wasserstein metrics, \( (4) \). When \( G \) is the unit RKHS norm ball, i.e., the IPM is MMD, Nath & Jawanpuria (2020) show that sample complexity of estimation may be very efficient. However, as far as we know, none of the existing works study metric properties with MMD regularization.

We fill this gap in literature by analyzing metric properties of \( (5) \) and \( (6) \) with general \( G \) in two special cases: the case of \( p = 1 \) is presented in Section 3.1 and that of \( p > 1 \) is presented in Section 3.2.

3.1 Case: \( p = 1 \)

The metric property in this case is given by the following theorem:

**Theorem 3.1.** Let \( G \) satisfy assumption 2.7 so that \( \gamma_G \) is a valid IPM. Let \( c \) be a ground metric over \( X \) and \( \lambda > 0, q \geq 1 \). Then, \( U_{G,c,\lambda,1,q} \) is a norm induced metric over \( \mathbb{R}^+(X) \).

**Proof.** To simplify notation, in this proof let \( U = U_{G,c,\lambda,1,q} \). It is easy to see that \( U \) satisfies the following properties by simple inheritance:

1. \( U \geq 0 \). Indeed, each of the objective terms in \( (5) \) is non-negative.
2. \( U(s_0, t_0) = 0 \iff s_0 = t_0 \). By above observation, sum of non-negative terms is zero if and only if each is zero. Since each term is a metric we have the result.
3. \( U(s_0, t_0) = U(t_0, s_0) \). Indeed, each objective term in \( (5) \) is symmetric.
4. \( U(\rho s_0, \rho t_0) = \rho U(s_0, t_0), \rho \geq 0 \). Follows by change of variables \((s, t) \mapsto (\rho s, \rho t) \) in \( (6) \) for \( U(\rho s_0, \rho t_0) \) and \( \gamma_G^q \) being a norm-induced metric satisfies the same property.
5. \( U(s_0, t_0) = u(|s_0 - t_0|) \) for some appropriate function \( u \). Indeed, each objective term in \( (6) \) is pointwise maximum of linear functions in \( s - t \), hence a shift of variables \((s, t) \mapsto (s + r, t + r) \) shows \( U(s_0, t_0) = U(s_0 + r, t_0 + r) \).

Towards proving the triangle inequality, we first observe that the \( q^{th} \) root of the objective in \( (6) \) can be written as \( h(x) = \| (h_1(x), h_2(x), h_3(x)) \|_q \), where \( x = (s, t, s_0, t_0) \). Now, each \( h_i \) is pointwise maximum of linear functions in \( x \) as each is either \( W_1 \) or \( \gamma_G^q \). Domains of \( h_i \) are also convex. Hence each \( h_i \) is convex. By convexity preserving vector composition rules (for e.g., Section 3.2.4 in Boyd & Vandenberghe 2004), we have that \( h(x) \) is also convex. Indeed, \( h_i \geq 0 \) are convex and \( |x|^{q} \) is convex and non-increasing in each entry over non-negative orthant. Now, since \( U(s_0, t_0) = \min_{x \in \mathbb{R}} h(x, s, t, s_0, t_0) \), where \( h \) is convex, we have that \( U \) is also convex (see for e.g., Section 3.2.5 in Boyd & Vandenberghe 2004).

Since \( U \) is convex and positively homogeneous, it is sub-additive. \( u(|s_0 - t_0|) = U(s_0, t_0) = U(s_0 + r, t_0 + r) \leq U(s_0, r_0) + U(r_0, t_0) = u(|s_0 - r_0|) + u(|r_0 - t_0|) \). Hence \( U \) is a norm-induced metric. \( \square \)

In general, when the IPM is not the total variation metric and not the Kantorovich metric, and \( q > 1 \), the proposed metrics \( U_{G,c,\lambda,1,q} \) are new. However in the case \( q = 1 \), as shown in the following theorem, \( U_{G,c,\lambda,1,1} \) is again an IPM:
Theorem 3.2. Whenever $G$ satisfies Assumptions $2.1$ and $2.2$, $c$ is a (continuous) ground metric over compact $\mathcal{X}$, and $\lambda > 0$, we have that:

$$U_{G,c,\lambda,1,1}(s_0,t_0) = \max_{f \in G(\lambda) \cap W_c} \int_\mathcal{X} f \, ds_0 - \int_\mathcal{X} f \, dt_0.$$ (7)

Here, $G(\lambda) = \{ \lambda g \mid g \in G \}$ and $W_c$ is all $1$-Lipschitz functions wrt. metric $c$.

The above theorem generalizes the well-known result about Dudley metrics being related to optimal transport (Piccoli & Rossi 2016; Scetbon et al. 2021). The theorem follows by deriving the Fenchel dual of (5) in the special case $p = q = 1$ (refer appendix A for details).

If the regularizer is a Kantorovich metric, i.e., $G = \mathcal{W}_c$ and $\lambda \geq 1$, $U_{\mathcal{W}_c,c,\lambda,1,1}$ gives back the Kantorovich metric, providing the “primal/OT” interpretation to the Kantorovich metric in the unbalanced case.

3.2 Case: $p > 1$

Though the novel metrics presented in the earlier section are norm-induced and may have interesting applications, they are essentially infimal convolutions of IPMs. However, the metrics $W_p$ for $p > 1$ are not IPMs, and hence we expect more interesting geometries to be induced when $W_p$ ($p > 1$) are regularized with IPMs. For example, Piccoli & Rossi (2014) present metrics induced when $W_p$ is TV-regularized, Liero et al. (2018) show that metrics are induced when $W_p$ is KL-regularized etc. Accordingly, in this section we focus on the case $p > 1$.

Note that the proof strategy of the earlier section does not apply in this case as $W_p$ need not be (jointly) convex when $p > 1$. Also, straight-forward application of the proof methodology of Piccoli & Rossi (2014) does not seem to extend for general IPMs. We believe this is because total variation can be understood as a variant of OT; whereas an IPM, in general, need not have an OT interpretation.

Interestingly, under some mild conditions we are able to show metric properties even when $p > 1$ with general IPM-regularizers:

Theorem 3.3. Let $G$ satisfy Assumption $2.1$, then $\gamma_G$ is a valid IPM. Further assume that $\max_{x \in G} |g(x)| = \beta$. Let the cost $c$ be a metric that is bounded i.e., $0 < r \leq c(x,y) \leq R \forall x,y \in \mathcal{X}$. Let $p > 1$, $q = 1$ and $\lambda \leq \frac{r^p}{pR^{p-1} \beta}$. Then, $U_{G,c,\lambda,p,1}$ is a metric over $\mathcal{R}^+(\mathcal{X})$.

Remark 3.4. if the IPM is the MMD induced by the Gaussian kernel, then $\beta = 1$. If the measures are discrete or sample based, then existence of $r, R$ is trivial. In the continuous case, consider the Gaussian kernel induced distance over a compact $\mathcal{X}$ as the cost. Then both $r, R$ do exist. The bound on $\lambda$ can be improved by making more assumptions. For example, by additionally assuming $\exists \alpha > 0 \exists \gamma_G(s,t) \geq \alpha |s-t|_{TV} \forall s,t \in \mathcal{R}^+(\mathcal{X})$, the bound improves to $\frac{r^p}{pR^{p-1}(\beta - \alpha)}$.

Note that $U$ trivially inherits all the metric properties except the triangle inequality. The proof for the triangle inequality, detailed in appendix B is technical and is inspired from standard gluing lemma style arguments.

Using derivations analogous to those presented in Nath & Jawanpuria (2020), we believe the novel family of metrics presented in this paper also might have attractive sample complexities whenever the IPM-regularizer is MMD based. However, such details are beyond the scope of this presentation.

3.3 Finite Sample Simplifications

Encouraged by the theoretical results proved above, we now focus on few pragmatic details for employing the proposed metrics in downstream applications.

For the sake of simplicity, we consider the following variant\footnote{The coefficients for the various objective terms is taken to be slightly different than that in \ref{5} merely for convenience.} in this section:

$$U(s_1, s_2) \equiv \min_{\pi \in \mathcal{R}^+(\mathcal{X} \times \mathcal{X})} \int c^2 \, d\pi + \lambda_1 \| \mu_{\pi_1} - \mu_{s_1} \|^2 + \lambda_2 \| \mu_{\pi_2} - \mu_{s_2} \|^2,$$ (8)

Here, $\mu_s \equiv \int \phi(x) \, ds(x)$ is the kernel mean embedding of $s$ (Muandet et al. 2017), $\phi$ is the canonical feature map, $\| \cdot \|$ denotes the RKHS norm associated with a given characteristic kernel $k$. We believe \ref{8} may also be of practical interest as it interpolates between the popular squared-2-Wasserstein and squared-MMD metrics.

In typical ML applications only samples from $s_i$ are available. Accordingly, the support of the optimal plan is assumed to be finite/fixed and estimation is performed. Let $m_i$ samples from $s_i$ be given: $D_i = \{x_{i1}, \ldots, x_{im_i}\}$. Let us denote the
Gram-matrix of $D_i$ by $G_{ii}$. Let $C_{12}$ be the $m_1 \times m_2$ cost matrix with entries as evaluations of function $c^2$ over $D_1 \times D_2$.

As mentioned earlier, let us assume the transport plan is supported only at the samples\(^2\) let $\alpha_{ij} \equiv \pi(x_{1i}, x_{2j})$. Then, 

$$\mu_{\pi_1} = \frac{1}{m_1} \sum_{i=1}^{m_1} \sum_{j=1}^{m_2} \alpha_{ij} \phi(x_{1i}), \quad \mu_{\pi_2} = \frac{1}{m_2} \sum_{j=1}^{m_2} \sum_{i=1}^{m_1} \alpha_{ij} \phi(x_{2j})$$

and the estimate of $\mu_s$, is $\frac{1}{m_s} \sum_{j=1}^{m_s} \phi(x_{ij})$.

With this notation, (8) simplifies as:

$$\min_{\alpha \geq 0 \in \mathbb{R}^{m_1 \times m_2}} tr(C_{12}^T) + \lambda_1 \|\alpha - \frac{\sigma_1}{m_1} 1\|^2_{G_{11}} + \lambda_2 \|\alpha^T 1 - \frac{\sigma_2}{m_2} 1\|^2_{G_{22}},$$

where $tr(M)$ denotes the trace of $M$ and $\|x\|^2_{M} \equiv x^T M x$.

A related problem is that of Barycenter interpolation of measures (Agueh & Carlier [2011]). This problem has many interesting applications (Solomon et al. [2014, 2015], Gramfort et al. [2015]). Given measures $s_1, \ldots, s_n$ with total masses $\sigma_1, \ldots, \sigma_n$ respectively, and interpolation weights $\rho_1, \ldots, \rho_n$, the Barycenter $s \in \mathcal{R}^+(X)$ is defined as the solution of the following problem:

$$\min_{s \in \mathcal{R}^+(X)} \sum_{i=1}^{n} \rho_i \mathcal{U}(s_i, s)$$

Following Cuturi & Doucet [2014] and other related works, we assume that the barycenter, $s$, is supported by $\bigcup_{i=1}^{n} D_i$ and $\beta \in \mathbb{R}^m$ denotes the corresponding probabilities. Here, $m = \sum_{i=1}^{n} m_i$. Accordingly, we assume that the transport plan $\pi^*$ corresponding to $\mathcal{U}(s_i, s)$ is supported by $D_i \times \mathbb{R}^{m_i}$ and let $\alpha_i \geq 0 \in \mathbb{R}^{m_i \times m}$ denote the corresponding probabilities. Let us denote the gram-matrix of $\bigcup_{i=1}^{n} D_i$ by $G$. Let $C_i$ be the $m_i \times m$ matrix with entries as evaluations of cost function, $c^2$. Then, the proposed Barycenter formulation simplifies as:

$$\min_{\alpha, \beta \geq 0} \sum_{i=1}^{n} \rho_i \left\{ tr(C_i^T) + \alpha_i^T 1 - \frac{\sigma_i}{m_i} 1 \right\}^2_{G_i} + \lambda_2 \|\alpha^T 1 - \beta\|^2_G$$

The minimization with respect to $\beta$ is a standard weighted least-squares problem, which gives the analytical solution:

$$\beta = \sum_{j=1}^{n} \rho_j \alpha_j^T 1.$$

Using this to eliminate $\beta$, leads to:

$$\min_{\alpha \geq 0} \sum_{i=1}^{n} \rho_i \left\{ tr(C_i^T) + \alpha_i^T 1 - \frac{\sigma_i}{m_i} 1 \right\}^2_{G_i} + \lambda_2 \|\alpha^T 1 - \frac{\lambda}{\sum_{j=1}^{n} \rho_j \alpha_j^T 1\|_G^2}$$

Problems (9), (10) are instances of convex quadratic programs with non-negativity constraints. In the setting where all involved measures are normalized, the non-negativity constraints can be replaced by simplex constraints. In either case, they can be solved using the projected gradient-descent or the mirror-descent algorithm.

### 4 Experiments

We empirically evaluate the proposed MMD regularized (unbalanced) OT formulation on synthetic as well as real world datasets. On synthetic datasets, we compare against Wasserstein formulation, Generalized Wasserstein (GW-TV) formulation Piccoli & Rossi (2016) and MMD formulation, and we show some desirable properties of the proposed formulation. We further validate the proposed formulation over KL-divergence regularized (unbalanced) OT formulation with entropy regularization Chizat (2017) (eKL-UOT) and MMD metric on downstream ML applications.

For experiments with the proposed MMD regularized formulation, we either use the characteristic Gaussian (RBF) kernel $k(x, y) = exp(-\frac{||x-y||^2}{2\sigma^2})$ for some $\sigma > 0$ or the characteristic Inverse Multi-Quadratic (IMQ) kernel $k(x, y) = (K^2 + ||x-y||^2)^{-0.5}$ for some $K > 0$. For GW-TV, we show qualitative results only with $p = 1$ case (solved using Linear Programming) due to computational constraints.

#### 4.1 Synthetic Experiments

##### 4.1.1 Level sets with the Proposed Metric

**Dataset and experimental setup.** Similar to Bottou et al. [2017], we consider a model family for source distributions as $\mathcal{F} = \{P_{\theta} = \frac{1}{2}(\delta_{\theta_0} + \delta_{\theta+}) : \theta \in [-1, 1] \times [-1, 1]\}$ and a fixed target distribution $Q$ as $P_{[2,2]} \notin \mathcal{F}$. We show distances between $P_{\theta}$ and $Q$ on varying $\theta$.

\(^2\)We can also assume the support is $D_1 \cup D_2$ on both sides.
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Figure 2: (a) Data (b) OT with no regularization (c) OT with TV regularization (d) OT with Proposed MMD regularization

Compared Methods. Figure 1 presents level sets showing distances \( \{d(P_\theta, Q) : \theta \in [-1,1] \times [-1,1]\} \) where the distance \( d(.,.) \) is measured using MMD, 2-Wasserstein, GW-TV and the Proposed OT regularized formulations respectively.

Parameter tuning and evaluation protocol. Several applications in ML like Generative modeling, deal with optimizing over parameter (\( \theta \)) of the source distribution to match the target distribution. In such a scenario, level sets showing lesser number of stationary points which are not global optima may be desirable.

The hyper-parameters chosen for this experiment are as follows. For MMD, RBF kernel is used with \( \sigma^2 \) as 3. Results of 2-Wasserstein (OT with no regularization) with squared-euclidean ground metric are shown. GW-TV results have euclidean distance as the ground metric and \( \lambda \) as 10. For the proposed method, the chosen hyper-parameters are: squared-Euclidean cost as the ground metric, \( \lambda \) as 10, squared-MMD regularization and RBF kernel with \( \sigma^2 \) as 2. MMD and the proposed method are solved using Mirror Descent.

Results. Figure 1 demonstrates that the level sets of MMD show spurious local minima’s. The level sets of Wasserstein (OT with no regularization) and GW-TV (TV regularized) show more number of local maxima’s compared to the level sets of the Proposed.

4.1.2 Synthetic case for Transport matrix

Dataset and experimental setup. We next show OT matrix for the data shown in Figure 2(a). The source data points are present on the left of the dashed line and the target data points are on the right of the dashed line. Both the source and the target data points are clustered into two groups. Additionally, the last data point of the target data has been made an outlier.

Compared Methods. We compare the transport matrices of Wasserstein (OT with no regularization), GW-TV (OT with TV regularization) and the proposed formulation.

Parameter tuning and evaluation protocol. In this set-up, the transport matrix between the source and target is expected to have a block diagonal structure with the last column as all zeros.

The hyper-parameters chosen for this experiment are as follows. For all the methods, euclidean distance metric is taken as ground cost. For GW-TV, \( \lambda \) is chosen as 0.3. The proposed method is solved using Mirror Descent, \( \lambda \) is chosen as 0.1, MMD regularization is employed with RBF kernel and \( \sigma^2 \) as \( 10^{-3} \).

Results. As shown in Figure 2, the transport matrix of the proposed formulation correctly captures this structure. The transport matrix of the Wasserstein formulation fails to do this and the transport matrix of GW-TV shows some block-diagonal structure but does not seem to distinguish between the outlier point from the rest.

4.1.3 Synthetic Bi-modal

In this section, we contrast the transport plan of the proposed method with the transport plan of GW-TV on synthetic data with bimodal distribution. Figures 3 and 4 show marginals of transport plans with normalized measures (balanced case) and un-normalized measures (unbalanced case) respectively. The source and target measures are shown using dashed lines. euclidean distance is used as the ground cost metric for both GW-TV and the proposed method. The row labeled ‘Prop. p=1, q=1’ shows results of the proposed formulation with MMD regularization and the row labeled ‘Prop. p=1, q=2’ shows results of the proposed formulation with squared-MMD regularization. The proposed method is solved using Projected Gradient Descent with Armijo rule. IMQ kernel with hyper-parameter \( K^2 \) as \( 10^{-5} \) is used in all our results. More results are in section C.1.
In Figure 4, we also show results of the proposed MMD regularized formulation with RBF kernel and with IMQ kernel.

GW-TV
(a) reg 1e-2 (b) reg 5e-2 (c) reg 1e-1 (d) reg 2e-1 (e) reg 5e-1
Prop. p=1, q=1
(a) reg 1e-2 (b) reg 2e-2 (c) reg 4e-2 (d) reg 5e-2 (e) reg 1e-1
Prop. p=1, q=2
(a) reg 1e-2 (b) reg 5e-2 (c) reg 1e-1 (d) reg 2e-1 (e) reg 5e-1
Prop. p=2, q=1
(a) reg 1e-2 (b) reg 5e-2 (c) reg 1e-1 (d) reg 2e-1 (e) reg 5e-1
Prop. p=2, q=2
(a) reg 1e-2 (b) reg 5e-2 (c) reg 1e-1 (d) reg 2e-1 (e) reg 5e-1

Figure 3: Synthetic Bimodal Balanced case

GW-TV
(a) RBF reg 1 (b) RBF reg 2 (c) RBF reg 4 (d) RBF reg 5
Prop. p=1, q=1
(a) reg 2e-2 (b) reg 5e-2 (c) reg 1e-1 (d) reg 2e-1
Prop. p=1, q=2
(a) reg 1e-3 (b) reg 4e-3 (c) reg 6e-3 (d) reg 1e-2
Prop. p=1, q=2
(a) RBF reg 1e-1 (b) RBF reg 5e-1 (c) RBF reg 1 (d) RBF reg 3

Figure 4: Synthetic Bimodal Unbalanced case

4.2 Single cell RNA sequencing

Single cell RNA sequencing technique (scRNA-seq) have received increased attention in developmental biology as it provides insights into cellular functionality by recording expression profiles of genes (Kolodziejczyk et al. 2015, Wagner et al. 2016). One popular application of this technology is to understand how the expression profile of the cells change over stages (Schiebinger et al. 2019), e.g., from embryonic stem cells to specified lineages such as hematopoietic or neuronal. An expression profile is a mathematical expression of cells as vectors in gene expression space, where
We next consider the class ratio estimation problem (Iyer et al., 2014). Given a multi-class labeled training dataset \( A \), the aim is to estimate the ratio of classes in an unlabeled test dataset \( B \) across different time steps. The ratio estimation problem with MMD, the formulation is:

\[
\min_{\theta \in \Delta_c} \frac{1}{m_2} \sum_{i=1}^{m_2} \frac{1}{m_1} \sum_{j=1}^{m_1} G_{11}[x_i, y_j] + \frac{z(\theta)^T G_{22} z(\theta) - 2 \frac{1}{m_2} \frac{1}{m_1} \sum_{i=1}^{m_2} \sum_{j=1}^{m_1} G_{12}[x_i, y_j]}{m_1}
\]

Table 1: EMD (lower is better) between computed barycenter and ground truth distribution

| Timestep | MMD  | εKL-UOT | PROPOSED |
|----------|------|---------|----------|
| T1       | 0.045| 0.028   | 0.020    |
| T2       | 0.012| 0.011   | 0.011    |
| T3       | 0.009| 0.018   | 0.008    |

A key advantage of IPM based regularization over KL based regularization is flexibility in parameterization for estimation. 

Barycenter in the optimal transport framework offers a principled approach to estimate the trajectory of a measure at an intermediate timestep \( t_i < t < t_j \) when we have measurements available only at \( t_i \) (source) and \( t_j \) (target) time steps. 

**Dataset and experimental setup.** We perform experiments on the Embryoid Body (EB) single cell dataset (Moon et al., 2019). The dataset has samples available at five timesteps (at 0, 2, 5, 12, 20 days of development of human embryo). Following Tong et al. (2020), we project the data onto two-dimensional space and associate uniform measures to the source and the target samples given at different timesteps. 

**Parameter tuning and evaluation protocol.** The computed barycenter is evaluated against the measure corresponding to the ground truth samples available at the corresponding timestep. We compute the distance between two measures at two different time steps.

**Results.** The results are reported in Table 1. We observe that the proposed method outperforms the baselines on all the three timesteps.
Table 2: Mean Absolute Deviation (lower is better) averaged across test splits

| DATASET      | MMD | αKL-UOT | PROPOSED |
|--------------|-----|---------|---------|
| Ionosphere   | 0.106 | 0.212 | 0.109   |
| SAHeart      | 0.169 | 0.102 | 0.091   |
| Diabetes     | 0.171 | 0.134 | 0.113   |
| Australian   | 0.175 | 0.114 | 0.092   |

squared-MMD regularized UOT formulation as follows:

$$\min_{\theta \in \Delta_e} \min_{\alpha \in \mathbb{R}^{m \times m}, \alpha \geq 0, 1^\top \alpha = 1} tr (\alpha C^\top) + \lambda \left( \frac{1}{m_1} 1^\top G_1 \alpha 1 + \frac{1}{m_2} 1^\top G_2 \alpha 1 - 2 \frac{1}{m_2} 1^\top [G_{11} G_{12}] \alpha 1 \right) + \lambda \left( \frac{1}{m_2} \alpha G \alpha^\top 1 + z(\theta)^\top G_2 z(\theta) - 2 z(\theta)^\top [G_{21} G_{22}] \alpha^\top 1 \right)$$

where $z(\theta) \in \mathbb{R}^{m_1}$, $z_i(\theta) = \frac{\theta_{i\cdot}}{n_i}$, and $n_j$ denotes the number of instances labeled $j$ in $L$. In section C.3, we show results where the transport matrix was parameterized with only source data on one side and with only target data on the other side.

The KL-divergence regularized UOT formulation for class-ratio estimation problem is as follows:

$$\min_{\theta \in \Delta_e} \min_{\alpha \in \mathbb{R}^{m_1 \times m_2}, \alpha \geq 0, 1^\top \alpha = 1} tr (\alpha C_{12}^\top) + \lambda KL(\alpha 1, \frac{1}{m_2} 1^\top) + \lambda KL(\alpha^\top 1, z(\theta)) + \epsilon \Omega(\alpha)$$

**Dataset and experimental setup.** We follow the experimental setup described in [Iyer et al., 2014] and show results on four binary classification datasets from the UCI repository ([Dua & Graff, 2017]). The fraction of positive class examples on the training set is fixed as 0.5. For each dataset, we create four test set with the fraction of positive class examples as [0.2, 0.4, 0.6, 0.8].

**Parameter tuning and evaluation protocol.** We report the average absolute deviation of the predicted class-ratios from the ground truth. We randomly generate train and test sets, where, for every train set, four test sets are generated corresponding to the four test class-ratios. Hyper-parameters are tuned separately for each class ratio using 30 validation sets that were randomly sampled from the training set. We repeat the whole setup with four random seeds. More details of hyper-parameters are in section C.3.

**Results.** The results, averaged across the four test set splits, are reported in Table 2. We observed that the proposed formulation outperforms other baselines for three out of four datasets and is second best by a small margin for the Ionosphere dataset.

### 4.4 Domain Adaptation in JUMBOT framework

Several works ([Courty et al., 2017], [Courty et al., 2017], [Seguy et al., 2018], [Damodaran et al., 2018]) have successfully employed the optimal transport (OT) in domain adaptation applications. We showcase the utility of our IPM regularized OT formulation in the recently proposed JUMBOT ([Fatras et al., 2021]) framework for Domain Adaptation.

Given a source and a target distribution, JUMBOT aims at finding a joint distribution map between them, similar to [Damodaran et al., 2018], but with the minibatch set-up. To this end, JUMBOT learns functions $g_\theta$ and $f_\gamma$ to map the inputs into the latent space and to map the latent space to target domain respectively. In implementation, JUMBOT employs the embedding space as the penultimate layer of neural network. JUMBOT’s loss function involves a cross entropy term on the source data and KL-UOT distance between source and target distribution.

**Dataset and experimental setup** We perform the Domain Adaptation experiment on Digits datasets comprising of MNIST [LeCun & Cortes, 2010], M-MNIST [Ganin et al., 2016], SVHN [Netzer et al., 2011], USPS [Hull, 1994] and VisDA 2017 [Peng et al., 2017] datasets. We replace the KL-UOT based loss with the proposed IPM-regularized UOT loss, keeping the other experimental set-up same as JUMBOT. We obtain JUMBOT’s result with KL-UOT with the best hyper-parameter reported ([Fatras et al., 2021]). Following JUMBOT, we tune our (IPM-regularized UOT loss) hyper-parameters for the Digits experiment on USPS to MNIST (U→M) domain adaptation task and used the same for SVHN to MNIST (S→M) and MNIST to MMNIST (M→MM) domain adaptation tasks. Following JUMBOT, we report validation accuracy on VisDA 2017.


### Table 3: Target accuracy (higher is better) in JUMBOT framework

| TASK        | eKL-UOT | PROPOSED |
|-------------|---------|----------|
| DIGITS U → M | 98.3    | 98.4     |
| DIGITS S → M | 98.8    | 97.6     |
| DIGITS M → MM | 96.1    | 96.2     |
| VISDA TRAIN → VAL | 70.9    | 72.2     |

The chosen hyper-parameters for Digits experiment are IMQ kernel with constant $K^2$ as 10, $\lambda$ as 10 and MMD regularization. We also added a ridge regularization on the transport matrix with coefficient 10. For VisDA experiment, the optimal hyper-parameters are Gaussian kernel with constant $\sigma^2$ as 60, $\lambda$ as 10 and squared-MMD regularization.

**Results** In Table 3, we report the accuracy obtained on target datasets. We observe that the proposed IPM-regularized UOT loss obtains better performance than KL-UOT based loss on three out of four datasets.

5 Conclusion

Optimal Transport literature seems to have an overwhelming number of results with KL/divergence based regularization. In comparison, IPM based regularization has received hardly any attention. We hope the theoretical as well as the empirical findings in this work will motivate further study in this direction.

References

Agrawal, R. and Horel, T. Optimal bounds between f-divergences and integral probability metrics. In *Proceedings of the 37th International Conference on Machine Learning*, 2020.

Agueh, M. and Carlier, G. Barycenters in the wasserstein space. *SIAM Journal on Mathematical Analysis*, 43(2):904–924, 2011.

Bot, R. I. *Conjugate Duality in Convex Optimization*, volume 637 of Lecture Notes in Economics and Mathematical Systems book series. Springer, 2010.

Bottou, L., Arjovsky, M., Lopez-Paz, D., and Oquab, M. Geometrical insights for implicit generative modeling. *arXiv preprint arXiv:1712.07822*, 2017.

Boyd, S. and Vandenberghe, L. *Convex optimization*. Cambridge university press, 2004.

Chizat, L. Unbalanced optimal transport : Models, numerical methods, applications. Technical report, Universite Paris sciences et lettres, 2017.

Chizat, L., Peyre, G., Schmitzer, B., and Vialard, F.-X. Unbalanced optimal transport: Dynamic and kantorovich formulations. *Journal of Functional Analysis*, 274(11):3090–3123, 2018a.

Chizat, L., Peyré, G., Schmitzer, B., and Vialard, F.-X. Scaling algorithms for unbalanced optimal transport problems. *Math. Comput.*, 87(314):2563–2609, 2018b. URL [https://doi.org/10.1090/mcom/3303](https://doi.org/10.1090/mcom/3303).

Courty, N., Flamary, R., Habrard, A., and Rakotomamonjy, A. Joint distribution optimal transportation for domain adaptation. In *Advances in Neural Information Processing Systems*, volume 30, pp. 3730–3739, 2017.

Courty, N., Flamary, R., Tuia, D., and Rakotomamonjy, A. Optimal transport for domain adaptation. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 39(9):1853–1865, 2017.

Cuturi, M. Sinkhorn distances: Lightspeed computation of optimal transport. In *Proceedings of the 26th International Conference on Neural Information Processing Systems - Volume 2*, pp. 2292–2300, 2013.

Cuturi, M. and Doucet, A. Fast computation of wasserstein barycenters. In *Proceedings of the 31st International Conference on International Conference on Machine Learning - Volume 32*, pp. II–685–II–693. JMLR.org, 2014.

Damodaran, B. B., Kellenberger, B., Flamary, R., Tuia, D., and Courty, N. Deepjdot: Deep joint distribution optimal transport for unsupervised domain adaptation, 2018.

Dua, D. and Graff, C. UCI machine learning repository, 2017. URL [http://archive.ics.uci.edu/ml](http://archive.ics.uci.edu/ml).

Fatras, K., Séjourné, T., Courty, N., and Flamary, R. Unbalanced minibatch optimal transport; applications to domain adaptation. In *Proceedings of the 38th International Conference on Machine Learning*, 2021.
Feydy, J., Séjourné, T., Vialard, F.-X., ichi Amari, S., Trouvé, A., and Peyré, G. Interpolating between optimal transport and mmd using sinkhorn divergences. In International Conference on Artificial Intelligence and Statistics, 2018.

Frogner, C., Zhang, C., Mobahi, H., Araya-Polo, M., and Poggio, T. Learning with a wasserstein loss. In Proceedings of the 28th International Conference on Neural Information Processing Systems - Volume 2, pp. 2053–2061, 2015.

Ganin, Y., Ustinova, E., Ajakan, H., Germain, P., Larochelle, H., Laviolette, F., Marchand, M., and Lempitsky, V. Domain-adversarial training of neural networks. The journal of machine learning research, 17(1):2096–2030, 2016.

Genevay, A., Chizat, L., Bach, F., Cuturi, M., and Peyré, G. Sample complexity of sinkhorn divergences. In The 22nd International Conference on Artificial Intelligence and Statistics, AISTATS 2019, 16–18 April 2019, Naha, Okinawa, Japan, pp. 1574–1583, 2019.

Georgiou, T. T., Karlsson, J., and Takyar, M. S. Metrics for power spectra: An axiomatic approach. IEEE Transactions on Signal Processing, 57(3):859–867, 2009.

Gramfort, A., Peyré, G., and Cuturi, M. Fast optimal transport averaging of neuroimaging data. In Proceedings of 24th International Conference on Information Processing in Medical Imaging, 2015.

Hanin, L. G. Kantorovich-rubinstein norm and its application in the theory of lipschitz spaces. In PROCEEDINGS OF THE AMERICAN MATHEMATICAL SOCIETY, volume 115, 1992.

Hull, J. A database for handwritten text recognition research. IEEE Transactions on Pattern Analysis and Machine Intelligence, 16(5):550–554, 1994. doi: 10.1109/34.291440.

Iyer, A., Nath, S., and Sarawagi, S. Maximum mean discrepancy for class ratio estimation. In ICML, 2014.

Kolodziejczyk, A. A., Kim, J. K., Svensson, V., Marioni, J. C., and Teichmann, S. A. The technology and biology of single-cell rna sequencing. Molecular Cell, 58(4):610–620, 2015.

LeCun, Y. and Cortes, C. MNIST handwritten digit database. http://yann.lecun.com/exdb/mnist/, 2010. URL http://yann.lecun.com/exdb/mnist/.

Liero, M., Mielke, A., and Savaré, G. Optimal transport in competition with reaction: The hellinger-kantorovich distance and geodesic curves. SIAM J. Math. Anal., 48:2869–2911, 2016.

Liero, M., Mielke, A., and Savaré, G. Optimal entropy-transport problems and a new hellinger–kantorovich distance between positive measures. Inventiones mathematicae, 211(3):969–1117, 2018.

Mena, G. and Niles-Weed, J. Statistical bounds for entropic optimal transport: sample complexity and the central limit theorem. In Wallach, H., Larochelle, H., Beygelzimer, A., d’Alché-Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems, volume 32. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/5acdc9ca5d99ae66afde1ee0e3b26b-Paper.pdf.

Moon, K. R., van Dijk, D., Wang, Z., Gigante, S., Burkhart, D. B., Chen, W. S., Yim, K., van den Elzen, A., Hirn, M. J., Coifman, R. R., Ivanova, N. B., Wolf, G., and Krishnaswamy, S. Visualizing structure and transitions for biological data exploration. Nature Biotechnology, 37(12):1482–1492, 2019.

Muandet, K., Fukumizu, K., Sriperumbudur, B., and Schölkopf, B. Kernel mean embedding of distributions: A review and beyond. Foundations and Trends® in Machine Learning, 10(1-2):1–141, 2017.

Muller, A. Integral probability metrics and their generating classes of functions. Advances in Applied Probability, 29:429–443, 1997.

Nath, J. S. and Jawanpuria, P. K. Statistical optimal transport posed as learning kernel embedding. In Advances in Neural Information Processing Systems, 2020.

Netzer, Y., Wang, T., Coates, A., Bissacco, A., Wu, B., and Ng, A. Reading digits in natural images with unsupervised feature learning. In NeurIPS, 2011.

Peng, X., Usman, B., Kaushik, N., Hoffman, J., Wang, D., and Saenko, K. Visda: The visual domain adaptation challenge. arXiv preprint arXiv:1710.06924, 2017.

Peyré, G. and Cuturi, M. Computational optimal transport. Foundations and Trends® in Machine Learning, 11(5-6):355–607, 2019.

Piccoli, B. and Rossi, F. Generalized wasserstein distance and its application to transport equations with source. Archive for Rational Mechanics and Analysis, 211:335–358, 2014.

Piccoli, B. and Rossi, F. On properties of the generalized wasserstein distance. Archive for Rational Mechanics and Analysis, 222, 12 2016. doi: 10.1007/s00205-016-1026-7.

Scetbon, M., Meunier, L., Atif, J., and Cuturi, M. Equitable and optimal transport with multiple agents. In AISTATS, 2021.
Schiebinger, G., Shu, J., Tabaka, M., Cleary, B., Subramanian, V., Solomon, A., Gould, J., Liu, S., Lin, S., Berube, P., Lee, L., Chen, J., Brumbaugh, J., Rigollet, P., Hochdelinger, K., Jaenisch, R., Regev, A., and Lander, E. S. Optimal-transport analysis of single-cell gene expression identifies developmental trajectories in reprogramming. *Cell*, 176(4):928–943.e22, 2019.

Schmitzer, B. and Wirth, B. Dynamic models of wasserstein-1-type unbalanced transport. *ESAIM: COCV*, 25:23, 2019. doi: 10.1051/cocv/2018017. URL https://doi.org/10.1051/cocv/2018017.

Seguy, V., Damodaran, B. B., Flamary, R., Courty, N., Rolet, A., and Blondel, M. Large-scale optimal transport and mapping estimation. In *International Conference on Learning Representations (ICLR)*, 2018.

Solomon, J., Rustamov, R., Guibas, L., and Butscher, A. Wasserstein propagation for semi-supervised learning. In Xing, E. P. and Jebara, T. (eds.), *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, pp. 306–314, 2014.

Solomon, J., de Goes, F., Peyré, G., Cuturi, M., Butscher, A., Nguyen, A., Du, T., and Guibas, L. Convolutional wasserstein distances: Efficient optimal transportation on geometric domains. *ACM Trans. Graph.*, 34(4), 2015.

Sriperumbudur, B. K., Fukumizu, K., Gretton, A., Schölkopf, B., and Lanckriet, G. R. G. On integral probability metrics, phi-divergences and binary classification. *arXiv preprint arXiv:0901.2698*, 2009.

Sriperumbudur, B. K., Fukumizu, K., and Lanckriet, G. R. G. Universality, characteristic kernels and RKHS embedding of measures. *Journal of Machine Learning Research*, 12:2389–2410, 2011.

Tong, A., Huang, J., Wolf, G., Van Dijk, D., and Krishnaswamy, S. TrajectoryNet: A dynamic optimal transport network for modeling cellular dynamics. In III, H. D. and Singh, A. (eds.), *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pp. 9526–9536. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/tong20a.html.

Villani, C. *Topics in Optimal Transportation Theory*, volume 58 of *Graduate Studies in Mathematics*. American Mathematical Society, 01 2003.

Wagner, A., Regev, A., and Yosef, N. Revealing the vectors of cellular identity with single-cell genomics. *Nature Biotechnology*, 34:1145–1160, 2016.

Zhang, K., Scholkopf, B., Muandet, K., and Wang, Z. Domain adaptation under target and conditional shift. In *ICML*, 2013.
A Proof of Theorem 3.2

We present a proof based on the classical Moreau-Rockafellar formula (Bot, 2010):

**Theorem A.1.** Let $X$ be a real Banach space and $f, g : X \mapsto \mathbb{R} \cup \{\infty\}$ be closed convex functions such that $\text{dom}(f) \cap \text{dom}(g)$ is not empty, then: $(f + g)^*(y) = \min_{x_1 + x_2 = y} f^*(x_1) + g^*(x_2) \forall y \in X^*$. Here, $f^*$ is the Fenchel conjugate of $f$ and $X^*$ is the topological dual of $X$.

Consider the indicator function $F_c : C(X \times X) \mapsto \mathbb{R} \cup \{\infty\}$ defined by: $F_c(f, g) = 0$ if $f(x) + g(y) \leq c(x, y) \forall x, y \in X$, and $\infty$ otherwise. Consider another indicator function: $F_G(f, g)$ defined as: $0$ if $f \in G, g \in \mathbb{G}$ and $\infty$ otherwise. Topological dual of $C(X \times X)$ is regular Radon measures $\mathcal{R}(X \times X)$ and the duality product $\langle h, \pi \rangle \equiv \int h \ d\pi$.

Now, it is easy to see that $F^*_c(s, t) = \max_{f \in C(X \times X)} \int f \ ds + \int g \ dt, s.t. f(x) + g(y) \leq c(x, y) \forall x, y \in X$, which under the assumptions that $X$ is compact and $c$ is continuous, is Wasserstein $W(s, t)$ with cost $c$ (Villani, 2003). On the other hand, $F^*_G(s, t) = \lambda \max_{f \in \mathcal{G}} \int f \ ds + \max_{g \in \mathcal{G}} \int g \ dt = \lambda (\gamma_G(s, 0) + \gamma_G(t, 0))$. Note that $U_{G, c, \lambda, 1}(s_0, t_0) = \min_{s(x), t(x) = (s_0, t_0)} F^*_c(s, t) + F^*_G(s_1, t_1)$.

Now, observe that $G$ is a closed, convex function because $G$ is a closed, convex set. On the other hand, $F_c$ is trivially convex and is closed because $c$ is continuous. Hence by applying the Moreau-Rockafellar formula we have that:

$$U_{G, c, \lambda, 1}(s_0, t_0) = \max_{f \in \mathcal{G}(\lambda), g \in \mathcal{G}(\lambda)} \int f \ ds + \int g \ dt, s.t. f(x) + g(y) \leq c(x, y) \forall x, y \in X$$

(B 10)

Now, the constraints in (10) are equivalent to: $g(y) \leq \min_{x \in X} c(x, y) - f(x) \forall y \in X$. The RHS is nothing but the $c$-conjugate (c-transform) of $f$. From proposition 6 in Peyré & Cuturi (2019), whenever $c$ is a metric, we have:

$$\min_{x \in X} d(x, y) - f(x) = \begin{cases} -f(y) & \text{if } f \in W_c, \\ -\infty & \text{otherwise}. \end{cases}$$

Thus the constraints are equivalent to: $g(y) \leq -f(y) \forall y \in X, f \in W_c$. By symmetry, we also obtain that $f(y) \leq -g(y) \forall y \in X, g \in W_c$. Now, since the dual, (10), seeks to maximize the objective with respect to $g$, and monotonically increases with values of $g$, at optimality we have that $g(y) = -f(y) \forall y \in X$. Note that this equality is possible to achieve as both $g, f \in G(\lambda) \cap W_c$. Eliminating $g$, one obtains (7).

B Proof of triangle inequality from theorem 3.3

To simplify notation we denote $U(G, c, \lambda, p, 1)$ by $U$. Also, we assume all measures involved admit (un-normalized) densities merely to simplify notation. Analogous derivations hold for those in $\mathcal{R}^+(X)$. To prove the triangle inequality, we need to show that $U(r_0, t_0) \leq U(r_0, s_0) + U(s_0, t_0)$ holds.

Let $r_1, s_1$ be the optimal solution in (6) that defines $U(r_0, s_0)$. Likewise, Let $s_2, t_2$ be the optimal solution in (6) that defines $U(s_0, t_0)$. Now if $s_1 = s_2$, then the triangle inequality trivially follows from that of $W_p, \gamma_{\mathcal{M}_b}$ (inheritance). Now, let’s assume that $s_1 \neq s_2$. We invoke the gluing lemma style argument for this case.

Define the gluing marginal $\bar{s} \equiv \min(s_1, s_2)$. Let $\pi_1, \pi_2$ denote the optimal transport plans for $W_p(r_1, s_1), W_p(s_2, t_2)$ respectively. Let $\bar{r}, \bar{t}$ be the projections of $\bar{s}$ onto $\pi_1, \pi_2$ respectively i.e., $\bar{r}(x) = \int \pi_1(x, y) \bar{s}(y) \ dy$ and $\bar{t}(z) = \int \pi_2(z, y) \bar{s}(y) \ dy$. Let $\bar{r}(x, y) \equiv \pi_1(x, y) \bar{s}(y)$ and $\bar{t}(x, y) \equiv \pi_2(x, y) \bar{s}(y)$. Since by definition $\bar{s} \leq \pi_i$, we have that $|s|W_p(\bar{r}, \bar{s}) \leq |s_1|W_p(r_1, s_1)$ and $|s\bar{W}_p(\bar{s}, \bar{t}) \leq |s_2|W_p(s_2, t_2)$. However, as we shall observe later, these trivial upper bounds are not enough to show triangle inequality with PPM regularization. Here we will need more tighter upper bounds, which can be obtained in view of the assumptions in the theorem statement. To this end, we present the following lemma:

**Lemma B.1.** $|s_1|W_p(r_1, s_1) - |s\bar{W}_p(\bar{r}, \bar{s}) \geq \frac{r^p |s_1 - \bar{s}|^{1/p} r^{-1/p}}{pR^{p-1}}$. Analogously, $|s_2|W_p(s_2, t_2) - |s\bar{W}_p(\bar{s}, \bar{t}) \geq \frac{r^p |s_2 - \bar{s}|^{1/p} r^{-1/p}}{pR^{p-1}}$.

**Proof.** Let $a^p \equiv |s^1|W_p(r_1, s_1), b^p \equiv |s\bar{W}_p(\bar{r}, \bar{s})$. Now, $a^p - b^p \geq \int E_{\pi_1}/y |c^p(X, y)/y| (s_1(y) - \bar{s}(y)) \ dy \geq r^p |s_1 - \bar{s}| r^{-1/p}$. This is because we assume the cost is lower bounded by $r$ and $\pi_1(x, y)$ is a probability density. Hence, $b \leq R |s_1|^{1/p}$. Hence, $\frac{|s_1 - \bar{s}|^{1/p} r^{-1/p}}{pR^{p-1}} \leq \frac{r^p |s_1 - \bar{s}|^{1/p} r^{-1/p}}{pR^{p-1}}$. Again, this is because the cost is upper bounded by $R$.

Now, $|s_1|W_p(r_1, s_1) - |s_1\bar{W}_p(\bar{r}, \bar{s}) = a - \frac{r^p |s_1 - \bar{s}|^{1/p} r^{-1/p}}{pR^{p-1}}$. Multiplying this final inequality by $|s_1|^{1/p}$ and observing that $|s| \leq |s_1|$ gives the required inequality.

\[ \square \]

\[ \text{In case of total variation regularization, these inequalities are sufficient to prove the triangle inequality} \] Piccoli & Rossi (2014).
Now, since $s_1 \neq s_2$, we have that $|s_i - \bar{s}|_{TV} > 0$ and the lower bound in lemma B.1 is (strictly) positive. While lemma B.1 lower bounds the improvement in the Wasserstein term by employing the gluing marginal, the following lemma upper bounds the slack introduced in the IPM terms because of the same:

**Lemma B.2.** $(\gamma_G(r_0, \bar{r}) + \gamma_G(t_0, \bar{t})) - (\gamma_G(r_0, t_1) + \gamma_G(t_0, t_2)) \leq \beta|s_1 - s_2|_{TV}$.

**Proof.** Recall that $\bar{r}(x) = \int \pi_1(x/y)\bar{s}(y) dy = \int [y < s_1(y)] \pi_1(x/y)s_1(y) dy + \int [y > s_1(y)] \pi_1(x/y)s_2(y) dy = \int \pi_1(x/y)s_1(y) dy + \int [y > s_1(y)] \pi_1(x/y)(s_2(y) - s_1(y)) dy = r_1(x) + \int [y > s_1(y)] \pi_1(x/y)(s_2(y) - s_1(y)) dy$. The last equality is because $\pi_1$ is the optimal plan for $W_p(r_1, s_1)$. Now subtracting both sides by $r_0(x)$ and equating the IPM value for both the sides gives: $\gamma_G(r_0, \bar{r}) = \max_{f \in G} \left( \int f(x)(r_0(x) - r_1(x)) dx + \int [y > s_1(y)] f(x)\pi_1(x/y)(s_1(y) - s_2(y)) dy \right) \leq \gamma_G(r_0, r_1) + \max_{f \in G} \int [y > s_1(y)] E_{\pi_{1/(y)}}[f(X)/y](s_1(y) - s_2(y)) dy$. Now, by the assumption on $G$ we have that $|f(x)| \leq \beta \Rightarrow E_{\pi_{1/(y)}}[f(X)/y] \leq \beta$. Hence, $\gamma_G(r_0, \bar{r}) \leq \gamma_G(r_0, r_1) + \beta \int [y > s_1(y)] (s_1(y) - s_2(y)) dy$. Similarly, we obtain $\gamma_G(t_0, \bar{t}) \leq \gamma_G(t_0, t_2) + \beta \int [y > s_1(y)] (s_2(y) - s_1(y)) dy$. Adding these two gives the required inequality. 

We are now ready to prove the triangle inequality:

$$U(r_0, t_0) \leq |\bar{s}|W_p(r_0, \bar{r}) + \lambda \gamma_G(r_0, \bar{r}) + \lambda \gamma_G(t_0, \bar{t})$$

$$\leq |\bar{s}|W_p(r_0, \bar{r}) + |\bar{s}|W_p(s_1, \bar{r}) + \lambda \gamma_G(r_0, \bar{r}) + \lambda \gamma_G(t_0, \bar{t})$$

$$\leq |s_1|W_p(r_1, s_1) + |s_2|W_p(s_2, t_2) + \lambda \gamma_G(r_0, \bar{r}) + \lambda \gamma_G(t_0, \bar{t}) - \frac{r^p}{pR^{p-1}}|s_2 - s_1|_{TV}$$

$$\leq |s_1|W_p(r_1, s_1) + |s_2|W_p(s_2, t_2) + \lambda \gamma_G(r_0, r_1) + \lambda \gamma_G(t_0, t_2) + \lambda \beta - \frac{r^p}{pR^{p-1}}|s_2 - s_1|_{TV}$$

Here, the first inequality is by definition of $U(r_0, t_0)$ in (6). Second is true because $W_p$ is a metric. Third is true because of Lemma B.1 and the fact that total variation is a metric. The fourth is because of Lemma B.2. The last follows from the upper bound on $\lambda$ and adding the required terms.

## C Experiments

We present more experimental details and additional results in this section. We will open-source the codes to reproduce all our experiments upon acceptance of the paper.

### C.1 Synthetic Experiments

**More Transport Plans for Synthetic Bimodal Experiment**

**Barycenter with Gaussian measures** We experiment with source and target measures as Gaussian and compare our barycenters with those obtained with MMD (Avg) and $\epsilon$KL-UOT. The rows in [7] are for the case with normalized and un-normalized Gaussian measures respectively.

**C.1.1 Level Sets with the Proposed Metric**

For plotting contour plots, the hyper-parameter specifying total number of lines is 20 for all methods.

### C.2 Single cell RNA sequencing

Embryoid Body dataset comprises of data at 5 timesteps with sample sizes as 2381, 4163, 3278, 3665 and 3332 respectively. For the task of prediction at timestep $t_1$, the data was standardized using statistics of data from $\{t_0, t_1, t_2, t_3, t_4\} \setminus \{t_1\}$. Mirror Descent was used to solve the barycenter formulations for the proposed method as well as for KL-UOT, with step size as the inverse of infinity norm of the gradient. During the validation phase, 100 iterations of Mirror Descent were performed and for reporting final performance on the chosen hyper-parameters 1000 iterations were performed. For the proposed method, constant $K^2$, of the IMQ kernel is chosen from $\{1e-3, 1e-4, 1e-5\}$ and $\lambda$ is chosen from $\{1, 1e-1, 1e-2\}$. For KL-UOT, $\lambda$ is chosen from $\{1, 1e-1, 1e-2\}$ and the coefficient of entropic regularization from $\{1e-1, 1e-3, 1e-5\}$. 

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C.3 Class Ratio Experiment

We experimented on four UCI datasets: Australian, Ionosphere, SA-Heart and Diabetes. Based on an initial random seed, we divided the data into a training set and a test set. The (training set size, test set size) for Australian, Ionosphere, SA-Heart and Diabetes datasets are (454, 100), (172, 50), (192, 80) and (376, 100) respectively. Hyper-parameters are
tuned on 30 validation sets that were randomly sampled from the training set. The ratio of classes in the training sets was kept as 0.5. We report the results on the test set with the best hyper-parameter after repeating the experiment with 4 initial random seeds. All methods are solved using Mirror Descent. During the validation phase, 500 iterations of Mirror Descent are performed and during the final test phase 1000 iterations are performed. We also present the results with the proposed method where the transport matrix \( \alpha \in \mathbb{R}^{m \times n^2} \). We refer to it as Proposed version 1.

For the Proposed version 1 and Proposed formulation, \( \lambda \) is chosen from \{0.1, 1, 10\} for Ionosphere dataset, from \{0.01, 0.1, 1\} for Australian dataset, from \{1, 10, 100\} for Diabetes dataset and from \{0.1, 1, 10\} for SAHeart dataset. The constant hyper-parameter used in IMQ kernel is chosen from \{1, 10, 20\} for Ionosphere and from \{100, 150, 200\} for all other datasets. The pool of hyper-parameters is chosen based on scale of terms in the involved objective functions and the condition numbers of Gram matrices.

For MMD, RBF kernel is used as it resulted in better optimization compared to IMQ kernel. For validation, the pool of \( \sigma^2 \) values was \{10, 20, 30\} for Australian, \{0.01, 0.05, 0.1\} for Ionosphere, \{30, 40, 50\} for SA-Heart and \{30, 40, 50\} for Diabetes dataset. The chosen \( \sigma^2 \) values are 20 for Australian, 0.1 for Ionosphere, 50 for SA-Heart and 50 for Diabetes dataset.

For KL-UOT, \( \lambda \) is chosen from \{0.1, 0.01, 0.001\} for Australian dataset and from \{0.1, 0.1, 0.01\} for all other datasets. The entropic regularizer, \( \epsilon \), is chosen from \{0.1, 0.01, 0.001\}. The pool of hyper-parameters is chosen based on the scale of terms in the objective. We note that for the KL-UOT optimization optimal \( \theta \) at iteration \( k \) is
\[
\theta_k = [\sum_{y_i = 0}\alpha_k^i \mathbf{1}_i, \sum_{y_i = 1}\alpha_k^i \mathbf{1}_i].
\]

**Australian** For KL-UOT, the chosen hyper-parameters (\( \lambda, \epsilon \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10^{-3}, 10^{-1}), (10^{-3}, 10^{-1}), (10^{-2}, 10^{-3}), (10^{-1}, 10^{-3})\) respectively. For Proposed version 1 method, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((1, 200), (1, 200), (0.01, 150), (0.01, 200)\) respectively. For Proposed, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((1, 200), (1, 200), (0.1, 150), (0.01, 200)\) respectively.

**Ionosphere** For KL-UOT, the chosen hyper-parameters (\( \lambda, \epsilon \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10^{-2}, 10^{-1}), (10^{-2}, 10^{-1}), (10^{-1}, 10^{-1})\) respectively. For Proposed version 1 method, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10, 1), (10, 1), (10, 1), (1, 1)\) respectively. For Proposed, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((1, 10), (0.1, 10), (0.1, 1), (1, 1)\) respectively.

**Diabetes** For KL-UOT, the chosen hyper-parameters (\( \lambda, \epsilon \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10^{-1}, 10^{-3}), (10^{-1}, 10^{-3}), (10^{-2}, 10^{-3}), (10^{-1}, 10^{-3})\) respectively. For Proposed version 1 method, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10, 200), (1, 200), (1, 150), (1, 200)\) respectively. For Proposed, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((1, 100), (1, 100), (1, 200), (1, 200)\) respectively.

**SAHeart** For KL-UOT, the chosen hyper-parameters (\( \lambda, \epsilon \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10^{-3}, 10^{-1}), (10^{-2}, 10^{-1}), (10^{-2}, 10^{-3}), (10^{-2}, 10^{-3})\) respectively. For Proposed version 1 method, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((10, 100), (10, 100), (10, 150), (1, 100)\) respectively. For Proposed, the chosen hyper-parameters (\( \lambda, K^2 \)) for class ratios 0.2, 0.4, 0.6, 0.8 are \((1, 200), (1, 100), (0.1, 200), (10, 200)\) respectively.

### Table 4: Australian: Absolute Deviation averaged across data splits

| DATASET | MMD   | \( \epsilon \)KL-UOT | PROPOSED VERSION 1 | PROPOSED         |
|---------|-------|-----------------------|--------------------|-----------------|
| 0.2     | 0.247±1.8E-2 | 0.305±4.49E-4 | 0.191±3.69E-2 | **0.181±4.21E-2** |
| 0.4     | 0.068±1.2E-2 | 0.105±5.30E-4 | 0.027±2.23E-2 | **0.012±3.98E-3** |
| 0.6     | 0.106±2.4E-2 | **0.02±2.17E-2** | 0.031±1.39E-2 | 0.032±2.37E-2    |
| 0.8     | 0.281±1.8E-2 | **0.025±1.97E-2** | 0.156±3.53E-2 | 0.144±4.44E-2    |

### Table 5: Diabetes: Absolute Deviation averaged across data splits

| DATASET | MMD   | \( \epsilon \)KL-UOT | PROPOSED VERSION 1 | PROPOSED         |
|---------|-------|-----------------------|--------------------|-----------------|
| 0.2     | 0.244±2.7E-2 | 0.206±5.24E-2 | 0.184±0.234 | **0.163±6.54E-2** |
| 0.4     | **0.077±3E-2** | 0.106±5.67E-2 | 0.115±6.62E-2 | 0.143±7.65E-2   |
| 0.6     | 0.098±3.3E-2 | **0.041±1.94E-2** | 0.096±6.76E-2 | **0.041±4E-2**  |
| 0.8     | 0.266±2.6E-2 | 0.182±1.48E-1 | **0.14±1.43E-1** | 0.105±9.51E-2   |
Table 6: Ionosphere: Absolute Deviation averaged across data splits

| DATASET | MMD       | ϵKL-UOT   | PROPOSED VERSION 1 | PROPOSED    |
|---------|-----------|-----------|--------------------|-------------|
| 0.2     | 0.17±3.3E-2 | 0.442±1.23E-2 | 0.101±7.79E-2     | 0.122±8.73E-2 |
| 0.4     | 0.069±3.9E-2 | 0.271±2.06E-2 | 0.124±6.74E-2     | 0.147±8.41E-2 |
| 0.6     | 0.038±1.3E-2 | 0.104±5.76E-2 | 0.08±4.28E-2      | 0.106±2.6E-2  |
| 0.8     | 0.147±2.2E-2 | 0.033±1.31E-2 | 0.024±1.62E-2     | 0.06±3.94E-2  |

Table 7: SAHeart: Absolute Deviation averaged across data splits

| DATASET | MMD       | ϵKL-UOT   | PROPOSED VERSION 1 | PROPOSED    |
|---------|-----------|-----------|--------------------|-------------|
| 0.2     | 0.28±7E-2  | 0.203±0.0766 | 0.23±0.198        | 0.138±0.116  |
| 0.4     | 0.131±5.1E-2 | 0.112±0.00523 | 0.199±0.148      | 0.072±0.0497 |
| 0.6     | 0.053±5.4E-2 | 0.023±0.0182  | 0.106±0.078      | 0.065±0.0333 |
| 0.8     | 0.211±6E-2  | 0.07±0.0685   | 0.083±0.069      | 0.088±0.0517 |

C.3.1 Classification Accuracy

For OT based methods, we further use the transport matrix for getting classification accuracy on test data. To this end, we first compute the barycentric projection of test data onto source data and label a test point based on the source point nearest to its barycentric projection. We note that this classification experiment was performed using the same set of hyper-parameters that were chosen after validating for Mean Absolute Deviation. The results are shown in [9] where we outperformed the baselines.

C.3.2 Domain Adaptation in JUMBOT framework

The accuracies shown in table 3 are averages across three independent trials. Mirror Descent with 500 iterations is used to solve the proposed UOT formulation. The digits experiment is done on NVIDIA RTX 2080 GPU and the VisDA experiment is done on NVIDIA GTX 1080 Ti GPU.
Table 8: Mean Absolute Deviation (lesser is better) averaged across data splits

| DATASET   | MMD-sq | \(\epsilon\)KL-UOT | PROPOSED VERSION 1 | PROPOSED |
|-----------|--------|---------------------|---------------------|----------|
| IONOSPHERE | 0.106  | 0.212               | 0.082               | 0.109    |
| SAHEART   | 0.169  | 0.102               | 0.155               | 0.091    |
| DIABETES  | 0.171  | 0.134               | 0.134               | 0.113    |
| AUSTRALIAN | 0.175  | 0.114               | 0.101               | 0.092    |

Table 9: Mean Accuracy (in \%) after Domain Adaptation (higher is better) averaged across data splits

| DATASET    | \(\epsilon\)KL-UOT | PROPOSED VERSION 1 | PROPOSED |
|------------|---------------------|---------------------|----------|
| IONOSPHERE | 51.1                | 82.3                | 80.3     |
| SAHEART    | 57.2                | 57.9                | 57.8     |
| DIABETES   | 59.3                | 64.5                | 63.9     |
| AUSTRALIAN | 44.2                | 45.3                | 44.8     |