

Appendix

A Proofs

A.1 Derivation of the smooth relaxed dual

Recall that

$$\text{OT}_\Omega(\mathbf{a}, \mathbf{b}) = \min_{T \in \mathcal{U}(\mathbf{a}, \mathbf{b})} \sum_{j=1}^n \mathbf{t}_j^\top \mathbf{c}_j + \Omega(\mathbf{t}_j). \quad (16)$$

We now add Lagrange multipliers for the two equality constraints but keep the constraint $T \geq 0$ explicitly:

$$\text{OT}_\Omega(\mathbf{a}, \mathbf{b}) = \min_{T \geq 0} \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \sum_{j=1}^n \mathbf{t}_j^\top \mathbf{c}_j + \Omega(\mathbf{t}_j) + \alpha^\top (T \mathbf{1}_n - \mathbf{a}) + \beta^\top (T^\top \mathbf{1}_m - \mathbf{b}).$$

Since (16) is a convex optimization problem with only linear equality and inequality constraints, Slater's conditions reduce to feasibility [Boyd and Vandenberghe, 2004, §5.2.3] and hence strong duality holds:

$$\begin{aligned} \text{OT}_\Omega(\mathbf{a}, \mathbf{b}) &= \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \min_{T \geq 0} \sum_{j=1}^n \mathbf{t}_j^\top \mathbf{c}_j + \Omega(\mathbf{t}_j) + \alpha^\top (T \mathbf{1}_n - \mathbf{a}) + \beta^\top (T^\top \mathbf{1}_m - \mathbf{b}) \\ &= \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \sum_{j=1}^n \min_{\mathbf{t}_j \geq 0} \mathbf{t}_j^\top (\mathbf{c}_j + \alpha + \beta_j \mathbf{1}_m) + \Omega(\mathbf{t}_j) - \alpha^\top \mathbf{a} - \beta^\top \mathbf{b} \\ &= \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} - \sum_{j=1}^n \max_{\mathbf{t}_j \geq 0} \mathbf{t}_j^\top (-\mathbf{c}_j - \alpha - \beta_j \mathbf{1}_m) - \Omega(\mathbf{t}_j) - \alpha^\top \mathbf{a} - \beta^\top \mathbf{b} \\ &= \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \alpha^\top \mathbf{a} + \beta^\top \mathbf{b} - \sum_{j=1}^n \max_{\mathbf{t}_j \geq 0} \mathbf{t}_j^\top (\alpha + \beta_j \mathbf{1}_m - \mathbf{c}_j) - \Omega(\mathbf{t}_j). \end{aligned}$$

Finally, plugging the expression of (6) gives the claimed result.

A.2 Derivation of the convex conjugate

The convex conjugate of $\text{OT}_\Omega(\mathbf{a}, \mathbf{b})$ w.r.t. the first argument is

$$\text{OT}_\Omega^*(\mathbf{g}, \mathbf{b}) = \sup_{\mathbf{a} \in \Delta^m} \mathbf{g}^\top \mathbf{a} - \text{OT}_\Omega(\mathbf{a}, \mathbf{b}).$$

Following a similar argument as [Cuturi and Peyré, 2016, Theorem 2.4], we have

$$\text{OT}_\Omega^*(\mathbf{g}, \mathbf{b}) = \max_{\substack{T \geq 0 \\ T^\top \mathbf{1}_m = \mathbf{b}}} \langle T, \mathbf{g} \mathbf{1}_n^\top - C \rangle - \sum_{j=1}^n \Omega(\mathbf{t}_j).$$

Notice that this is an easier optimization problem than (5), since there are equality constraints only in one direction. Cuturi and Peyré [2016] showed that this optimization problem admits a closed form in the case of entropic regularization. Here, we show how to compute OT_Ω^* for any strongly-convex regularization.

The problem clearly decomposes over columns and we can rewrite it as

$$\begin{aligned} \text{OT}_\Omega^*(\mathbf{g}, \mathbf{b}) &= \sum_{j=1}^n \max_{\substack{\mathbf{t}_j \geq 0 \\ \mathbf{t}_j^\top \mathbf{1}_m = b_j}} \mathbf{t}_j^\top (\mathbf{g} - \mathbf{c}_j) - \Omega(\mathbf{t}_j) \\ &= \sum_{j=1}^n b_j \max_{\boldsymbol{\tau}_j \in \Delta^m} \boldsymbol{\tau}_j^\top (\mathbf{g} - \mathbf{c}_j) - \frac{1}{b_j} \Omega(b_j \boldsymbol{\tau}_j) \\ &= \sum_{j=1}^n b_j \max_{\Omega_j} (\mathbf{g} - \mathbf{c}_j), \end{aligned}$$

where we defined $\Omega_j(\mathbf{y}) := \frac{1}{b_j}\Omega(b_j\mathbf{y})$ and where \max_{Ω} is defined in (8).

A.3 Expression of the strongly-convex duals

Using a similar derivation as before, we obtain the duals of (13) and (14).

Proposition 3 *Duals of (13) and (14)*

$$\begin{aligned} \text{ROT}_{\Phi}(\mathbf{a}, \mathbf{b}) &= \max_{\alpha, \beta \in \mathcal{P}(C)} -\frac{1}{2}\Phi^*(-2\alpha, \mathbf{a}) - \frac{1}{2}\Phi^*(-2\beta, \mathbf{b}) \\ \widetilde{\text{ROT}}_{\Phi}(\mathbf{a}, \mathbf{b}) &= \max_{\alpha, \beta \in \mathcal{P}(C)} -\Phi^*(-\alpha, \mathbf{a}) + \beta^{\top} \mathbf{b} \\ &= \max_{\alpha \in \mathbb{R}^m} -\Phi^*(-\alpha, \mathbf{a}) - \sum_{j=1}^n b_j \max_{i \in [m]} (\alpha_i - c_{i,j}), \end{aligned}$$

where Φ^* is the conjugate of Φ in the first argument.

The duals are strongly convex if Φ is smooth.

When $\Phi(\mathbf{x}, \mathbf{y}) = \frac{1}{2\gamma}\|\mathbf{x} - \mathbf{y}\|^2$, $\Phi^*(-\alpha, \mathbf{a}) = \frac{\gamma}{2}\|\alpha\|^2 - \alpha^{\top} \mathbf{a}$. Plugging that expression in the above, we get

$$\text{ROT}_{\Phi}(\mathbf{a}, \mathbf{b}) = \max_{\alpha, \beta \in \mathcal{P}(C)} \alpha^{\top} \mathbf{a} + \beta^{\top} \mathbf{b} - \gamma (\|\alpha\|^2 + \|\beta\|^2) \quad (17)$$

and

$$\begin{aligned} \widetilde{\text{ROT}}_{\Phi}(\mathbf{a}, \mathbf{b}) &= \max_{\alpha, \beta \in \mathcal{P}(C)} \alpha^{\top} \mathbf{a} + \beta^{\top} \mathbf{b} - \frac{\gamma}{2}\|\alpha\|^2 \\ &= \max_{\alpha \in \mathbb{R}^m} \alpha^{\top} \mathbf{a} - \sum_{j=1}^n b_j \max_{i \in [m]} (\alpha_i - c_{i,j}) - \frac{\gamma}{2}\|\alpha\|^2. \end{aligned}$$

This corresponds to the original dual and semi-dual with squared 2-norm regularization on the variables.

A.4 Proof of Theorem 1

Before proving the theorem, we introduce the next two lemmas, which bound the regularization value achieved by any transportation plan.

Lemma 2 *Bounding the entropy of a transportation plan*

Let $H(\mathbf{a}) := -\sum_i a_i \log a_i$ and $H(T) := -\sum_{i,j} t_{i,j} \log t_{i,j}$ be the joint entropy. Let $\mathbf{a} \in \Delta^m$, $\mathbf{b} \in \Delta^n$ and $T \in \mathcal{U}(\mathbf{a}, \mathbf{b})$. Then,

$$\max\{H(\mathbf{a}), H(\mathbf{b})\} \leq H(T) \leq H(\mathbf{a}) + H(\mathbf{b}).$$

Proof. See, for instance, [Cover and Thomas, 2006].

Together with $0 \leq H(\mathbf{a}) \leq \log m$ and $0 \leq H(\mathbf{b}) \leq \log n$, this provides lower and upper bounds for the entropy of a transportation plan. As noted in [Cuturi, 2013], the upper bound is tight since

$$\max_{T \in \mathcal{U}(\mathbf{a}, \mathbf{b})} H(T) = H(\mathbf{a}\mathbf{b}^{\top}) = H(\mathbf{a}) + H(\mathbf{b}).$$

Lemma 3 *Bounding the squared 2-norm of a transportation plan*

Let $\mathbf{a} \in \Delta^m$, $\mathbf{b} \in \Delta^n$ and $T \in \mathcal{U}(\mathbf{a}, \mathbf{b})$. Then,

$$\sum_{i=1}^m \sum_{j=1}^n \left(\frac{a_i}{n} + \frac{b_j}{m} - \frac{1}{mn} \right)^2 \leq \|T\|^2 \leq \min\{\|\mathbf{a}\|^2, \|\mathbf{b}\|^2\}.$$

Proof. The tightest lower bound is given by $\min_{T \in \mathcal{U}(\mathbf{a}, \mathbf{b})} \|T\|^2$. An exact iterative algorithm was proposed in [Calvillo and Romero, 2016] to solve this problem. However, since we are interested in an explicit formula, we consider instead the lower bound $\min_{\substack{T \mathbf{1}_n = \mathbf{a} \\ T^\top \mathbf{1}_m = \mathbf{b}}} \|T\|^2$ (i.e., we ignore the non-negativity constraint). It is known [Romero, 1990]

that the minimum is achieved at $t_{i,j} = \frac{a_i}{n} + \frac{b_j}{m} - \frac{1}{mn}$, hence our lower bound. For the upper bound, we have

$$\begin{aligned} \|T\|^2 &= \sum_{i=1}^m \sum_{j=1}^n t_{i,j}^2 \\ &= \sum_{i=1}^m \sum_{j=1}^n \left(a_i \frac{t_{i,j}}{a_i} \right)^2 \\ &= \sum_{i=1}^m a_i^2 \sum_{j=1}^n \left(\frac{t_{i,j}}{a_i} \right)^2 \\ &\leq \sum_{i=1}^m a_i^2 \sum_{j=1}^n \left(\frac{t_{i,j}}{a_i} \right) \\ &= \|\mathbf{a}\|^2. \end{aligned}$$

We can do the same with $\mathbf{b} \in \Delta^n$ to obtain $\|T\|^2 \leq \|\mathbf{b}\|^2$, yielding the claimed result. \square

Together with $0 \leq \|\mathbf{a}\|^2 \leq 1$ and $0 \leq \|\mathbf{b}\|^2 \leq 1$, this provides lower and upper bounds for the squared 2-norm of a transportation plan.

Proof of the theorem. Let T^* and T_Ω^* be optimal solutions of (2) and (5), respectively. Then,

$$\text{OT}(\mathbf{a}, \mathbf{b}) + \Omega(T_\Omega^*) = \langle T^*, C \rangle + \Omega(T_\Omega^*) \leq \langle T_\Omega^*, C \rangle + \Omega(T_\Omega^*) = \text{OT}_\Omega(\mathbf{a}, \mathbf{b}).$$

Likewise,

$$\text{OT}_\Omega(\mathbf{a}, \mathbf{b}) = \langle T_\Omega^*, C \rangle + \Omega(T_\Omega^*) \leq \langle T^*, C \rangle + \Omega(T^*) = \text{OT}(\mathbf{a}, \mathbf{b}) + \Omega(T^*).$$

Combining the two, we obtain

$$\text{OT}(\mathbf{a}, \mathbf{b}) + \Omega(T_\Omega^*) \leq \text{OT}_\Omega(\mathbf{a}, \mathbf{b}) \leq \text{OT}(\mathbf{a}, \mathbf{b}) + \Omega(T^*).$$

Using $T^*, T_\Omega^* \in \mathcal{U}(\mathbf{a}, \mathbf{b})$ together with Lemma 2 and Lemma 3 gives the claimed results.

A.5 Proof of Theorem 2

To prove the theorem, we first need the following two lemmas.

Lemma 4 *Bounding the 1-norm of $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ for $(\boldsymbol{\alpha}, \boldsymbol{\beta}) \in \mathcal{P}(C)$*

Let $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{P}(C)$ with extra constraints $\boldsymbol{\alpha}^\top \mathbf{1}_m = 0$ and $\boldsymbol{\alpha}^\top \mathbf{a} + \boldsymbol{\beta}^\top \mathbf{b} \geq 0$, where $\mathbf{a} \in \Delta^m$ and $\mathbf{b} \in \Delta^n$. Then,

$$0 \leq \|\boldsymbol{\alpha}\|_1 + \|\boldsymbol{\beta}\|_1 \leq \|C\|_\infty (\nu + n)$$

where

$$\nu = \max \left\{ (2 + n/m) \|\mathbf{a}^{-1}\|_\infty, \|\mathbf{b}^{-1}\|_\infty \right\}.$$

Proof. The proof technique is inspired by [Meshi et al., 2012, Supplementary material Lemma 1.2].

The 1-norm can be rewritten as

$$\|\boldsymbol{\alpha}\|_1 + \|\boldsymbol{\beta}\|_1 = \max_{\substack{\mathbf{r} \in \{-1, 1\}^m \\ \mathbf{s} \in \{-1, 1\}^n}} \mathbf{r}^\top \boldsymbol{\alpha} + \mathbf{s}^\top \boldsymbol{\beta}.$$

Our goal is to upper bound the following objective

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \quad & \mathbf{r}^\top \alpha + \mathbf{s}^\top \beta \quad \text{s.t.} \quad 0 \leq \alpha^\top \mathbf{a} + \beta^\top \mathbf{b}, \\ & \alpha_i + \beta_j \leq c_{i,j}, \\ & \alpha^\top \mathbf{1}_m = 0, \end{aligned}$$

with a constant that does not depend on \mathbf{r} and \mathbf{s} . We call the above the dual problem. Its Lagrangian is

$$\begin{aligned} L(\alpha, \beta, \mu, \nu, T) &= \mathbf{r}^\top \alpha + \mathbf{s}^\top \beta + \mu \alpha^\top \mathbf{1}_m + \nu (\alpha^\top \mathbf{a} + \beta^\top \mathbf{b}) + \sum_{i,j=1}^{m,n} t_{i,j} (c_{i,j} - \alpha_i - \beta_j) \\ &= (\mathbf{r} + \mu \mathbf{1}_m + \nu \mathbf{a} - T \mathbf{1}_n)^\top \alpha + (\mathbf{s} + \nu \mathbf{b} - T^\top \mathbf{1}_m)^\top \beta + \langle T, C \rangle \end{aligned}$$

with $\mu \in \mathbb{R}$, $\nu \geq 0$, $T \geq \mathbf{0}$. Maximizing the Lagrangian w.r.t. α and β gives the corresponding primal problem

$$\begin{aligned} \min_{T \geq \mathbf{0}, \mu \in \mathbb{R}, \nu \geq 0} \quad & \langle T, C \rangle \quad \text{s.t.} \quad T \mathbf{1}_n = \nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m, \\ & T^\top \mathbf{1}_m = \nu \mathbf{b} + \mathbf{s}. \end{aligned}$$

By weak duality, any feasible primal point provides an upper bound of the dual problem. We start by choosing $\mu = \frac{1}{m}(\sum_j s_j - \sum_i r_i)$ so that $\sum_{i,j} t_{i,j}$ provides the same values w.r.t. the last two constraints. Next, we choose

$$\nu = \max \left\{ \max_i \frac{2 + n/m}{a_i}, \max_j \frac{1}{b_j} \right\}$$

which ensures the non-negativity of $\nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m$ and $\nu \mathbf{b} + \mathbf{s}$ regardless of \mathbf{r} and \mathbf{s} . It follows that the transportation plan T defined by

$$T = \frac{1}{(\nu \mathbf{b} + \mathbf{s})^\top \mathbf{1}_n} (\nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m)(\nu \mathbf{b} + \mathbf{s})^\top$$

is feasible. We finally bound the objective, $\langle T, C \rangle \leq \|C\|_\infty \sum_{i,j} t_{i,j} \leq \|C\|_\infty (\nu + n)$. \square

Lemma 5 *Bounding the 1-norm of α for $(\alpha, \cdot) \in \mathcal{P}(C)$*

Let $\alpha, \beta \in \mathcal{P}(C)$ with extra constraints $\sum_{i=1}^m \alpha_i = 0$ and $\alpha^\top \mathbf{a} + \beta^\top \mathbf{b} \geq 0$, where $\mathbf{a} \in \Delta^m$ and $\mathbf{b} \in \Delta^n$. Then,

$$0 \leq \|\alpha\|_1 \leq 2\|C\|_\infty \|\mathbf{a}^{-1}\|_\infty.$$

Proof. Similarly as before, our goal is to upper bound

$$\begin{aligned} \max_{\alpha \in \mathbb{R}^m, \beta \in \mathbb{R}^n} \quad & \mathbf{r}^\top \alpha \quad \text{s.t.} \quad 0 \leq \alpha^\top \mathbf{a} + \beta^\top \mathbf{b}, \\ & \alpha_i + \beta_j \leq c_{i,j}, \\ & \alpha^\top \mathbf{1}_m = 0, \end{aligned}$$

with a constant which does not depend on \mathbf{r} . The corresponding primal is

$$\begin{aligned} \min_{T \geq \mathbf{0}, \mu \in \mathbb{R}, \nu \geq 0} \quad & \langle T, C \rangle \quad \text{s.t.} \quad T \mathbf{1}_n = \nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m, \\ & T^\top \mathbf{1}_m = \nu \mathbf{b}. \end{aligned}$$

By weak duality, any feasible primal point gives us an upper bound. We start by choosing $\mu = \frac{1}{m} \sum_i r_i$ so that $\sum_{i,j} t_{i,j}$ provides the same values w.r.t. the last two constraints. Next, we choose, $\nu = \max_i \frac{2}{a_i}$, which ensures the non-negativity of $\nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m$ ($\nu \mathbf{b} \geq 0$ is also satisfied since $\nu \geq 0$) which appears in the r.h.s. of the second constraint, independently of \mathbf{r} . It follows that the transportation plan T defined by

$$T = \frac{1}{\nu \mathbf{b}^\top \mathbf{1}_n} (\nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m)(\nu \mathbf{b})^\top = (\nu \mathbf{a} + \mathbf{r} + \mu \mathbf{1}_m) \mathbf{b}^\top$$

is feasible. We finally bound the objective

$$\langle T, C \rangle \leq \|C\|_\infty \sum_{i,j} t_{i,j} \leq \nu \|C\|_\infty = 2 \|C\|_\infty \|\mathbf{a}^{-1}\|_\infty,$$

which concludes the proof. \square

Proof of the theorem. We begin by deriving the bound for the relaxed primal. Let $(\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*)$ and $(\boldsymbol{\alpha}_\Phi^*, \boldsymbol{\beta}_\Phi^*)$ be optimal solutions of (3) and (17), respectively. Since $(\boldsymbol{\alpha}_\Phi^*)^\top \mathbf{a} + (\boldsymbol{\beta}_\Phi^*)^\top \mathbf{b} \leq (\boldsymbol{\alpha}^*)^\top \mathbf{a} + (\boldsymbol{\beta}^*)^\top \mathbf{b}$, we have

$$\text{ROT}_\Phi(\mathbf{a}, \mathbf{b}) \leq \text{OT}(\mathbf{a}, \mathbf{b}) - \frac{\gamma}{2} (\|\boldsymbol{\alpha}_\Phi\|^2 + \|\boldsymbol{\beta}_\Phi\|^2).$$

Likewise,

$$\text{OT}(\mathbf{a}, \mathbf{b}) - \frac{\gamma}{2} (\|\boldsymbol{\alpha}^*\|^2 + \|\boldsymbol{\beta}^*\|^2) \leq \text{ROT}_\Phi(\mathbf{a}, \mathbf{b}).$$

Combining the two, we get

$$\text{OT}(\mathbf{a}, \mathbf{b}) - \frac{\gamma}{2} (\|\boldsymbol{\alpha}^*\|^2 + \|\boldsymbol{\beta}^*\|^2) \leq \text{ROT}_\Phi(\mathbf{a}, \mathbf{b}) \leq \text{OT}(\mathbf{a}, \mathbf{b}) - \frac{\gamma}{2} (\|\boldsymbol{\alpha}_\Phi\|^2 + \|\boldsymbol{\beta}_\Phi\|^2). \quad (18)$$

Hence we need to bound variables $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathcal{P}(C)$. Since $\|\cdot\|_2 \leq \|\cdot\|_1$, we can upper bound $\|\boldsymbol{\alpha}^*\|_1 + \|\boldsymbol{\beta}^*\|_1$. In addition, we can always add the additional constraint that $\boldsymbol{\alpha}^\top \mathbf{a} + \boldsymbol{\beta}^\top \mathbf{b} \geq \mathbf{0}^\top \mathbf{a} + \mathbf{0}^\top \mathbf{b} = 0$ since $(\mathbf{0}, \mathbf{0})$ is dual feasible for (3). Since for any optimal pair $\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*$, the pair $\boldsymbol{\alpha}^* - \sigma \mathbf{1}, \boldsymbol{\beta}^* + \sigma \mathbf{1}$ is also feasible and optimal for any $\sigma \in \mathbb{R}$, we can also add the constraint $\boldsymbol{\alpha}^\top \mathbf{1}_m = 0$. The obtained bound will obviously hold for any optimal pair $\boldsymbol{\alpha}^*, \boldsymbol{\beta}^*$. Hence, we can apply Lemma 4. By the same reasoning but using the constraint $\boldsymbol{\beta}^\top \mathbf{1}_n = 0$ in place of $\boldsymbol{\alpha}^\top \mathbf{1}_m = 0$, we can obtain a similar bound. By combining these two bounds, we obtain our final bound:

$$\|\boldsymbol{\alpha}\|_1 + \|\boldsymbol{\beta}\|_1 \leq \|C\|_\infty \min\{\nu_1 + n, \nu_2 + m\}$$

where

$$\begin{aligned} \nu_1 &= \max \left\{ (2 + n/m) \|\mathbf{a}^{-1}\|_\infty, \|\mathbf{b}^{-1}\|_\infty \right\} \\ \nu_2 &= \max \left\{ \|\mathbf{a}^{-1}\|_\infty, (2 + m/n) \|\mathbf{b}^{-1}\|_\infty \right\}. \end{aligned}$$

Taking the square of this bound and plugging the result in (18) gives the claimed result. Applying the same reasoning with Lemma 5 gives the claimed result for the semi-relaxed primal.

B Alternating minimization with exact block updates

General case. Let $\boldsymbol{\beta}(\boldsymbol{\alpha})$ be an optimal solution of (7) given $\boldsymbol{\alpha}$ fixed, and similarly for $\boldsymbol{\alpha}(\boldsymbol{\beta})$. From the first-order optimality conditions,

$$\nabla \delta_\Omega(\boldsymbol{\alpha} + \beta_j(\boldsymbol{\alpha}) \mathbf{1}_m - \mathbf{c}_j)^\top \mathbf{1}_m = b_j \quad \forall j \in [n] \quad (19)$$

and similarly for $\boldsymbol{\alpha}$ given $\boldsymbol{\beta}$ fixed. Solving these equations is non-trivial in general. However, because

$$\nabla \delta_\Omega(\boldsymbol{\alpha} + \beta_j(\boldsymbol{\alpha}) \mathbf{1}_m - \mathbf{c}_j) = b_j \nabla \max_{\Omega_j}(\boldsymbol{\alpha} - \mathbf{c}_j)$$

holds $\forall \boldsymbol{\alpha} \in \mathbb{R}^m, j \in [n]$, we can retrieve $\beta_j(\boldsymbol{\alpha})$ if we know how to compute $\nabla \max_{\Omega}(\mathbf{x})$ and the inverse map $(\nabla \delta_\Omega)^{-1}(\mathbf{y})$ exists. That map exists and equals $\nabla \Omega(\mathbf{y})$ provided that Ω is differentiable and $\mathbf{y} > \mathbf{0}$.

Entropic regularization. It is easy to verify that (19) is satisfied with

$$\beta(\boldsymbol{\alpha}) = \gamma \log \left(\frac{\mathbf{b}}{K^\top e^{\frac{\boldsymbol{\alpha}}{\gamma} - \mathbf{1}_m}} \right) \quad \text{where} \quad K := e^{\frac{-c}{\gamma}}$$

and similarly for $\boldsymbol{\alpha}(\boldsymbol{\beta})$. These updates recover the iterates of the Sinkhorn algorithm [Cuturi, 2013].

Squared 2-norm regularization. Plugging the expression of $\nabla \delta_\Omega$ in (19), we get that $\boldsymbol{\beta}(\boldsymbol{\alpha})$ must satisfy

$$[\boldsymbol{\alpha} + \beta_j(\boldsymbol{\alpha}) \mathbf{1}_m - \mathbf{c}_j]_+^\top \mathbf{1}_m = \gamma b_j \quad \forall j \in [n].$$

Close inspection shows that it is exactly the same optimality condition as the Euclidean projection onto the simplex $\operatorname{argmin}_{\mathbf{y} \in \Delta^m} \|\mathbf{y} - \mathbf{x}\|^2$ must satisfy, with $\mathbf{x} = \frac{\boldsymbol{\alpha} - \mathbf{c}_j}{\gamma b_j}$. Let $x_{[1]} \geq \dots \geq x_{[m]}$ be the values of \mathbf{x} in sorted order.

Following [Michelot, 1986, Duchi et al., 2008], if we let

$$\rho := \max \left\{ i \in [m] : x_{[i]} - \frac{1}{i} \left(\sum_{r=1}^i x_{[r]} - 1 \right) > 0 \right\}$$

then \mathbf{y}^* is *exactly* achieved at $[\mathbf{x} + \frac{\beta_j(\boldsymbol{\alpha})}{\gamma b_j} \mathbf{1}_m]_+$, where

$$\beta_j(\boldsymbol{\alpha}) = -\frac{\gamma b_j}{\rho} \left(\sum_{r=1}^{\rho} x_{[r]} - 1 \right).$$

The expression for $\boldsymbol{\alpha}(\boldsymbol{\beta})$ is completely symmetrical. While a projection onto the simplex is required for each coordinate, as discussed in §3.3, this can be done in expected linear time. In addition, each coordinate-wise solution can be computed in parallel.

Alternating minimization. Once we know how to compute $\boldsymbol{\beta}(\boldsymbol{\alpha})$ and $\boldsymbol{\alpha}(\boldsymbol{\beta})$, there are a number of ways we can build a proper algorithm to solve the smoothed dual. Perhaps the simplest is to alternate between $\boldsymbol{\beta} \leftarrow \boldsymbol{\beta}(\boldsymbol{\alpha})$ and $\boldsymbol{\alpha} \leftarrow \boldsymbol{\alpha}(\boldsymbol{\beta})$. For entropic regularization, this two-block coordinate descent (CD) scheme is known as the Sinkhorn algorithm and was recently popularized in the context of optimal transport by Cuturi [2013]. A disadvantage of this approach, however, is that computational effort is spent updating coordinates that may already be near-optimal. To address this issue, we can instead adopt a greedy CD scheme as recently proposed for entropic regularization by Altschuler et al. [2017].

C Additional experiments

We ran the same experiments as Figure 2 and Figure 3 on one more image pair: “Graffiti” by Jon Ander and “Rainbow Bridge National Monument Utah”, by Bernard Spragg. Both images are in the public domain. The results, presented in Figure 5 and Figure 6 below, confirm the empirical findings described in §6.1 and §6.2. The images are available at <https://github.com/mblondel/smooth-ot/tree/master/data>.

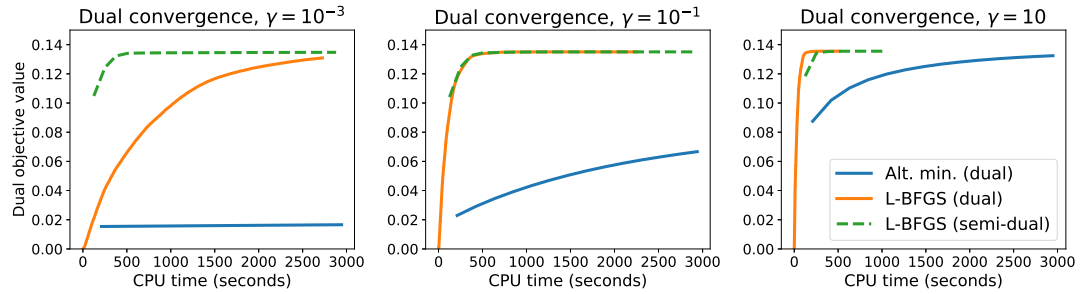


Figure 5: Same experiment as Figure 3 on one more image pair.

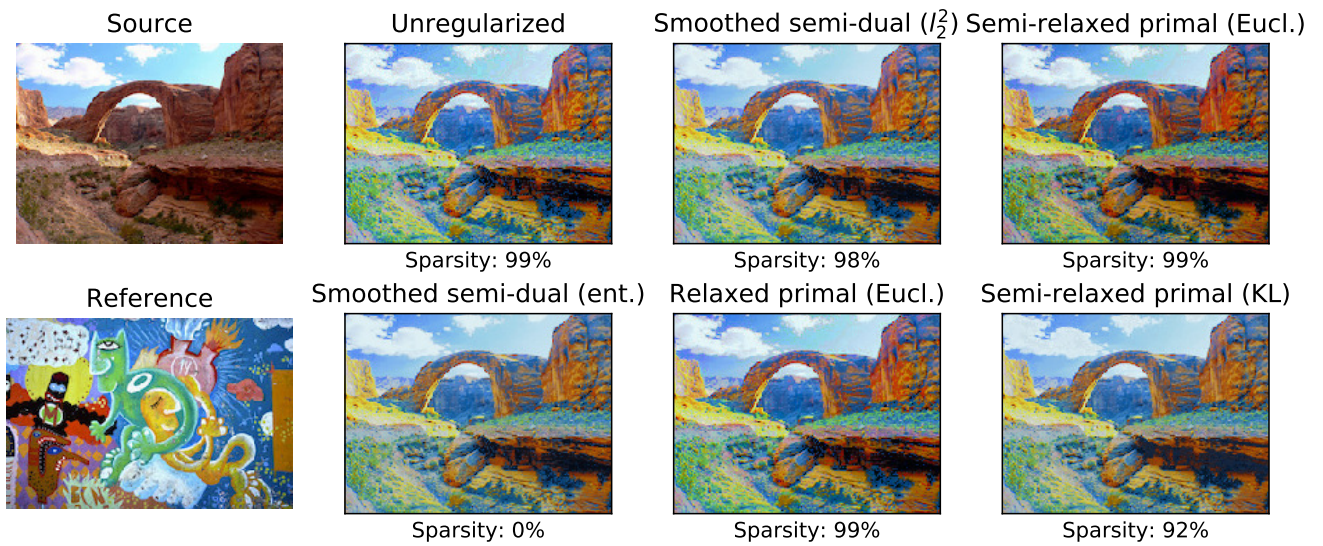


Figure 6: Same experiment as Figure 2 on one more image pair.