RELAXATION OF OPTIMAL TRANSPORT PROBLEM VIA STRICTLY CONVEX FUNCTIONS

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ABSTRACT. An optimal transport problem on finite spaces is a linear program. Recently, a relaxation of the optimal transport problem via strictly convex functions, especially via the Kullback–Leibler divergence, sheds new light on data sciences. This paper provides the mathematical foundations and an iterative process based on a gradient descent for the relaxed optimal transport problem via Bregman divergences.

1. Introduction

A optimal transport problem discussed in this paper is a variational problem as follows. Given \( C = (c_{ij})_{1 \leq i,j \leq N} \in M_N(\mathbb{R}) \) and \( x = (x_i)_{i=1}^N, y = (y_j)_{j=1}^N \in \mathbb{R}^N \) with

\[
x_i, y_j \geq 0 \quad \text{for } 1 \leq i, j \leq N \quad \text{and} \quad \sum_{i=1}^N x_i = \sum_{i=1}^N y_i = 1,
\]

find \( \Pi = (\pi_{ij})_{1 \leq i,j \leq N} \in M_N(\mathbb{R}) \) minimizing

\[
\sum_{i,j=1}^N c_{ij} \pi_{ij}
\]

under the constraints

\[
\pi_{ij} \geq 0, \quad \sum_{k=1}^N \pi_{ik} = x_i, \quad \sum_{k=1}^N \pi_{kj} = y_j, \quad \text{for } 1 \leq i, j \leq N.
\]

Since this variational problem is a linear program, a minimizer may lie on the boundary of the constraint set and not be unique. Furthermore, a gradient descent is not useful to find a minimizer.

In data sciences, a relaxation of the optimal transport problem via strictly convex functions achieves substantial success, where one of pioneering works is a fast algorithm for the relaxed transport problem via the Kullback–Leibler divergence proposed by Cuturi [2]. The Kullback–Leibler divergence between \( \Pi \in M_N(\mathbb{R}) \) satisfying (1.1) and \( x \otimes y \) is defined by

\[
\text{KL}(\Pi, x \otimes y) := \sum_{1 \leq i,j \leq N, \pi_{ij} \neq 0} \pi_{ij} \log \frac{\pi_{ij}}{x_i y_j}.
\]

The fast algorithm is called Sinkhorn’s algorithm since the convergence of this algorithm is attributed to an iterative process by Sinkhorn [5, 6] (for historical perspective, see [4, Remark 4.5] and the references therein). We notice that if we run Sinkhorn’s iteration and stop at the finite step, then the output \( \Pi \in M_N(\mathbb{R}) \) may not satisfy (1.1).

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As another strictly convex functions, we focus attention on a Bregman divergence, which is a generalization of the Kullback–Leibler divergence via a strictly convex, continuous function \( f : [0, 1] \to \mathbb{R} \) with \( f \in C^1((0, 1]) \). The \textit{Bregman divergence} associated to \( f \) between \( \Pi \in M_N(\mathbb{R}) \) satisfying (1.1) and \( x \otimes y \) is defined by

\[
D_f(\Pi, x \otimes y) := \sum_{1 \leq i,j \leq N, x_i y_j \neq 0} \left( f(\pi_{ij}) - f(x_i y_j) - f'(x_i y_j) (\pi_{ij} - x_i y_j) \right).
\]

If \( f(r) = r \log r \), where by convention \( 0 \log 0 := 0 \), then \( D_f(\Pi, x \otimes y) = KL(\Pi, x \otimes y) \). We notice that Sinkhorn’s iterative process is not applicable for Bregman divergences other than the Kullback–Leibler divergence. In Section 4, we provide an iterative process to find the relaxed minimizer via Bregman divergences, where the output \( \Pi \in M_N(\mathbb{R}) \) always satisfies (1.1) even if we stop the iteration at the finite step (Theorem 4.2, Corollary 4.3). The iterative process is based on a gradient descent.

For a relaxed optimal transport problem, although there are a lot of successful applications, mathematical argument is sometimes not rigorous. After a brief review of the optimal transport problem in Section 2, we provide the mathematical foundations of the relaxed optimal transport problem in Section 3. We first provide a criterion for a strictly convex function \( f \) such that a relaxed minimizer lies in the interior of the constraint set (Lemma 3.7). Then we prove the continuity (Theorem 3.11) and the monotonicity (Theorem 3.13) in the relaxed optimal transport problem. Moreover, we justify a dual relaxed optimal transport problem (Theorem 3.4).

2. Optimal transport problem

We briefly recall some notions in the optimal transport problem. When it will introduce no confusion, we shall use the same notation \( \langle \cdot, \cdot \rangle \) for the standard inner product on Euclidean space and the Frobenius inner product on the space of matrices of a fixed size.

The norm induced from \( \langle \cdot, \cdot \rangle \) is denoted by \( \| \cdot \|_2 \).

For \( N \in \mathbb{N} \) with \( N \geq 2 \), define

\[
P_N := \left\{ x = (x_i)_{i=1}^N \in \mathbb{R}^N \mid x_i \geq 0 \text{ for } 1 \leq i \leq N, \sum_{i=1}^N x_i = 1 \right\},
\]

\[
P_{N \times N} := \left\{ \Pi = (\pi_{ij})_{i,j=1}^N \in M_N(\mathbb{R}) \mid \pi_{ij} \geq 0 \text{ for } 1 \leq i, j \leq N, \sum_{i,j=1}^N \pi_{ij} = 1 \right\}.
\]

We call \( \Pi \in P_{N \times N} \) a \textit{coupling} (or \textit{transport plan}) between \( x, y \in P_N \) if

\[
\sum_{k=1}^N \pi_{ik} = x_i, \quad \sum_{k=1}^N \pi_{kj} = y_j, \quad \text{for } 1 \leq i, j \leq N.
\]

We denote by \( \Pi(x, y) \) the set of couplings between \( x, y \in P_N \). Then \( \Pi(x, y) \) is nonempty due to \( x \otimes y \in \Pi(x, y) \), where \( x \otimes y \) is the outer product of \( x, y \), that is,

\[
(x \otimes y)_{ij} = x_i y_j \quad \text{for } 1 \leq i, j \leq N.
\]

It is easy to see that \( \Pi(x, y) \) is a convex compact subset of \( (M_N(\mathbb{R}), \| \cdot \|_2) \).

For \( x \in P_N \) and \( \Pi \in P_{N \times N} \), define

\[
\text{supp } x := \{ i \mid 1 \leq i \leq N, \ x_i \neq 0 \}, \quad \text{supp } \Pi := \{ (i, j) \mid 1 \leq i, j \leq N, \pi_{ij} \neq 0 \}.
\]
Lemma 2.1. For \( x, y \in \mathcal{P}_N \) and \( \Pi \in \Pi(x, y) \),
\[
\text{supp } x \times \text{supp } y = \text{supp } x \otimes y, \quad \text{supp } \Pi \subset \text{supp } x \otimes y.
\]

Proof. It is trivial that \( \text{supp } x \times \text{supp } y = \text{supp } x \otimes y \). For \((i, j) \in \text{supp } \Pi\), we find that
\[
0 < \pi_{ij} = \sum_{k=1}^{N} \pi_{ik} = x_i, \quad 0 < \pi_{ij} = \sum_{k=1}^{N} \pi_{ik} = y_j,
\]
which implies \((i, j) \in \text{supp } x \otimes y\). \(\square\)

For \(C = (c_{ij})_{1 \leq i,j \leq N} \in M_N(\mathbb{R})\), we define a function \(C : \mathcal{P}_N \times \mathcal{P}_N \to \mathbb{R}\) by
\begin{equation}
C(x, y) := \inf_{\Pi \in \Pi(x, y)} \langle C, \Pi \rangle = \inf_{\Pi \in \Pi(x, y)} \left( \sum_{i,j=1}^{N} c_{ij} \pi_{ij} \right).
\end{equation}

Since \(\Pi(x, y)\) is compact and the function on \((\Pi(x, y), \| \cdot \|_2)\) sending \(\Pi\) to \(\langle C, \Pi \rangle\) is continuous, there exists a coupling \(\Pi \in \Pi(x, y)\) attaining the infimum in (2.2). Such a coupling is called an optimal coupling between \(x, y\). Throughout this paper, we choose a matrix \(C \in M_N(\mathbb{R})\) arbitrarily and fix it unless otherwise indicated.

The following characterization of optimal couplings is well-known. Although the proof in the case of finite spaces is easy, the direct proof is less common. For the sake of completeness, we give a direct proof. Let \(\mathcal{G}_M\) be the set of permutations on \(M\)-letters.

Definition 2.2. A subset \(S \subset \{1, \ldots, N\}^2\) is called \(C\)-cyclically monotone if
\begin{equation}
\sum_{m=1}^{M} c_{im,jm} \leq \sum_{m=1}^{M} c_{i\sigma(m),jm}.
\end{equation}
holds for any family \(\{(i_m, j_m)\}_{m=1}^{M}\) of points in \(S\) and any \(\sigma \in \mathcal{G}_M\).

It is easy to see that a subset of a \(C\)-cyclically monotone set is \(C\)-cyclically monotone.

Proposition 2.3. (cf. [7, Theorem 5.10]) Given \(x, y \in \mathcal{P}_N\), \(\Pi \in \Pi(x, y)\) is optimal if and only if \(\text{supp } \Pi\) is \(C\)-cyclically monotone.

Proof. Let \(\Pi \in \Pi(x, y)\) be an optimal coupling. If there exist \(\{(i_m, j_m)\}_{m=1}^{M} \subset \text{supp } \Pi\) and \(\sigma \in \mathcal{G}_M\) for which (2.3) is not valid, then, for \(\varepsilon := \min_{1 \leq m \leq M} \{\pi_{im,jm}\}\), we define \(\Pi^\varepsilon \in M_N(\mathbb{R})\) by
\[
\pi_{ij}^\varepsilon := \begin{cases} 
\pi_{ij} - \varepsilon & \text{if } (i, j) \in \{(i_m, j_m)\}_{m=1}^{M}, \\
\pi_{ij} + \varepsilon & \text{if } (i, j) \in \{(i_{\sigma(m)}, j_m)\}_{m=1}^{M}, \\
\pi_{ij} & \text{otherwise}.
\end{cases}
\]
We see that \(\Pi^\varepsilon \in \Pi(x, y)\) and
\[
0 \leq \langle C, \Pi^\varepsilon \rangle - \langle C, \Pi \rangle = -\varepsilon \sum_{m=1}^{M} c_{im,jm} + \varepsilon \sum_{m=1}^{M} c_{i\sigma(m),jm} = \varepsilon \sum_{m=1}^{M} (c_{i\sigma(m),jm} - c_{im,jm}) < 0,
\]
which is a contradiction. Thus \(\text{supp } \Pi\) is \(C\)-cyclically monotone.

Conversely, assume that \(\text{supp } \Pi\) is \(C\)-cyclically monotone. We define \(\xi \in \mathbb{R}^N\) by
\[
\xi_i := \sup_{M \in \mathbb{N}} \max \left\{ \sum_{m=1}^{M} (c_{im,jm} - c_{im+1,jm}) \mid (i_m, j_m) \in \text{supp } \Pi \text{ for } 1 \leq m \leq M, \ i_{M+1} = i \right\}.
\]
For $z \in \mathbb{R}^N$, if we define $z^C \in \mathbb{R}^N$ by
\[ z^C_j := \min_{1 \leq i \leq N}\{z_i + c_{ij}\} \quad \text{for } 1 \leq j \leq N, \]
then we observe that
\[ \sum_{j=1}^N \xi^C_j y_j - \sum_{i=1}^N \xi_i x_i = \sum_{i,j=1}^N (\xi^C_j - \xi_i) \pi^\prime_{ij} \leq \sum_{i,j=1}^N c_{ij} \pi^\prime_{ij} = \langle C, \Pi' \rangle \quad \text{for } \Pi' \in \Pi(x, y). \]
For $(i', j') \in \text{supp } \Pi$, it follows that
\[ \xi_i \geq \sup_{M \in \mathbb{N}} \max \left\{ \sum_{m=1}^M (c_{im,jm} - c_{im+1,jm}) \mid (i_m, j_m) \in \text{supp } \Pi, 1 \leq m \leq M - 1, (i_M, j_M) = (i', j'), i_{M+1} = i \right\} \]
\[ = \xi_i + (c_{ij'} - c_{ij}). \]
Thus we find that
\[ \xi^C_j = \min_{1 \leq i \leq N}\{z_i + c_{ij}\} \geq \xi_i + (c_{ij'} - c_{ij}). \]
which means that $\xi^C_j - \xi_i = c_{ij}$ if $(i, j) \in \text{supp } \Pi$. It turns out that
\[ \sum_{i=1}^N \xi^C_i x_i \leq \langle C, \Pi \rangle = \sum_{i,j=1}^N (\xi^C_j - \xi_i) \pi_{ij} = \sum_{i,j=1}^N \xi^C_j y_j - \sum_{i=1}^N \xi_i x_i, \]
implies the optimality of $\Pi$. \hfill $\square$

By the proof, we notice the following relation.
\[ \mathcal{C}(x, y) = \sup \left\{ \langle (-\xi, \eta), (x, y) \rangle \mid (\xi, \eta) \in \mathbb{R}^N \times \mathbb{R}^N, \eta_j - \xi_i \leq c_{ij} \quad \text{for } 1 \leq i, j \leq N \right\} \]
\[ = \sup \left\{ \langle (-z, z^C), (x, y) \rangle \mid z \in \mathbb{R}^N \right\}. \]
This relation called the Kantorovich duality (see [7, Chapter 5] for more details).

**Corollary 2.4.** Let $((x^n, y^n))_{n \in \mathbb{N}}$ be a sequence in $(\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2)$ converging to $(x, y)$.

For an optimal coupling $\Pi^n \in \Pi(x^n, y^n)$, $(\Pi^n)_{n \in \mathbb{N}}$ contains a convergent subsequence and the limit of any convergent subsequence is an optimal coupling between $x, y$. Hence $\mathcal{C}$ is continuous on $(\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2)$.

Conversely, for an optimal coupling $\Pi_* \in \Pi(x, y)$, there exists a sequence of optimal couplings $\Pi^n \in \Pi(x^n, y^n)$ containing a subsequence converging to $\Pi_*$. \hfill $\square$

**Proof.** By the compactness of $(\mathcal{P}_{N \times N}, \| \cdot \|_2)$, there is a convergent subsequence $(\Pi^n_{l})_{l \in \mathbb{N}}$ of $(\Pi^n)_{n \in \mathbb{N}}$. Set $\Pi := \lim_{l \to \infty} \Pi^n_{l}$. We see that
\[ \sum_{k=1}^N \pi_{ik} = \sum_{k=1}^N \lim_{l \to \infty} \pi^n_{ik} = x_i, \quad \sum_{k=1}^N \pi_{kj} = \sum_{k=1}^N \lim_{l \to \infty} \pi^n_{kj} = y_j, \quad \text{for } 1 \leq i, j \leq N, \]
hence $\Pi \in \Pi(x, y)$. For $l \in \mathbb{N}$ large enough, $\text{supp } \Pi \subset \text{supp } \Pi^n_{l}$ holds. By Proposition 2.3, $\text{supp } \Pi^n_{l}$ is $C$-cyclically monotone and so is $\text{supp } \Pi$, hence $\Pi$ is optimal.
To prove the converse implication, we choose a subsequence of \(((x^n, y^n))_{n \in \mathbb{N}}\), still denoted by \(((x^n, y^n))_{n \in \mathbb{N}}\), such that \((x^n, y^n) \neq (x, y)\) and \(\text{supp } x \otimes y \subset \text{supp } x^n \otimes y^n\) for \(n \in \mathbb{N}\). Define \(\delta_n \in (0, 1)\) and \(\tilde{x}^n, \tilde{y}^n \in \mathcal{P}_N\) by

\[
\delta_n := \min_{(i,j) \in \text{supp } x \otimes y} \left\{ \frac{x^n_i}{x_i}, \frac{y^n_j}{y_j} \right\}, \quad \left(1 - \sqrt{\max_{(i,j) \in \text{supp } x^n \otimes y^n} \{ |x^n_i - x_i|, |y^n_j - y_j| \}} \right) \overset{n \to \infty}{\longrightarrow} 1,
\]

\[
\tilde{x}^n := \frac{x^n - \delta_n x}{1 - \delta_n} \overset{n \to \infty}{\longrightarrow} x, \quad \tilde{y}^n := \frac{y^n - \delta_n y}{1 - \delta_n} \overset{n \to \infty}{\longrightarrow} y,
\]

respectively. For an optimal coupling \(Q^n \in \Pi(\tilde{x}^n, \tilde{y}^n)\), we denote by \((Q^{n(l)})_{l \in \mathbb{N}}\) and \(Q\) a convergent subsequence of \((Q^n)_{n \in \mathbb{N}}\) and its limit, respectively. Then \(Q \in \Pi(x, y)\) is optimal. If we set

\[
Q^n_* := \delta_n Q + (1 - \delta_n)Q^n, \quad \Pi^n_* := \delta_n \Pi_* + (1 - \delta_n)\Pi^n,
\]

then \(Q^n_* \in \Pi(x^n, y^n)\) and \(\lim_{n \to \infty} \Pi^n_* = \Pi_*\). It follows that

\[
\langle C, Q^n_* \rangle = \delta_n C(x, y) + (1 - \delta_n)C(\tilde{x}^n, \tilde{y}^n) = \langle C, \Pi^n_* \rangle.
\]

For \(l \in \mathbb{N}\) large enough, \(\text{supp } Q \subset \text{supp } Q^{n(l)}\) holds, hence \(\text{supp } Q^{n(l)} = \text{supp } Q^n\), which is \(C\)-cyclically monotone. Then \(Q^{n(l)}\) is optimal by Proposition 2.3 and \(\Pi^{n(l)}\) is also optimal. This completes the proof of the corollary. \(\square\)

**Remark 2.5.** By Corollary 2.4, a sequence of optimal couplings contains a convergent subsequence, however the sequence itself may not converge. Indeed, if \(C \in M_N(\mathbb{R})\) is the all 1s matrix, then \(\text{supp } x \otimes y\) is \(C\)-cyclically monotone for any \(x, y \in \mathcal{P}_N\), consequently every element in \(\Pi(x, y)\) is optimal by Proposition 2.3.

3. RELAXATION

We introduce a relaxation of the optimal transport problem \((2.2)\) via strictly convex functions. Throughout this section, we choose a strictly convex, continuous function \(f\) on \([0, 1]\) such that \(f \in C^1([0, 1])\) and fix it unless otherwise indicated. Then the limit \(f'(0) := \lim_{\varepsilon \downarrow 0} f'(\varepsilon)\) exists in \([-\infty, \infty)\) and \(\lim_{\varepsilon \downarrow 0} \varepsilon f'(\varepsilon) = 0\) by the convexity of \(f\). To make sense of the latter function when \(r_0 = 0\), we employ throughout the convention that \(\pm \infty \cdot 0 := 0\). Define \(D_f : [0, 1] \times [0, 1] \to (-\infty, \infty]\) by

\[
D_f(r, r_0) = f(r) - f(r_0) - f'(r_0)(r - r_0).
\]

It follows from the strict convexity of \(f\) that \(D_f(r, r_0) \in [0, \infty]\) and \(D_f(r, r_0) = 0\) if and only if \(r = r_0\). The function \(D_f\) is continuous on \([0, 1] \times (0, 1]\) and lower semicontinuous on \([0, 1] \times [0, 1]\). Moreover, for \(r_0 \in (0, 1]\), the function \(D_f(\cdot, r_0)\) is strictly convex, continuous on \([0, 1]\).

**Definition 3.1.** Fix \(C \in M_N(\mathbb{R})\) and a strictly convex, continuous function \(f\) on \([0, 1]\) such that \(f \in C^1([0, 1])\).

1. We define the Bregman divergence associated to \(f\) on \(\mathcal{P}_{N \times N} \times \mathcal{P}_{N \times N}\) by

\[
D_f(\Pi, \tilde{\Pi}) := \sum_{i,j=1}^N D_f(\pi_{ij}, \tilde{\pi}_{ij})
\]
Remark 3.2. A relaxed optimal transport problem via Bregman divergences is also studied by Dessein, Papadakis and Rouas [3], where a Bregman divergence is determined by a convex function \( f \) appearing and the assumption of convex functions is milder than theirs. For example, the Kullback–Leibler divergence. In our method, the Bregman projection does not appear as a base point. The choice of the base point is crucial for Bregman divergences other than the Kullback–Leibler divergence. In our method, the Bregman projection does not appear and the assumption of convex functions is milder than theirs. For example, the function \( f(r) := -r^{1/2}e^{-r} - r \) can be treated in our setting, but \( \phi(\Pi) := \sum_{i,j=1}^{N} f(\pi_{ij}) \) cannot be treated in the setting in [3].

It is trivial that an \((f,0)\)-coupling is an optimal coupling and \( C^0 = C \). For \( x, y \in \mathcal{P}_N \) and \( \Pi \in \Pi(x,y) \), we see that
\[
\mathcal{D}_f(\Pi, x \otimes y) = \sum_{(i,j) \in \text{supp} \, x \otimes y} D_f(\pi_{ij}, x_i y_j) \in [0, \infty),
\]
and \( \mathcal{D}_f(\Pi, x \otimes y) = 0 \) if and only if \( \Pi = x \otimes y \). By the strict convexity and the continuity of \( \mathcal{D}_f(\cdot, x \otimes y) \) on the compact set \( (\Pi(x,y), \| \cdot \|_2) \), we have the following.

Proposition 3.3. For \( x, y \in \mathcal{P}_N \) and \( \gamma > 0 \), an \((f,\gamma)\)-coupling between \( x, y \) is uniquely determined. Moreover, there exists a unique optimal coupling \( \Pi_* \in \Pi(x,y) \) such that \( \mathcal{D}_f(\Pi_*, x \otimes y) = \Lambda(x,y) \).

Computing \( \mathcal{C}_\lambda(x,y) \) is equivalent to solving the variational problem (2.2) under the constraint \( \mathcal{D}_f(\Pi, x \otimes y) = \lambda \), and reduces to computing \( \mathcal{C}_\gamma(x, y) \). In the case \( f(r) = r \log r \), this property is mentioned (but not proved) in [2]. See also [3, Theorem 15].

Theorem 3.4. Given \( x, y \in \mathcal{P}_N \) and \( \lambda \in [0, \Lambda(x,y)] \), it follows that
\[
\mathcal{C}_\lambda(x,y) = \inf \{ \langle C, \Pi \rangle \mid \Pi \in \Pi(x,y), \mathcal{D}_f(\Pi, x \otimes y) = \lambda \}.
\]
Furthermore, if \( \lambda = \mathcal{D}_f(P^\gamma, x \otimes y) \) holds for some \( \gamma \geq 0 \), where \( P^\gamma \) is an \((f,\gamma)\)-coupling between \( x, y \), then \( \mathcal{C}_\lambda(x,y) = \mathcal{C}_\gamma(x,y) \).

Proof. If \( \lambda \in [0, \Lambda(x,y)] \), then (3.1) trivially holds. Assume \( \lambda \in (0, \Lambda(x,y)) \neq \emptyset \). By the continuity of \( \mathcal{D}_f(\cdot, x \otimes y) \) on \( \Pi(x,y) \), the set
\[
\{ \Pi \in \Pi(x,y) \mid \mathcal{D}_f(\Pi, x \otimes y) \leq \lambda \}
\]
is compact in $(\Pi(x, y), \| \cdot \|_2)$. Then there exists $\Pi_\lambda \in \Pi(x, y)$ such that
\[
\mathcal{D}_f(\Pi_\lambda, x \otimes y) \leq \lambda, \quad C_\lambda(x, y) = \langle C, \Pi_\lambda \rangle > C(x, y).
\]
If $\mathcal{D}_f(\Pi_\lambda, x \otimes y) < \lambda$, then there exists $t \in (0, 1)$ such that
\[
\mathcal{D}_f((1 - t)\Pi_\lambda + t\Pi_\star, x \otimes y) = \lambda
\]
by the intermediate value theorem, where $\Pi_\star \in \Pi(x, y)$ is an optimal coupling such that $\mathcal{D}_f(\Pi_\star, x \otimes y) = \Lambda(x, y)$. However,
\[
C_\lambda(x, y) \leq \langle C, (1 - t)\Pi_\lambda + t\Pi_\star \rangle = (1 - t)C_\lambda(x, y) + tC(x, y) < C_\lambda(x, y),
\]
which is a contradiction. Thus $\mathcal{D}_f(\Pi_\star, x \otimes y) = \lambda$ and (3.1) holds. In addition, in the case of $\lambda = \mathcal{D}_f(\Pi^\gamma, x \otimes y)$, we see that
\[
\mathcal{F}^\gamma_{x,y}(\Pi_\lambda) = C_\lambda(x, y) + \gamma \lambda \leq \langle C, \Pi^\gamma \rangle + \gamma \lambda = \mathcal{F}^\gamma_{x,y}(\Pi^\gamma) \leq \mathcal{F}^\gamma_{x,y}(\Pi_\lambda),
\]
which implies $C_\lambda(x, y) = C^\gamma(x, y)$. □

By Theorems 3.11 and 3.13 and Proposition 3.15 below, for $x, y \in \mathcal{P}_N$, if $\text{supp} x \otimes y$ is not $C$-cyclically monotone and $f'(0) = -\infty$, then
\[
(0, \Lambda(x, y)) = \{ \mathcal{D}_f(\Pi^\gamma, x \otimes y) \mid \gamma > 0 \text{ and } \Pi^\gamma \in \Pi(x, y) \text{ is an } (f, \gamma)\text{-coupling} \}.
\]

We prove the continuity of $\Lambda$.

**Proposition 3.5.** The function $\Lambda$ is lower semicontinuous on $\mathcal{P}_N \times \mathcal{P}_N$ and continuous on the interior of $\mathcal{P}_N \times \mathcal{P}_N$. Moreover, if either $f'(0) \in \mathbb{R}$ or $f(r) = r \log r$, then $\Lambda$ is continuous on $\mathcal{P}_N \times \mathcal{P}_N$.

**Proof.** Let $((x^n, y^n))_{n \in \mathbb{N}}$ be a sequence in $(\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2)$ converging to $(x, y)$. Set
\[
S' := \text{supp } x^n \otimes y^n \setminus \text{supp } x \otimes y,
\]
which is empty if $(x, y)$ is an interior point of $\mathcal{P}_N \times \mathcal{P}_N$. Passing to subsequences if necessary, we may assume that $\text{supp } x \otimes y \subset \text{supp } x^n \otimes y^n$ and $\text{supp } x^n \otimes y^n$ does not depend on $n \in \mathbb{N}$ without loss of generally. Let $\Pi^n_\star \in \Pi(x^n, y^n)$ be an optimal coupling such that $\mathcal{D}_f(\Pi^n_\star, x^n \otimes y^n) = \Lambda(x^n, y^n)$. Since any convergent subsequence of $(\Pi^n_\star)_{n \in \mathbb{N}}$ converges to an optimal coupling between $x, y$ by Corollary 2.4, we have
\[
\Lambda(x, y) \leq \liminf_{n \to \infty} \Lambda(x^n, y^n),
\]
which implies the lower semicontinuity of $\Lambda$ on $\mathcal{P}_N \times \mathcal{P}_N$. Again by Corollary 2.4, there is a sequence of optimal couplings $\Pi^n \in \Pi(x^n, y^n)$ such that $\lim_{l \to \infty} \Pi^{n(l)} = \Pi_\star$ for some $(n(l))_{l \in \mathbb{N}} \subset \mathbb{N}$. If $(i, j) \in \text{supp } x \otimes y$, then
\[
\lim_{l \to \infty} f'(x_i^{n(l)} y_j^{n(l)}) \pi_{i,j}^{n(l)} = f'(x_i y_j) \pi_{i,j}
\]
by $f \in C^1((0, 1])$. On the other hand, since $\pi_{i,j}^{n(l)} \leq \min\{x_i^{n(l)}, y_j^{n(l)}\}$ holds for $1 \leq i, j \leq N$, if either $f'(0) \in \mathbb{R}$ or $f(r) = r \log r$, then
\[
\lim_{l \to \infty} \left| f'(x_i^{n(l)} y_j^{n(l)}) \pi_{i,j}^{n(l)} \right| \leq \lim_{l \to \infty} \left| f'(x_i^{n(l)} y_j^{n(l)}) \cdot \min\{x_i^{n(l)}, y_j^{n(l)}\} \right| = 0 \quad \text{for } (i, j) \in S'.
\]
Thus if $f'(0) \in \mathbb{R}$, $f(r) = r \log r$, or $(x, y)$ is an interior point of $\mathcal{P}_N \times \mathcal{P}_N$, then
\[
\limsup_{n \to \infty} \Lambda(x^n, y^n) \leq \lim_{l \to \infty} \mathcal{D}_f(\Pi^{n(l)}, x^n \otimes y^n) = \mathcal{D}_f(\Pi_\star, x \otimes y) = \Lambda(x, y).
\]
This completes the proof of the proposition. □
Remark 3.6. In Proposition 3.5 if \( f'(0) = -\infty \), then \( \Lambda \) is not necessarily continuous on \( P_N \times P_N \). Indeed, let \( f(r) = -r^p/p \) for \( p \in (0, 1/2) \) and \( C = (\delta_{ij})_{1 \leq i, j \leq 2} \in M_2(\mathbb{R}) \). We choose \( x^a, y^a \in P_2 \) and \( P^{a} \in P_{2 \times 2} \) as

\[
x^a_1 = a, \quad x^a_2 = 1 - a, \quad y^a_1 = 1 - a, \quad y^a_2 = a, \quad \text{where} \ a \in [0, 1/2],
\]

\[
\pi^{a,s}_{11} = s, \quad \pi^{a,s}_{12} = a - s, \quad \pi^{a,s}_{21} = 1 - a - s, \quad \pi^{a,s}_{22} = s, \quad \text{where} \ s \in [0, a],
\]

respectively. Then \( P^{a,0} \) is an unique optimal coupling. We see that

\[
\Lambda(x^0, y^0) = 0, \quad \lim_{a \downarrow 0} \Lambda(x^a, y^a) = -\lim_{a \downarrow 0} f'(a^2)a = \lim_{a \downarrow 0} a^{2p-1} = \infty.
\]

We consider a condition such that \((f, \gamma)\)-couplings lie in the interior of \( \Pi(x, y) \).

Lemma 3.7. For \( x, y \in P_N \) and \( \gamma > 0 \), let \( P^\gamma \in \Pi(x, y) \) be an \((f, \gamma)\)-coupling. Assume that \( f'(0) = -\infty \). Then

\[
\text{supp } P^\gamma = \text{supp } x \otimes y
\]

and there exists \((\alpha, \beta) \in \mathbb{R}^{\text{supp } x \otimes y}\) such that

\[(3.2) \quad c_{ij} + \gamma \left( f'(p^\gamma_{ij}) - f'(x_iy_j) \right) = \alpha_i + \beta_j \quad \text{for} \ (i, j) \in \text{supp } x \otimes y.\]

Proof. It follows form Lemma 2.1 that

\[
\text{supp } P^\gamma \subset \text{supp } x \otimes y := S.
\]

Assume that \( \text{supp } P^\gamma \neq S \). For \( t \in (0, 1) \), set

\[
\Pi^t := (1 - t)P^\gamma + tx \otimes y \in \Pi(x, y).
\]

Since \( P^\gamma \) is a unique minimizer of \( F^\gamma_{x,y} \) on \( \Pi(x, y) \), it turns out that

\[
0 \leq \lim_{t \downarrow 0} \frac{d}{dt} F^\gamma_{x,y}(\Pi^t) = \sum_{i,j \in \text{supp } P^\gamma} (x_iy_j - p^\gamma_{ij}) \left\{ c_{ij} + \gamma \left( f'(p^\gamma_{ij}) - f'(x_iy_j) \right) \right\}
\]

\[
+ \sum_{i,j \in S(\text{supp } P^\gamma)} x_iy_j \left\{ c_{ij} + \gamma \left( \lim_{t \downarrow 0} f'(tx_iy_j) - f'(x_iy_j) \right) \right\}
\]

\[
= -\infty.
\]

This is a contradiction, hence \( \text{supp } P^\gamma = \text{supp } x \otimes y \).

Assume \( |\text{supp } x| = |\text{supp } y| = N \). If we regard \( P_{N \times N} \) as a subset of \( \mathbb{R}^{N \times N} \), then \( P^\gamma \) lies in an open set \((\mathbb{R}_{>0})^{N \times N}\). For \( 1 \leq i, j \leq N \), define \( X_i, Y_j : (\mathbb{R}_{>0})^{N \times N} \to \mathbb{R} \) by

\[
X_i(Z) := \sum_{k=1}^N z_{ik}, \quad Y_j(Z) := \sum_{k=1}^N z_{kj}.
\]

We see that, for \( Z \in (\mathbb{R}_{>0})^{N \times N} \), \( Z \in \Pi(x, y) \) if and only if

\[
X_i(Z) = x_i \quad \text{for} \ 1 \leq i \leq N, \quad Y_j(Z) = y_j \quad \text{for} \ 1 \leq j \leq N - 1.
\]

Since the Jacobian matrix of \((X_1, \cdots, X_N, Y_1, \cdots, Y_{N-1})\) has always rank \( 2N - 1 \), the method of Lagrange multipliers yields that there is \((\alpha, \beta) \in \mathbb{R}^{N \times N} \) such that \( \beta_N = 0 \) and

\[
c_{ij} + \gamma \left( f'(p^\gamma_{ij}) - f'(x_iy_j) \right) = \nabla_{z_{ij}} F^\gamma_{x,y}(P^\gamma)
\]

\[
= \sum_{k=1}^N \left( \alpha_k \nabla_{z_{ij}} X_k(P^\gamma) + \beta_k \nabla_{z_{ij}} Y_k(P^\gamma) \right) = \alpha_i + \beta_j.
\]

The case of either \( |\text{supp } x| \neq N \) or \( |\text{supp } y| \neq N \) is proved analogously. \( \square \)
Remark 3.8. To apply the method of Lagrange multipliers, an extremum should be attained in the interior of the constraint set as in the proof of Lemma 3.7. Note that the number of the constraint conditions is \(|\text{supp} x| + |\text{supp} y| - 1\), not \(|\text{supp} x| + |\text{supp} y|\).

Remark 3.9. In Lemma 3.7, the assumption \(f'(0) = -\infty\) is necessary. Indeed, if \(f'(0) \in \mathbb{R}\) then \(f \in C^1([0,1])\). We choose \(x, y^a \in \mathcal{P}_2\) and \(P^{a,s} \in \mathcal{P}_{2 \times 2}\) as

\[
x_1 = x_2 = \frac{1}{2}, \quad y_1^a = 1 - a, \quad y_2^a = a, \quad \text{where } a \in [0,1/2],
\]

\[
p^{a,s}_{11} = \frac{1}{2} - s, \quad p^{a,s}_{12} = s, \quad p^{a,s}_{21} = \frac{1}{2} - a + s, \quad p^{a,s}_{22} = a - s, \quad \text{where } s \in [0,a],
\]

respectively. Then \(P(x, y^a) = \{P^{a,s}\}_{s \in [0,a]}\). We see that

\[
M_a := \sup_{s \in (0,a)} |f'(p^{a,s}_{11}) + f'(p^{a,s}_{12}) + f'(p^{a,s}_{21}) - f'(p^{a,s}_{22})| + 1
\]

is finite by the continuity of \(f'\) on [0,1]. If we take \(C = (\delta_{ij})_{1 \leq i,j \leq 2} \in M_2(\mathbb{R})\) and \(\gamma \in (0,2/M_a)\), then, for \(s \in (0,a)\) with \(a \neq 0\), it turns out that

\[
\frac{\partial}{\partial s} \mathcal{F}^\gamma_{x,y}(P^{a,s}) = -2 + \gamma (-f'(p^{a,s}_{11}) + f'(p^{a,s}_{12}) + f'(p^{a,s}_{21}) - f'(p^{a,s}_{22})) \leq -2 + \gamma M_a < 0,
\]

implying that \(P^{a,s}\) is an \((f,\gamma)\)-coupling, where \(\text{supp} P^{a,s} \neq \text{supp} x \otimes y^a\).

If we define \(\tilde{f} : [0,1] \to \mathbb{R}\) by

\[
\tilde{f}(r) := f(r) - f(0) - r(f(1) - f(0)),
\]

then \(\tilde{f}\) is again strictly convex, continuous on [0,1] and \(\tilde{f} \in C^1((0,1])\). We see that \(\tilde{f}(0) = \tilde{f}(1) = 0\). Moreover, \(D \tilde{f} = D f\) on \([0,1] \times [0,1]\). Thus, when we discuss the relaxed optimal transport problem via the Bregman divergences associated to \(f\), we may assume \(f(0) = f(1) = 0\) without loss of generality. In this case, the convexity of \(f\) yields that \(f \leq 0\) on [0,1]. We estimate the difference between \(C\) and \(C^\gamma\).

Proposition 3.10. Given \(x, y \in \mathcal{P}_N\) and \(\gamma > 0\), let \(P^\gamma \in \Pi(x,y)\) be an \((f,\gamma)\)-coupling. Then

\[
\frac{1}{\gamma} (C^\gamma(x,y) - C(x,y)) \leq \Lambda(x,y) - D_f(P^\gamma, x \otimes y) \leq \Lambda(x,y).
\]

In the case of \(f'(0) = -\infty\),

\[
\frac{1}{\gamma} (C^\gamma(x,y) - C(x,y)) = -D_f(\Pi_*, P^\gamma) + \Lambda(x,y) - D_f(\Pi^\gamma, x \otimes y),
\]

where \(\Pi_* \in \Pi(x,y)\) is an optimal coupling such that \(\Lambda(x,y) = D_f(\Pi_*, x \otimes y)\). On the other hands, if \(f(0) = f(1) = 0\), then

\[
\Lambda(x,y) \leq -f' \left( \min_{(i,j) \in \text{supp} x \otimes y} x_i y_j \right) + \sum_{(i,j) \in \text{supp} x \otimes y} (-f(x_i y_j) + f'(x_i y_j) x_i y_j).
\]

Proof. It follows from the definition of \(\mathcal{F}_{x,y}^\gamma\) with the nonnegativity of \(D_f\) that

\[
C^\gamma(x,y) \leq C^\gamma(x,y) + \gamma D_f(P^\gamma, x \otimes y) = \mathcal{F}_{x,y}^\gamma(P^\gamma) \leq \mathcal{F}_{x,y}^\gamma(\Pi_*) = C(x,y) + \gamma \Lambda(x,y),
\]

implying the inequalities in (3.3).
Assume \( f'(0) = -\infty \). By Lemma (3.2) there exists \( (\alpha, \beta) \in \mathbb{R}^{\text{supp } x \otimes y} \) satisfying (3.2). Since we have
\[
\sum_{(i,j) \in \text{supp } x \otimes y} (\alpha_i + \beta_j) \pi_{ij} = \sum_{i \in \text{supp } x} \alpha_i x_i + \sum_{j \in \text{supp } y} \beta_j y_j \quad \text{for } \Pi \in \Pi(x,y),
\]
we multiply (3.2) by \( \pi_{ij} - p_{ij}^\gamma \) and take the sum over \((i,j) \in \text{supp } x \otimes y\) to have
\[
\frac{1}{\gamma} (C^\gamma(x,y) - C(x,y)) = \sum_{(i,j) \in \text{supp } x \otimes y} (\pi_{ij} - p_{ij}^\gamma) \left( f'(p_{ij}^\gamma) - f'(x_i y_j) \right) = -D_f(\Pi, P^\gamma) + D_f(\Pi, x \otimes y) - D_f(P^\gamma, x \otimes y).
\]
In the case of \( f(0) = f(1) = 0 \), the convexity of \( D_f(\cdot, r_0) \) on \([0,1]\) yields that
\[
\Lambda(x,y) = D_f(\Pi, x \otimes y) = \sum_{(i,j) \in \text{supp } x \otimes y} D_f(\pi_{ij}, x_i y_j)
\]
\[
\leq \sum_{(i,j) \in \text{supp } x \otimes y} \left\{ (1 - \pi_{ij})D_f(0, x_i y_j) + \pi_{ij}D_f(1, x_i y_j) \right\}
\]
\[
= \sum_{(i,j) \in \text{supp } x \otimes y} (\pi_{ij} - f(x_i y_j) - f'(x_i y_j)(\pi_{ij} - x_i y_j))
\]
\[
\leq -f'(\min_{(i,j) \in \text{supp } x \otimes y} x_i y_j) + \sum_{(i,j) \in \text{supp } x \otimes y} (f(x_i y_j) + f'(x_i y_j)x_i y_j),
\]
where the last inequality follows from the monotonicity of \( f' \) on \([0,1]\).

This completes the proof of the proposition. \( \square \)

We prove the continuity of \((f, \gamma)\)-couplings. The limit of \((f, \gamma)\)-coupling between two given points in \( \mathcal{P}_N \) as \( \gamma \downarrow 0 \) and \( \gamma \uparrow \infty \) are discussed in [3] Properties 7–9] for Bregman divergences, and in [4 Proposition 4.1] for the Kullback–Leibler divergences. In Euclidean setting, \( C^\gamma \) is lower semicontinuous, but not continuous in general (see [1 Lemma 2.4]).

**Theorem 3.11.** Let \( ((x^n, y^n))_{n \in \mathbb{N}} \) be a sequence in \( (\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2) \) converging to \((x, y)\) and \( (\gamma^n)_{n \in \mathbb{N}} \) a sequence in \((0, \infty)\) converging to \( \gamma \in [0, \infty) \), respectively. For an \((f, \gamma^n)\)-coupling \( P^{\gamma^n} \) between \( x^n, y^n \),
\[
\lim_{n \to \infty} P^{\gamma^n} = \begin{cases} x \otimes y & \gamma = \infty, \\ P^\gamma & \gamma \in (0, \infty), \\ \Pi_n & \gamma = 0, \end{cases}
\]
where \( P^\gamma \) is an \((f, \gamma)\)-coupling between \( x, y \), and \( \Pi_n \) is an optimal coupling between \( x, y \) such that \( D_f(\Pi_n, x \otimes y) = \Lambda(x,y) \). Hence the function on \((0, \infty) \times \mathcal{P}_N \times \mathcal{P}_N \) sending \((\gamma, x, y)\) to \( C^\gamma(x,y) \) is continuous and can be extended to \([0, \infty] \times \mathcal{P}_N \times \mathcal{P}_N \) continuously.

**Proof.** By the compactness of \( (\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2) \), \( (P^{\gamma^n})_{n \in \mathbb{N}} \) contains a convergent subsequence, still denoted by \( (P^{\gamma^n})_{n \in \mathbb{N}} \). An argument similar to that in (2.4) yields that \( \Pi := \lim_{n \to \infty} P^{\gamma^n} \in \Pi(x,y) \). We may assume that \( \text{supp } x \otimes y \subset \text{supp } x^n \otimes y^n \) and \( \text{supp } x^n \otimes y^n \) does not depend on \( n \in \mathbb{N} \) without loss of generally. Set \( S' := \text{supp } x^n \otimes y^n \setminus \text{supp } x \otimes y \).

Then \( \pi_{ij} = \lim_{n \to \infty} p^n_{ij} = 0 \) for \((i,j) \in S'\).
Claim 3.12. Assume one of $S' = \emptyset$, $f'(0) \in \mathbb{R}$ or \( \gamma \neq 0 \). Then
\[
\lim_{n \to \infty} D_f(P^{\gamma_n}, x^n \otimes y^n) = D_f(\Pi, x \otimes y).
\]

Proof. Recall that
\[
D_f(P^{\gamma_n}, x^n \otimes y^n) = \sum_{(i,j) \in \text{supp } x^n \otimes y^n} f'(p_{ij}^{\gamma_n}) - f'(x_i^n y_j^n) - f'(x_i^n y_j^n)(p_{ij}^{\gamma_n} - x_i^n y_j^n).
\]
Since \( f \in C([0,1]) \cap C^1((0,1]) \) and \( \lim_{\varepsilon \downarrow 0} f'(\varepsilon) = 0 \), it is enough to show that
\[
\lim_{n \to \infty} f'(x_i^n y_j^n)p_{ij}^{\gamma_n} = 0 \quad \text{for } (i,j) \in S'.
\]
This trivially holds if either $S' = \emptyset$ or $f'(0) \in \mathbb{R}$.

Assume $S' \neq \emptyset$ and $f'(0) = -\infty$. Lemma 3.17 yields that supp $P^{\gamma_n} = \text{supp } x^n \otimes y^n$. Fix $(i_1, j_1) \in S'$ and $(i_2, j_2) \in \text{supp } \Pi$. Then $f'(x_i^n y_j^n)p_{ij}^{\gamma_n} \leq 0$ for $n \in \mathbb{N}$ large enough and
\[
\lim_{n \to \infty} f'(p_{ij}^{\gamma_n})p_{ij}^{\gamma_n} = \lim_{n \to \infty} f'(x_i^n y_j^n)p_{ij}^{\gamma_n} = 0.
\]
By $\lim_{\varepsilon \downarrow 0} f'(\varepsilon) = 0$, $\lim_{n \to \infty} f'(p_{ij}^{\gamma_n})p_{ij}^{\gamma_n} = 0$. In addition, it follows from $p_{ij}^{\gamma_n} \leq x_i^n$ that
\[
\lim_{n \to \infty} f'(x_i^n y_j^n)p_{ij}^{\gamma_n} \leq \lim_{n \to \infty} f'(x_i^n y_j^n) \cdot x_i^n y_j^n \cdot \frac{1}{y_j^n} = 0.
\]
Similarly, $\lim_{n \to \infty} f'(x_i^n y_j^n)p_{ij}^{\gamma_n} = 0$ holds.

Let $\Pi' \in M_N(\mathbb{R})$ by
\[
\pi_{ij}^{\varepsilon} := \begin{cases} 
p_{ij}^{\gamma_n} + \text{sgn}(\sigma)\varepsilon & \text{if } (i,j) = (i_{\sigma(m)}, j_m) \text{ with } m = 1,2 \text{ and } \sigma \in \mathfrak{S}_2, \\
p_{ij}^{\gamma_n} & \text{otherwise},
\end{cases}
\]
then $\Pi' \in \Pi(x^n, y^n)$ and
\[
0 = \frac{d}{d\varepsilon} \mathcal{F}_{x^n, y^n}(\Pi') \bigg|_{\varepsilon = 0} = \sum_{m \in \{1,2\}, \sigma \in \mathfrak{S}_2} \text{sgn}(\sigma) \left\{ c_{\sigma(m), j_m} + \gamma_n \left( f'(p_{\sigma(m), j_m}^{\gamma_n}) - f'(x_{\sigma(m)}^n y_{j_m}^n) \right) \right\}.
\]
If \( \gamma \neq 0 \), then
\[
0 = -\lim_{n \to \infty} \sup_{p_{ij}^{\gamma_n}} \sum_{m \in \{1,2\}, \sigma \in \mathfrak{S}_2} \text{sgn}(\sigma) \left\{ c_{\sigma(m), j_m} + \frac{f'(p_{\sigma(m), j_m}^{\gamma_n}) - f'(x_{\sigma(m)}^n y_{j_m}^n)}{\gamma_n} \right\}
\leq \lim_{n \to \infty} \inf_{p_{ij}^{\gamma_n}} f'(x_i^n y_j^n) \leq \lim_{n \to \infty} \inf_{p_{ij}^{\gamma_n}} f'(x_i^n y_j^n) \leq 0,
\]
implies $\lim_{n \to \infty} f'(x_i^n y_j^n)p_{ij}^{\gamma_n} = 0$. This completes the proof of the claim.

We see that
\[
\frac{1}{\gamma_n} \langle C, P^\gamma \rangle + D_f(P^{\gamma_n}, x^n \otimes y^n) = \frac{1}{\gamma_n} \mathcal{F}_{x^n, y^n}^{\gamma_n}(P^{\gamma_n})
\leq \frac{1}{\gamma_n} \mathcal{F}_{x^n, y^n}(x^n \otimes y^n) = \frac{1}{\gamma_n} \langle C, x^n \otimes y^n \rangle.
\]
Since $|\langle C, \Pi \rangle|$ is uniformly bounded in $\Pi \in \mathcal{P}_{N \times N}$ by $\max_{1 \leq i,j \leq N} |c_{ij}|$, in the case of $\gamma = \infty$, letting $n \to \infty$ and applying Claim 3.12 lead to $D_f(\Pi, x \otimes y) \leq 0$, that is, $\Pi = x \otimes y$. \(\diamondsuit\)
Assume one of $S' = \emptyset$ or $f'(0) \in \mathbb{R}$. Then, similarly to the proof of Claim 3.12
\[
\lim_{n \to \infty} D_f(\Pi^n, x^n \otimes y^n) = D_f(\lim_{n \to \infty} \Pi^n, x \otimes y)
\]
holds for any convergent sequence of $\Pi^n \in \Pi(x^n, y^n)$. Let $\delta_n \in (0, 1)$ and $\tilde{x}^n, \tilde{y}^n \in \mathcal{P}_N$ as in (2.5). For $\gamma \in (0, \infty)$, it follows from the definition of $P^n$ that
\[
\mathcal{F}^{\gamma}_{x,y}(P^n) \leq \mathcal{F}^{\gamma}_{x,y}(\Pi) = \lim_{n \to \infty} \mathcal{F}^{\gamma}_{x^n,y^n}(P^n)
\]
\[
\leq \lim_{n \to \infty} \mathcal{F}^{\gamma}_{x^n,y^n}(\delta_n \gamma + (1 - \delta_n)\tilde{x}^n \otimes \tilde{y}^n) = \mathcal{F}^{\gamma}_{x,y}(P^n).
\]
By the uniqueness of an $(\alpha, \beta)$-coupling, we find that $\Pi = P^n$. On the other hand, there exists a sequence of optimal couplings $\Pi^n \in \Pi(x^n, y^n)$ such that $\lim_{l \to \infty} \Pi^{n(l)} = \Pi_\ast$ for some $(n(l))_{l \in \mathbb{N}} \subset \mathbb{N}$ by Corollary 2.4. In the case of $\gamma = 0$, it turns out that
\[
\mathcal{C}(x, y) = \mathcal{C}(\Pi) = \lim_{n \to \infty} \mathcal{F}^{\gamma}_{x^n,y^n}(P^n) = \lim_{n \to \infty} \mathcal{F}^{\gamma}_{x^n,y^n}(\Pi^n) = \mathcal{C}(x, y),
\]
\[
D_f(\Pi, x \otimes y) - \Lambda(x, y) = \lim_{l \to \infty} \left( D_f(\Pi^{n(l)}, x^{n(l)} \otimes y^{n(l)}) - D_f(\Pi^{n(l)}, x^{n(l)} \otimes y^{n(l)}) \right)
\]
\[
\leq \lim sup_{l \to \infty} \frac{1}{\gamma(n(l))} \left( \mathcal{C}(\Pi^{n(l)}) - \mathcal{C}(P^n) \right) \leq 0.
\]
Thus $\Pi \in \Pi(x, y)$ is optimal and $D_f(\Pi, x \otimes y) \leq \Lambda(x, y)$, that is, $\Pi = \Pi_\ast$.

It remains to prove the case $\gamma \in [0, \infty)$ under the conditions $S' \neq \emptyset$ and $f'(0) = -\infty$. In this case, it follows from Lemma 3.7 that there exists $(\alpha^n, \beta^n) \in \mathbb{R}^{\text{supp } \otimes y^n}$ such that
\[
c_{ij} + \gamma_n \left( f'(p^n_{ij}) - f'(x_i^n y_j^n) \right) = \alpha^n_i + \beta^n_j \quad \text{for } (i, j) \in \text{supp } x^n \otimes y^n.
\]
If $(i, j) \in \text{supp } \Pi$, then letting $n \to \infty$ leads to
\[
c_{ij} + \gamma \left( f'(\pi_{ij}) - f'(x_i y_j) \right) = \lim_{n \to \infty} (\alpha^n_i + \beta^n_j).
\]
Moreover, if $(i, j), (i, j') \in \text{supp } \Pi$, then
\[
\lim_{n \to \infty} \left( \beta^n_j - \beta^n_j' \right) = c_{ij} + \gamma \left( f'(\pi_{ij}) - f'(x_i y_j) \right) - \left\{ c_{ij'} + \gamma \left( f'(\pi_{ij'}) - f'(x_i y_j') \right) \right\},
\]
hence the right-hand side is independent of $i$. Similarly, if $(i, j), (i', j) \in \text{supp } \Pi$, then
\[
c_{ij} + \gamma \left( f'(\pi_{ij}) - f'(x_i y_j) \right) - \left\{ c_{ij'} + \gamma \left( f'(\pi_{ij'}) - f'(x_i y_j' \right) \right\}
\]
is independent of $j$. Thus there exists $(\alpha, \beta) \in \mathbb{R}^{\text{supp } \Pi}$ solving the linear equations of the form
\[
\alpha_i + \beta_j = c_{ij} + \gamma \left( f'(\pi_{ij}) - f'(x_i y_j) \right) \quad (i, j) \in \text{supp } \Pi.
\]
In the case of $\gamma \in (0, \infty)$, if $(i, j), (i', j') \in \text{supp } \Pi$, then $(i, j), (i', j') \in \text{supp } x \otimes y$ and
\[
\lim_{n \to \infty} \left( f'(p^n_{ij}) + f'(p^n_{ij'}) \right) = \frac{1}{\gamma} \left( \alpha_i + \beta_j + \alpha_i' + \beta_j' - c_{ij} - c_{ij'} \right) + f'(x_i y_j) + f'(x_i y_j')
\]
by (2.4), which implies $(i, j), (i, j) \in \text{supp } \Pi$, that is, $\Pi \supseteq \Pi(x, y)$. Assume that $\min\{|\text{supp } x|, |\text{supp } y|\} > 1$, otherwise $|\Pi(x, y)| = 1$ hence $\Pi = P^n$ holds. If we set
\[
I := \{i \mid i \in \text{supp } x, \ i \neq \max_{k \in \text{supp } x} k\}, \quad J := \{j \mid j \in \text{supp } y, \ j \neq \max_{k \in \text{supp } y} k\},
\]
\[
O := \left\{ Z \in (0, 1)^{I \times J} \mid \sum_{k \in I} z_{ik} < x_i, \ \sum_{k \in J} z_{kj} < y_j, \ \text{for } (i, j) \in I \times J \right\},
\]
and define $\Phi : O \to M_N(\mathbb{R})$ by

\[
\phi_{ij}(Z) := \begin{cases} 
z_{ij} & \text{if } (i, j) \in I \times J, \\
x_i - \sum_{k \in J} z_{ik} & \text{if } j = \max_{k \in \text{supp } y} k, i \in I, \\
y_j - \sum_{k \in I} z_{kj} & \text{if } i = \max_{k \in \text{supp } x} k, j \in J, \\
1 - \sum_{i \in I} x_i - \sum_{j \in J} y_j + \sum_{(i, j) \in I \times J} z_{ij} & \text{if } i = \max_{k \in \text{supp } x} k, j = \max_{k \in \text{supp } y} k, \\
0 & \text{otherwise},
\end{cases}
\]

(3.6)

then $\Pi(x, y) = \Phi(O)$ and $P^\gamma, \Pi \in \Phi(O)$. Moreover, $F_{x,y}^\gamma \circ \Phi$ is strictly convex on $O$ and

$\nabla F_{x,y}^\gamma \circ \Phi|_{\Phi^{-1}(\Pi)} = 0$

by (3.5). Thus $\Pi$ is a unique minimizer of $F_{x,y}^\gamma \circ \Phi$ on $O$, that is, $\Pi = P^\gamma$.

Assume $\gamma = 0$. Then $\text{supp } \Pi$ is $C$-cyclically monotone by (3.5) hence $\Pi$ is optimal by Proposition 2.3. Furthermore, multiplying (3.4) by $\pi_{ij}$ (resp. $\pi_{*ij}$) and taking sum over $(i, j) \in \text{supp } x \otimes y$ lead to

$\sum_{(i,j) \in \text{supp } \Pi} \left(f'(p_{ij}^n) - f'(x^n_i y^n_j)\right) \pi_{ij} = \frac{1}{\gamma_n} \left(\sum_{i \in \text{supp } x} \alpha_i^n x_i + \sum_{j \in \text{supp } y} \beta_j^n y_j - C(x, y)\right)$

$= \sum_{(i,j) \in \text{supp } \Pi_*} \left(f'(p_{ij}^n) - f'(x^n_i y^n_j)\right) \pi_{*ij}.$

Since the left-hand side converges as $n \to \infty$, so does the right-hand side, which implies $\text{supp } \Pi_* \subset \text{supp } \Pi$ and

$\sum_{(i,j) \in \text{supp } \Pi} \left(f'(\pi_{ij}) - f'(x_i y_j)\right) (\pi_{*ij} - \pi_{ij}) = 0.$

For $t \in [0, 1]$, setting $\Pi_t := (1 - t)\Pi + t\Pi_* \in \Pi(x, y)$, we find that

$\lim_{t \to 0} \frac{d}{dt} D_f(\Pi_t, x \otimes y) = \sum_{(i,j) \in \text{supp } \Pi} \left(f'(\pi_{ij}) - f'(x_i y_j)\right) (\pi_{*ij} - \pi_{ij}) = 0.$

By the strict convexity $D_f(\cdot, x \otimes y)$ on $\Pi(x, y)$, if $\Pi \neq \Pi_*$, then $D_f(\Pi_t, x \otimes y)$ is strictly increasing in $t \in [0, 1]$ hence

$\Lambda(x, y) \leq D_f(\Pi, x \otimes y) = D_f(\Pi^0, x \otimes y) < D_f(\Pi_1, x \otimes y) = D_f(\Pi_*, x \otimes y) = \Lambda(x, y),$

which is a contradiction. Thus $\Pi = \Pi_*$ and the proof of Theorem 3.11 is complete. \hfill \Box

We prove the monotonicity of the functions on $(0, \infty)$ sending $\gamma$ to $C^\gamma(x, y), D_f(P^\gamma, x \otimes y)$. Note that the nondecreasing property of $C^\gamma(x, y)$ is discussed in [3, Property 6].

**Theorem 3.13.** Given $x, y \in \mathcal{P}_N$ and $\gamma \in (0, \infty)$, let $P^\gamma$ be an $(f, \gamma)$-coupling between $x, y$. Then the two functions on $(0, \infty)$ sending $\gamma$ to $C^\gamma(x, y), -D_f(P^\gamma, x \otimes y)$ are increasing on $(0, \infty)$. If either $C^{\gamma_0}(x, y) = C^{\gamma_1}(x, y)$ or $D_f(P^{\gamma_0}, x \otimes y) = D_f(P^{\gamma_1}, x \otimes y)$ holds for $\gamma_0, \gamma_1 \in (0, \infty)$, then $P^{\gamma_0} = P^{\gamma_1}$.

Moreover, if $\text{supp } x \otimes y$ is not $C$-cyclically monotone and $f'(0) = -\infty$, then the both functions are strictly increasing.
Proof. If there exist distinct $\gamma_0, \gamma_1 \in (0, \infty)$ such that

$$\mathcal{D}_f(P^{\gamma_0}, x \otimes y) = \mathcal{D}_f(P^{\gamma_1}, x \otimes y),$$

then, for $\gamma := 1 - t\gamma_0 + t\gamma_1$ with $t \in (0, 1)$, the strict convexity of $\mathcal{D}_f(\cdot, x \otimes y)$ leads to

$$\mathcal{F}_{x,y}^\gamma(P^\gamma) \leq \mathcal{F}_{x,y}^\gamma ((1 - t)P^{\gamma_0} + tP^{\gamma_1})$$

$$\leq (1 - t)\mathcal{F}_{x,y}^\gamma (P^{\gamma_0}) + t\mathcal{F}_{x,y}^\gamma (P^{\gamma_1}) = (1 - t)\mathcal{F}_{x,y}^{\gamma_0} (P^{\gamma_0}) + t\mathcal{F}_{x,y}^{\gamma_1} (P^{\gamma_1})$$

$$\leq (1 - t)\mathcal{F}_{x,y}^{\gamma_0} (P^\gamma) + t\mathcal{F}_{x,y}^{\gamma_1} (P^\gamma) = \mathcal{F}_{x,y}^\gamma (P^\gamma).$$

Hence the inequalities above all become equalities and $P^\gamma = P^{\gamma_0} = P^{\gamma_1}$ by the uniqueness of an $(f, \gamma)$-coupling. Moreover, since $\mathcal{D}_f(P^\gamma, x \otimes y)$ is nonnegative, continuous in $\gamma > 0$ and $\lim_{\gamma \to 0} \mathcal{D}_f(P^\gamma, x \otimes y) = 0$, we find that $\mathcal{D}_f(P^\gamma, x \otimes y)$ is decreasing in $\gamma > 0$.

For $\gamma_0, \gamma_1 \in (0, \infty)$ with $\gamma_0 < \gamma_1$, the monotonicity of $\mathcal{D}_f(P^\gamma, x \otimes y)$ in $\gamma > 0$ yields that

$$C^{\gamma_0}(x, y) + \gamma_0 \mathcal{D}_f(P^{\gamma_0}, x \otimes y) = \mathcal{F}_{x,y}^{\gamma_0} (P^{\gamma_0}) \leq \mathcal{F}_{x,y}^{\gamma_0} (P^{\gamma_1}) \leq C^{\gamma_1}(x, y) + \gamma_1 \mathcal{D}_f(P^{\gamma_1}, x \otimes y).$$

Thus the function on $(0, \infty)$ sending $\gamma$ to $C^\gamma(x, y)$ is increasing. If $C^{\gamma_0}(x, y) = C^{\gamma_1}(x, y)$, then the inequalities above all become equalities, in particular $\mathcal{F}_{x,y}^{\gamma_0} (P^{\gamma_0}) = \mathcal{F}_{x,y}^{\gamma_0} (P^{\gamma_1})$. By the uniqueness of $(f, \gamma)$-couplings, $P^{\gamma_0} = P^{\gamma_1}$.

Suppose that $\supp x \otimes y$ is not $C$-cyclically monotone and $f'(0) = -\infty$. In addition, we assume that there exist $\gamma_0, \gamma_1 \in (0, \infty)$ with $\gamma_0 < \gamma_1$ such that either $C^{\gamma_0}(x, y) = C^{\gamma_1}(x, y)$ or $\mathcal{D}_f(P^{\gamma_0}, x \otimes y) = \mathcal{D}_f(P^{\gamma_1}, x \otimes y)$ holds. Then $P^\gamma = P^{\gamma_0}$ for $\gamma \in [\gamma_0, \gamma_1]$. Then, for $\gamma \in [\gamma_0, \gamma_1]$, it follows from Lemma 3.7 that $\psi_{ij} := f'(p^\gamma_{ij}) - f'(x_{ij})$ is well-defined for $(i, j) \in \supp x \otimes y$ and is independent of $\gamma$. Furthermore, there exists $(\alpha^\gamma, \beta^\gamma) \in \mathbb{R}^{\supp x \otimes y}$ such that

$$c_{ij} + \gamma \psi_{ij} = \alpha^\gamma_i + \beta^\gamma_j \quad \text{for } (i, j) \in \supp x \otimes y.$$  

Since $\supp x \otimes y$ is not $C$-cyclically monotone, we find that $\min \{|\supp x|, |\supp y|\} > 1$. Set $i_0 := \max_{i \in \supp x} i$ and $j_0 := \max_{j \in \supp y} j$. Then it turns out that

$$\alpha^\gamma_i + \beta^\gamma_j = c_{i_0 j} + c_{i_0 j_0} - c_{i_0 j_0} + \gamma (\psi_{i_0 j_0} + \psi_{i_0 j} - \psi_{i_0 j_0}) \quad \text{for } (i, j) \in \supp x \otimes y.$$  

This with (3.7) yields that

$$c_{ij} + c_{i_0 j_0} - (c_{i_0 j} + c_{i_0 j_0}) = -\gamma \{\psi_{ij} + \psi_{i_0 j_0} - (\psi_{i_0 j} + \psi_{i_0 j_0})\} \quad \text{for } (i, j) \in \supp x \otimes y.$$  

Since $\gamma \in [\gamma_0, \gamma_1]$ is arbitrary, $c_{ij} + c_{i_0 j_0} = c_{i_0 j} + c_{i_0 j_0}$ holds for $(i, j) \in \supp x \otimes y$. Moreover, it is possible to replace $(i_0, j_0)$ with any element $(i, j) \in \supp x \otimes y$, consequently

$$c_{ij} + c_{kl} = c_{uj} + c_{kj} \quad \text{for } (i, j), (k, l) \in \supp x \otimes y.$$  

This leads to the $C$-cyclical monotonicity of $\supp x \otimes y$, which is a contradiction. Thus the two functions on $(0, \infty)$ sending $\gamma$ to $C^\gamma(x, y), \mathcal{D}_f(P^\gamma, x \otimes y)$ are strictly increasing. \qed

We prepare a lemma to provide an equality condition in $0 \leq \mathcal{D}_f(P^\gamma, x \otimes y) \leq \Lambda(x, y)$.

**Lemma 3.14.** For $x, y \in \mathcal{P}_N$, the following three conditions are equivalent to each other.

1. $x \otimes y$ is an $(f, \gamma)$-coupling for some $\gamma > 0$.
2. $x \otimes y$ is an $(f, \gamma)$-coupling for any $\gamma > 0$.
3. $\supp x \otimes y$ is $C$-cyclically monotone.

**Proof.** The implication from (2) to (1) is trivial. Assume (1). By Lemma 3.7, there exists $(\alpha, \beta) \in \mathbb{R}^{\supp x \otimes y}$ satisfying (3.2) for $P^\gamma = x \otimes y$, that is, $c_{ij} = \alpha_i + \beta_j$ for $(i, j) \in \supp x \otimes y$. This leads to the $C$-cyclical monotonicity of $\supp x \otimes y$, hence (3) holds.
Assume (3). By Proposition 2.3, $x \otimes y$ is optimal. For $\Pi \in \Pi(x, y)$ and $\gamma > 0$, we have
\[
\mathcal{F}_{x,y}(x \otimes y) = \langle C, x \otimes y \rangle + \gamma \mathcal{D}_f(x \otimes y, x \otimes y) = C(x, y) \leq \langle C, \Pi \rangle \leq \mathcal{F}_{x,y}(\Pi).
\]
Thus $x \otimes y$ is an $(f, \gamma)$-coupling for any $\gamma > 0$, that is, (2) holds.

**Proposition 3.15.** For $x, y \in \mathcal{P}_N$ and $\gamma > 0$, the following two conditions are equivalent to each other.

1. $\text{supp}\, x \otimes y$ is $C$-cyclically monotone.
2. $\mathcal{D}_f(\Pi^\gamma, x \otimes y) = 0$.

Moreover, these conditions lead to the following condition.

3. $\mathcal{D}_f(\Pi^\gamma, x \otimes y) = \Lambda(x, y)$. If $f'(0) = -\infty$, then the condition (3) is equivalent to the other conditions (1) and (2).

**Proof.** If $\text{supp}\, x \otimes y$ is $C$-cyclically monotone, then
\[
\mathcal{D}_f(\Pi^\gamma, x \otimes y) = \Lambda(x, y) = 0 \quad \text{for } \gamma > 0
\]
by Proposition 2.3 and Lemma 3.14. Thus the implication from (1) to (2) and (3) holds.

Conversely, for $\gamma > 0$, if $\mathcal{D}_f(\Pi^\gamma, x \otimes y) = 0$, then $\Pi^\gamma = x \otimes y$ hence $\text{supp}\, x \otimes y$ is $C$-cyclically monotone by Lemma 3.14. Thus the implication from (2) to (1) holds.

Assume $f'(0) = -\infty$ and fix $\gamma > 0$. If $\text{supp}\, x \otimes y$ is not $C$-cyclically monotone, then $P^\gamma$ is not optimal by Proposition 2.3 and Lemma 3.7 hence $C^\gamma(x, y) > C(x, y)$. Let $\Pi_\ast \in \Pi(x, y)$ an optimal coupling such that $\mathcal{D}_f(\Pi_\ast, x \otimes y) = \Lambda(x, y)$. It turns out that
\[
C^\gamma(x, y) + \gamma \mathcal{D}_f(\Pi^\gamma, x \otimes y) = \mathcal{F}_{x,y}(\Pi^\gamma) < \mathcal{F}_{x,y}(\Pi_\ast) = C(x, y) + \gamma \Lambda(x, y)
\]
by definition. Thus $\mathcal{D}_f(\Pi^\gamma, x \otimes y) < \Lambda(x, y)$, that is, (3) implies (1). This concludes the proof of the proposition.

**Remark 3.16.** For the strict monotonicity of $C^\gamma(x, y)$, $\mathcal{D}_f(\Pi^\gamma, x \otimes y)$ with respect to $\gamma > 0$ in Theorem 3.13 and the implication from (3) to (1) in Proposition 3.15, the assumption $f'(0) = -\infty$ is necessary. Indeed, in the setting as in Remark 3.9 for $\gamma \in (0, 2/M_a)$ with $a \neq 0$, $\Pi^\gamma = P^{\alpha,\gamma} \in \Pi(x, y)$ is an unique optimal coupling, hence $\mathcal{D}_f(\Pi^\gamma, x \otimes y) = \Lambda(x, y)$ holds. However $\text{supp}\, x \otimes y^a$ is not $C$-cyclically monotone.

**Remark 3.17.** It is easy to see that $C$ is convex on $(\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2)$. However, $C^\gamma$ is not convex on $(\mathcal{P}_N \times \mathcal{P}_N, \| \cdot \|_2)$ in general. For example, we choose $y^b \in \mathcal{P}_2$ and $Q^{b,s} \in \mathcal{P}_{2 \times 2}$ as
\[
y^b_1 = b, \quad y^b_2 = 1 - b, \quad \text{where } b \in [1/2, 1],
\]
\[
q_{11}^{b,s} = s, \quad q_{12}^{b,s} = q_{21}^{b,s} = b - s, \quad q_{22}^{b,s} = 1 - 2b + s, \quad \text{where } s \in [2b - 1, b],
\]
respectively. Then $\Pi(y^b, y^b) = \{Q^{b,s}\}_{s \in [2b - 1, b]}$, especially $\Pi(y^1, y^1) = \{Q^{1,1}\}$. We take $C = (1 - \delta_{ij})_{1 \leq i,j \leq 2} \in M_2(\mathbb{R})$ and $f(r) = r \log r$. For $\gamma > 0$ and $s \in (2b - 1, b)$ with $b \neq 1$, we find that
\[
\frac{\partial}{\partial s} \mathcal{F}_{x,y}(Q^{b,s}) = -2 + \gamma \log s \frac{(1 - 2b + s)}{(b - s)^2}.
\]
This yields that an unique $(f, \gamma)$-coupling between $y^b, y^b$ is $Q^{b,s(b)}$, where
\[
s(b) := \frac{1}{2(e^{2/\gamma} - 1)} \left( 2e^{2/\gamma}b - 2b + 1 - \sqrt{4(e^{2/\gamma} - 1)b(1 - b) + 1} \right).
\]
This means that $C^\gamma(y^b, y^b) = 2(b - s(b))$ for $b \in [1/2, 1)$. It is natural to set $s(1) := 1$. 
If \( C^\gamma \) is convex, then, for \( b_t := (1 - t)b_0 + tb_1 \) with \( b_0, b_1 \in [1/2, 1] \) and \( t \in (0, 1) \),
\[
2 \left( b_t - s(b_t) \right) = C^\gamma(y^{b_t}, y^{b_t}) = C^\gamma((1 - t)(y^{b_0}, y^{b_0}) + t(y^{b_1}, y^{b_1})) \\
\leq (1 - t)C^\gamma(y^{b_0}, y^{b_0}) + tC^\gamma(y^{b_1}, y^{b_1}) \\
= 2(1 - t)(b_0 - s(b_0)) + 2t(b_1 - s(b_1))
\]
holds, which is equivalent to the concavity of \( s(b) \) on \( b \in [1/2, 1] \). However, we find that \( \lim_{t \to 1} s'(b) = 2e^{2/\gamma} > 0 \). Thus \( C^\gamma \) is not convex.

4. Gradient descent on a space of couplings

We construct an iterative process to find the relaxed minimizer via the Bregman divergences associated to a strictly convex, continuous function \( f \) on \([0, 1]\) such that \( f \in C^2((0, 1]) \) with \( f'(0) = -\infty \), where the output \( \Pi \in \mathcal{P}_{N \times N} \) is always a coupling between two given points in \( \mathcal{P}_N \) even if we stop the iteration at the finite step. Note that \( f(r) = r \log r \) satisfies this condition.

For this purpose, we regard \( \Pi(x, y) \) as a submanifold of \( M_N(\mathbb{R}) \) and consider the gradient of \( \mathcal{F}_{x,y} \) with respect to the induced Riemannian metric. Note that an algorithm for general convex functions is already introduced (for instance, see \[3\], Section 4) and \[4\], Remark 4.10, Section 4.6] and the references therein) and a gradient descent of a convex function on \( \mathcal{P}_N \) is mentioned in \[4\], Section 9.3]. However, these are different from our method.

In what follows, we fix \( x, y \in \mathcal{P}_N \). For simplicity, we assume \(|\text{supp} \, x| = |\text{supp} \, y| = N \).

Let \( \Phi : O \to M_N(\mathbb{R}) \) be as in \[3.2\]. Then \( M := \Phi(O) \subset \Pi(x, y) \) becomes a submanifold of \( M_N(\mathbb{R}) \) of dimension \((N - 1)^2\), where \((M, \Phi^{-1}|_M)\) determines a global coordinate system of \( M \). Let \((\partial_{ij})_{1 \leq i,j \leq N}\) be coordinate vector fields of this global coordinate system. We denote by \( g \) the induced Riemannian metric on \( O \). We see that
\[
g(i,j)(k,l) := g(\partial_{ij}, \partial_{kl}) = (1 + \delta_{ik})(1 + \delta_{jl}) \quad \text{for} \quad 1 \leq i, j, k, l \leq N - 1,
\]
and its inverse matrix, denoted by \((g^{(i,j)(k,l)})_{1 \leq i,j,k,l \leq N-1}\), is
\[
g^{(i,j)(k,l)} := \left( \frac{1}{N} - \delta_{ik} \right) \left( \frac{1}{N} - \delta_{jl} \right) \quad \text{for} \quad 1 \leq i, j, k, l \leq N - 1.
\]
This ensures that \( M \) is a totally geodesic submanifold of \( M_N(\mathbb{R}) \), that is, \((\Pi^t)_{t \in [0,1]}\) is a geodesic in \( M \) if and only if there exist \( Z_0, Z_1 \in O \) such that
\[
\Pi^t = \Phi((1 - t)Z_0 + tZ_1) \quad \text{for} \quad t \in [0, 1].
\]

Fix \( \gamma > 0 \) and a strictly convex, continuous function \( f \) on \([0,1]\) such that \( f \in C^2((0,1]) \). Then \( \mathcal{F}_{x,y} \in C^2(M) \) and the composition of \( \mathcal{F}_{x,y} \) and a nonconstant geodesic on \((M, g)\) is always strictly convex. Hence the function \( \mathcal{F} : O \to \mathbb{R} \) defined by
\[
\mathcal{F}(Z) := \mathcal{F}_{x,y}(\Phi(Z))
\]
is \( C^2 \), strictly convex on \( O \). Moreover, \( \mathcal{F} \) is continuously extended to the closure \( \overline{O} \) of \( O \).

For \( 1 \leq i, j \leq N - 1 \), we write
\[
\nabla_{ij}\mathcal{F} := \left( \frac{\partial \mathcal{F}}{\partial z_{ij}} \right) = \sum_{(k,l) = (i,j),(N,N),(N,i),(i,N),(N,j)} \text{sgn}(k,l) \left\{ c_{kl} + \gamma \left( f'(\phi_{kl}) - f'(x_{kly}) \right) \right\}
\]
and \( \nabla \mathcal{F} := (\nabla_{ij}\mathcal{F})_{1 \leq i,j \leq N-1} \), where \( \text{sgn}(k,l) := 1 \) if \((k,l) = (i,j),(N,N)\), otherwise \( \text{sgn}(k,l) := -1 \). Then \( \nabla \mathcal{F}(Z) = 0 \) if and only if \( \Phi(Z) \) is an \((f, \gamma)\)-coupling between \( x, y \).
To define a sequence \((Z^n)_{n \in \mathbb{N}}\) in \(O\), we prepare a lemma.

**Lemma 4.1.** Let \(f\) be a strictly convex, continuous function on \([0,1]\) so that \(f \in C^2([0,1])\) with \(f'(0) = -\infty\). Given \(\gamma > 0\) and \(x, y \in \mathcal{P}_N\) with \(\text{supp } x = \text{supp } y = N\), define functions \(\varepsilon_{ij}, \varepsilon_i, \varepsilon_j, \varepsilon : O \to \mathbb{R}\) for \(1 \leq i, j \leq N-1\) by

\[
\varepsilon_{ij}(Z) := \begin{cases} 
\frac{z_{ij}}{2\nabla_{ij}F(Z)} & \text{if } \nabla_{ij}F(Z) > 0, \\
1 & \text{otherwise},
\end{cases}
\]

\[
\varepsilon_i(Z) := \begin{cases} 
\frac{x_i - \sum_{k=1}^{N-1} z_{ik}}{2\sum_{k=1}^{N-1} \nabla_{ik}F(Z)} & \text{if } \sum_{k=1}^{N-1} \nabla_{ik}F(Z) < 0, \\
1 & \text{otherwise},
\end{cases}
\]

\[
\varepsilon_j(Z) := \begin{cases} 
\frac{y_j - \sum_{k=1}^{N-1} z_{kj}}{2\sum_{k=1}^{N-1} \nabla_{kj}F(Z)} & \text{if } \sum_{k=1}^{N-1} \nabla_{kj}F(Z) < 0, \\
1 & \text{otherwise},
\end{cases}
\]

\[
\varepsilon(Z) := \min_{1 \leq i, j \leq N} \{\varepsilon_i(Z), \varepsilon_j(Z), \varepsilon_{ij}(Z)\},
\]

respectively. Then \(Z - t\nabla F(Z) \in O\) for \(t \in [0, \varepsilon(Z)]\) and

\[H(Z) := \max_{t \in [0,\varepsilon(Z)]} \frac{d^2}{dt^2}F(Z - t\nabla F(Z)) \geq 0\]

with equality if and only if \(\nabla F(Z) = 0\).

**Proof.** Set \(Z^t := Z - t\nabla F(Z)\). For \(1 \leq i, j \leq N-1\) and \(t \in [0, \varepsilon(Z)]\), we see that

\[
z_{ij}^t \geq \begin{cases} 
\frac{1}{2}z_{ij} & \text{if } \nabla_{ij}F(Z) > 0, \\
z_{ij} & \text{otherwise},
\end{cases}
\]

\[
\sum_{k=1}^{N-1} z_{ik}^t = \sum_{k=1}^{N-1} z_{ik} - t \sum_{k=1}^{N-1} \nabla_{ik}F(Z) \leq \begin{cases} 
\frac{1}{2} \left(x_i + \sum_{k=1}^{N-1} z_{ik} \right) & \text{if } \sum_{k=1}^{N-1} \nabla_{ik}F(Z) < 0, \\
\sum_{k=1}^{N-1} z_{ik} & \text{otherwise},
\end{cases}
\]

\[
\sum_{k=1}^{N-1} z_{kj}^t = \sum_{k=1}^{N-1} z_{kj} - t \sum_{k=1}^{N-1} \nabla_{kj}F(Z) \leq \begin{cases} 
\frac{1}{2} \left(y_j + \sum_{k=1}^{N-1} z_{kj} \right) & \text{if } \sum_{k=1}^{N-1} \nabla_{kj}F(Z) < 0, \\
\sum_{k=1}^{N-1} z_{kj} & \text{otherwise},
\end{cases}
\]

implying \(Z^t \in O\). Since \(F\) is strictly convex on \(O\), \(H(Z) \geq 0\) with equality if and only if \(\nabla F(Z) = 0\). \(\square\)

We compute that

\[
\frac{d^2}{dt^2}F(Z - t\nabla F(Z)) = \frac{\partial^2 F}{\partial z_{ij} \partial z_{kl}}(Z - t\nabla F(Z)) \cdot \nabla_{ij}F(Z) \cdot \nabla_{kl}F(Z),
\]

\[
\frac{\partial^2 F}{\partial z_{ij} \partial z_{kl}} = \gamma(f''(\phi_{ij})\delta_{ik}\delta_{jl} + f'(\phi_{NN}) + f''(\phi_{iN})\delta_{ik} + f''(\phi_{Nj})\delta_{ij}).
\]
Theorem 4.2. With the same assumptions and notation as in Lemma 4.1, define a sequence \((Z^n)_{n \in \mathbb{N}} \subset O\) inductively as follows.: Let \(Z^1 := \Phi^{-1}(x \otimes y) = (x; y_1)_{1 \leq i, j \leq N-1}\). If \(Z^n \in O\) has been defined, let \(Z^{n+1} := Z^n\) if \(\nabla F(Z^n) = 0\), and otherwise let

\[
Z^{n+1} := Z^n - t_n \nabla F(Z^n), \quad \text{where } t_n := \min \left\{ \frac{\|\nabla F(Z^n)\|^2_2}{H(Z^n)}, \varepsilon(Z^n) \right\}.
\]

Then \(Z^\infty := \lim_{n \to \infty} Z^n\) exists and \(\Phi(Z^\infty)\) is an \((f, \gamma)\)-optimal coupling between \(x, y\).

Proof. It is enough to show the case that \(\nabla F(Z^n) \neq 0\) for any \(n \in \mathbb{N}\). The Taylor expansion of \(F\) implies

\[
F(Z^{n+1}) - F(Z^n) \leq -t_n \langle \nabla F(Z^n), \nabla F(Z^n) \rangle + \frac{t_n^2}{2} \max_{t \in [0, t_n]} \frac{d^2}{dt^2} F(Z^n - t \nabla F(Z^n))
\]

Thus \(F(Z^n))_{n \in \mathbb{N}}\) is a strictly decreasing sequence. By

\[
\inf_{n \in \mathbb{N}} F(Z^n) \geq F(\Phi^{-1}(P^\gamma)),
\]

where \(P^\gamma\) is an \((f, \gamma)\)-optimal coupling between \(x, y\), the limit \(F^\infty := \lim_{n \to \infty} F(Z^n)\) exists. Then

\[
(4.1) \quad 0 = \lim_{n,L \to \infty} \left| F(Z^{n+L}) - F(Z^n) \right| \geq \lim_{n,L \to \infty} \sum_{l=0}^{L-1} \frac{t_{n+l}}{2} \|\nabla F(Z^{n+l})\|^2_2.
\]

If \(\lim \inf_{n \to \infty} \|\nabla F(Z^n)\|^2_2 = 0\), then there exists a subsequence of \((Z^n)\) converging to \(P^\gamma\). This implies that \(F^\infty = 0\), hence \(\lim_{n \to \infty} Z^n = P^\gamma\).

Assume \(\lim \inf_{n \to \infty} \|\nabla F(Z^n)\|^2_2 \in (0, \infty]\). Then it follows from (4.1) that

\[
\lim_{n,L \to \infty} \sum_{l=0}^{L-1} t_{n+l} = 0,
\]

\[
\|Z^{n+L} - Z^n\|^2_2 = \left\| \sum_{l=0}^{L-1} t_{n+l} \nabla F(Z^{n+l}) \right\|^2_2 \leq \sum_{l=0}^{L-1} t_{n+l} \|\nabla F(Z^{n+l})\|^2_2 \leq \left( \sum_{l=0}^{L-1} t_{n+l} \right)^{\frac{1}{2}} \left( \sum_{l=0}^{L-1} \|\nabla F(Z^{n+l})\|^2_2 \right)^{\frac{1}{2}} \xrightarrow{n,L \to \infty} 0,
\]

hence \(Z^\infty := \lim_{n \to \infty} Z^n \in \overline{O}\) exists. By the assumption that \(\lim \inf_{n \to \infty} \|\nabla F(Z^n)\|^2_2 \neq 0\), \(\Phi(Z^\infty) \neq P^\gamma\) holds. Since all of \(\varepsilon, H, \nabla F : O \to \mathbb{R}\) are continuous, if \(Z^\infty \in O\), then

\[
\inf_{n \in \mathbb{N}} t_n := \inf_{n \in \mathbb{N}} \min \left\{ \frac{\|\nabla F(Z^n)\|^2_2}{H(Z^n)}, \varepsilon(Z^n) \right\} > 0,
\]

which is a contradiction to \(\lim_{n \to \infty} t_n = 0\). Thus \(Z^\infty \in \partial O\) holds, that is, there exists \(1 \leq i, j \leq N\) such that \(\phi_{ij}(Z^\infty) = 0\). If \(1 \leq i, j \leq N-1\) and \(\phi_{iN}(Z^\infty), \phi_{Nj}(Z^\infty) > 0\), then

\[
\lim_{n \to \infty} \nabla_{ij} F(Z^n) = -\infty,
\]

consequently \((z^n_{ij} = \phi_{ij}(Z^n))_{n \in \mathbb{N}}\) is an increasing sequence, which is a contradiction to \(\phi_{ij}(Z^\infty) = 0\). The other cases are similar. Thus \(\lim_{n \to \infty} \|\nabla F(Z^n)\|^2_2 = 0\) and \(Z^\infty = P^\gamma\) follow. This completes the proof of the theorem. \(\square\)
In Theorem 4.2, we consider a gradient descent of \( F \) in \( O \). One can give a similar discussion for a gradient descent of \( F^\gamma_{x,y} \) in \( M \). To do this, we identify the tangent space \( T_\Pi M \) at \( \Pi \in M \) with \( M_{N-1}(\mathbb{R}) \) by a natural isomorphism

\[
\sum_{i,j=1}^{N-1} \zeta^{ij} \partial_{ij} \bigg|_\Pi \in T_\Pi M \iff (\zeta^{ij})_{1 \leq i,j \leq N-1} \in M_{N-1}(\mathbb{R}).
\]

Then the gradient of \( \nabla^\gamma_{g} F^\gamma_{x,y} \), denoted by \( \nabla^\gamma_{g} F^\gamma_{x,y} \), at \( \Phi(Z) \in M \) is identified with

\[
D(Z) = (d^{ij}(Z))_{1 \leq i,j \leq N-1} := \left( \sum_{k,l=1}^{N-1} g^{(i,j)(k,l)} \nabla_{ij}^{} F(Z) \right)_{1 \leq i,j \leq N-1},
\]

where \( D(Z) = 0 \) if and only if \( \Phi(Z) \) is an \((f,\gamma)\)-coupling between \( x,y \). Note that

\[
G(Z) := g(\nabla^\gamma_{g} F^\gamma_{x,y}^{}, \nabla^\gamma_{g} F^\gamma_{x,y}^{}) (\Phi(Z)) = \sum_{i,j,k,l=1}^{N-1} g^{(i,j)(k,l)} d^{ij}(Z) d^{kl}(Z) = \sum_{i,j,k,l=1}^{N-1} g^{(i,j)(k,l)} \nabla_{ij}^{} F(Z) \nabla_{kl}^{} F(Z).
\]

For a geodesic \( \Pi^t \in M \) defined by

\[
\Pi^t := \exp_\Pi (-t \nabla^\gamma_{g} F^\gamma_{x,y}^{}(\Pi)) = \Phi(\Pi - tD(Z)), \quad \text{where } Z := \Phi^{-1}(\Pi),
\]

we observe that

\[
\frac{d^2}{dt^2} F^\gamma_{x,y}^{}(\Pi^t) = \sum_{i,j,k,l=1}^{N-1} \frac{\partial^2 F}{\partial z_{ij} \partial z_{kl}} (Z - tD(Z)) \cdot d^{ij}(Z) \cdot d^{kl}(Z).
\]

The following corollary is proved in analogy with Theorem 4.2.

**Corollary 4.3.** With the same assumptions as in Lemma 4.1, for \( 1 \leq i, j \leq N-1 \), define functions \( \epsilon_{ij}, \epsilon^i, \epsilon_j, \epsilon : O \rightarrow \mathbb{R} \) by

\[
\epsilon_{ij}(Z) := \begin{cases} 
\frac{z_{ij}}{2d^{ij}(Z)} & \text{if } d^{ij}(Z) > 0, \\
1 & \text{otherwise}, 
\end{cases}
\]

\[
\epsilon^i(Z) := \begin{cases} 
\frac{x_i - \sum_{k=1}^{N-1} z_{ik}}{-2 \sum_{k=1}^{N-1} d^{ik}(Z)} & \text{if } \sum_{k=1}^{N-1} d^{ik}(Z) < 0, \\
1 & \text{otherwise}, 
\end{cases}
\]

\[
\epsilon_j(Z) := \begin{cases} 
\frac{y_j - \sum_{k=1}^{N-1} z_{kj}}{-2 \sum_{k=1}^{N-1} d^{kj}(Z)} & \text{if } \sum_{k=1}^{N-1} d^{kj}(Z) < 0, \\
1 & \text{otherwise}, 
\end{cases}
\]

\[
\epsilon(Z) := \min_{1 \leq i,j \leq N} \{ \epsilon^i(Z), \epsilon_j(Z), \epsilon_{ij}(Z) \},
\]

respectively. Then \( Z - tD(Z) \in O \) for \( t \in [0, \epsilon(Z)] \) and

\[
D_2(Z) := \max_{t \in [0, \epsilon(Z)]} \frac{d^2}{dt^2} F^\gamma_{x,y} (\Phi(Z - tD(Z))) \geq 0.
\]
with equality if and only if $D(Z) = 0$.

Furthermore, define $(Z^n)_{n \in \mathbb{N}} \subset O$ inductively as follows.: Let $Z^1 := \Phi^{-1}(x \otimes y)$. If $Z^n \in O$ has been defined, let $Z^{n+1} := Z^n$ if $D(Z^n) = 0$, and otherwise let

$$Z^{n+1} := Z^n - t_n D(Z^n),$$

where $t_n := \min \left\{ \frac{G(Z^n)}{D_2(Z^n)}, \epsilon(Z^n) \right\}$.

Then $Z^{\infty} := \lim_{n \to \infty} Z^n$ exists and $\Phi(Z^{\infty})$ is an $(f, \gamma)$-optimal coupling between $x, y$.

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