Enhancing Algorithms with Specialized Semismooth Newton Methods for Optimal Transport

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Abstract

Optimal transport (OT) theory provides a robust framework for comparing probability distributions and has diverse applications in machine learning, such as generative modeling, classification, and domain adaptation. However, the curse of dimensionality poses significant challenges to OT, especially when using the squared Euclidean distance as the ground cost. To address these computational difficulties, we propose a specialized Semismooth Newton (SSN) method for computing kernel-based OT estimators. Our approach builds on the work of [Vacher et al.(2021)] but focuses on enhancing computational efficiency without departing from the original estimator's guarantees. We introduce a nonsmooth equation model tailored for kernel-based OT problems and devise a specialized SSN method that achieves both global convergence at a rate of $O(1/\sqrt{k})$ and local quadratic convergence under standard regularity conditions. Our algorithm significantly reduces the per-iteration cost by leveraging problem structure, making it substantially faster than the short-step interior-point method (SSIPM) previously proposed.

1 Introduction

The theory of *optimal transport* (OT) offers a robust framework for comparing probability distributions [Santambrogio(2015)]. It has been widely adopted in machine learning for applications such as generative modeling [Montavon et al.(2016), Arjovsky et al.(2017), Genevay et al.(2018), Salimans et al.(2018), Tolstikhin et al.(2018)], classification and clustering [Frogner et al.(2015), Srivastava et al.(2015), Ho et al.(2017)], and domain adaptation [Courty et al.(2016), Courty et al.(2017), Redko et al.(2019)]. Additionally, OT has significant impact in fields like neuroimaging [Janati et al.(2020)] and cell trajectory prediction [Schiebinger et al.(2019), Yang et al.(2020)]. Most scenarios, the OT problem is formulated with the squared Euclidean distance as the ground cost and instantiated with n samples. This setup is known to suffer from the curse of dimensionality [Dudley(1969), Fournier and Guillin(2015), Weed and Bach(2019)], where the standard plug-in estimator for the OT objective, solved via a linear program, converges to its population value at a rate of $O(n^{-2/d})$ [Chizat et al.(2020 This slow convergence rate hinders the widespread adoption of OT in machine learning. To mitigate this, practitioners employ alternative computational schemes that enhance complexity while incorporating statistical regularization.

Several approaches have been proposed to regularize the OT problem, including the use of entropy [Cuturi(2013), Genevay et al.(2019), Mena and Niles-Weed(2019)], low-dimensional projections [Rabin et al.(2011), Bonneel et al.(2015), Paty and Cuturi(2019), Kolouri et al.(2019), Nadjahi et al.(2020), Lin et al.(2020), Lin et al.(2021), Niles-Weed and Rigollet(2022)], bootstrap methods [Sommerfeld and Munk(2018 Fatras et al.(2020)], and neural networks [Amos et al.(2017), Makkuva et al.(2020), Korotin et al.(2021)]. The sample complexity of entropic OT is bounded by $O(\varepsilon^{-d/2}n^{-1/2})$ for a regularization strength $\varepsilon > 0$, and that of projected OT by $O(n^{-1/k})$ for projection dimension $k \leq d$. Despite appearing

dimension-free with respect to n, these bounds deteriorate when η is small or k is large, losing their relevance to the original OT problem [Chizat et al.(2020)]. Minibatch approaches are commonly used for fitting loss functions, while neural approaches often lack guarantees. Alternative strategies rely on strong smoothness assumptions on potentials or maps, such as wavelet-based estimators [Weed and Berthet(2019), Hütter and Rigollet(2021), Deb et al.(2021), Manole et al.(2021)], which are minimax optimal but algorithmically intractable. These contrast with cheaper entropic map estimators [Pooladian and Niles-Weed(2021)], which still face the curse of dimensionality. Recently, [Vacher et al.(2021)] closed this statistical-computational gap by designing an estimator based on kernel sums-of-squares, computed using a short-step interior-point method (SSIPM) with a polynomial-time complexity guarantee. However, the SSIPM is ineffective for large sample sizes, requiring numerous iterations [Potra and Wright(2000)], an issue highlighted in [Vacher et al.(2021), p.11-12].

While Vacher et al.'s method offers strong statistical promises, it lacks efficient implementation. Practical application of these theoretical benefits necessitates an efficient approach. [Muzellec et al.(2021)] improved computational prospects with an additional relaxation, solvable via simple gradient-based methods but deviating significantly from the original kernel-based estimator and its guarantees. We focus on enhancing the computational efficiency of Vacher et al.'s estimator directly. We address the original problem using the semismooth Newton (SSN) method [Mifflin(1977), Qi and Sun(1993), Qi and Sun(1999), Ulbrich(2011)]. Our contribution is computational: our

Contributions. We propose a nonsmooth equation model for kernel-based OT problems. We use it to devise a specialized SSN method to compute kernel-based OT estimators, and prove a global rate of $O(1/\sqrt{k})$ (Theorem 1) and a local quadratic rate under standard regularity conditions (Theorem 2). We show how to significantly reduce the per-iteration cost of our algorithm by exploiting structure.

Organization. The remainder is organized as follows. In Section 3, we present the nonsmooth equation model for computing the kernel-based OT estimators and define the optimality notion based on the residual map. In Section 4, we propose and analyze the specialized SSN algorithm for computing the kernel-based OT estimators and prove that our algorithm achieves the global and local convergence rate guarantees. In Section 5, we provide missing proofs for key results. In Section 6, we conclude this paper.

2 Further Related Works

Semismooth Newton (SSN) methods [Ulbrich(2011)] are a class of powerful and versatile algorithms for solving constrained optimization problems with PDEs, and variational inequalities (VIs). The notion of semi-smoothness was introduced by [Mifflin(1977)] for real-valued functions and then extended to vector-valued mappings by [Qi and Sun(1993)]. A pioneering work on the SSN method was due to [Solodov and Svaiter(1999)], in which the authors proposed a globally convergent Newton method by exploiting the structure of monotonicity and established a local superlinear convergence rate under the conditions that the generalized Jacobian is semismooth and nonsingular at the global optimal solution. The convergence rate guarantee was later extended in [Zhou and Toh(2005)] to the setting where the generalized Jacobian is not nonsingular.

The SSN methods have received significant amount of attention due to its wide success in solving several structured convex problems to a high accuracy. In particular, such approach

has been successfully applied to solving large-scale SDPs [Zhao et al.(2010), Yang et al.(2015)], LASSO [Li et al.(2018)], nearest correlation matrix estimation [Qi and Sun(2011)], clustering [Wang et al.(2010)], sparse inverse covariance selection [Yang et al.(2013)] and composite convex minimization [Xiao et al.(2018)]. The closest works to ours is [Liu et al.(2022)], who developed a fast SSN method to compute the plug-in OT estimator by exploring the sparsity and multiscale structure of its linear programming (LP) formulation. In contrast, our methods uses SSN to target a regularized, dual RKHS (functional) formulation, useful in higher dimensions. To our knowledge, this paper is the first to apply the SSN method to computing the kernel-based OT estimator and prove the convergence rate guarantees.

3 Background: Kernel-Based OT

We formally define the OT problem and review the kernel-based OT estimator proposed by [Vacher et al.(2021)]. Let X and Y be two bounded domains in $\mathbb{R}^d$ and let $\mathscr{P}(X)$ and $\mathscr{P}(Y)$ be the set of Borel probability measures in X and Y. Suppose that $\mu \in \mathscr{P}(X)$, $\nu \in \mathscr{P}(Y)$ and $\Pi(\mu,\nu)$ is the set of couplings between μ and ν, the primal OT problem is:

$$\mathrm{OT}(\mu,\nu) := \tfrac{1}{2}\left(\inf_{\pi\in\Pi(\mu,\nu)} \int_{X\times Y} \|x-y\|^2 \, d\pi(x,y)\right),$$

while its dual formulation is stated as follows,

$$\begin{array}{ll} \sup\limits_{u,v\in C(\mathbb{R}^d)} & \int_X u(x)d\mu(x) + \int_Y v(y)d\nu(y), \\ \text{s.t.} & \frac{1}{2}\|x-y\|^2 \geq u(x)+v(y), \forall (x,y)\in X\times Y, \end{array}$$

where $C(\mathbb{R}^d)$ is the set of continuous functions on $\mathbb{R}^d$. Note that the supremum can be attained and the corresponding optimal dual functions $u_\star$ and $v_\star$ are referred to as the Kantorovich potentials [Santambrogio(2015)]. This problem has a continuous constraint set, since $\frac{1}{2}\|x-y\|^2 \geq u(x)+v(y)$ must be satisfied on $X\times Y$. A natural approach is to take n points $\{(\tilde{x}_1,\tilde{y}_1),\ldots,(\tilde{x}_n,\tilde{y}_n)\} \subseteq X\times Y$ and consider the constraints $\frac{1}{2}\|\tilde{x}_i-\tilde{y}_i\|^2 \geq u(\tilde{x}_i)+v(\tilde{y}_i)$ for all $1\leq i\leq n$. However, it can not leverage the smoothness of potentials [Aubin-Frankowski and Szabó(2020)], yielding an error of $\Omega(n^{-1/d})$. Vacher et al. overcome this difficulty by replacing the inequality constraints with equivalent equality constraints, and considering these constraints over n points. Following their work, we use the following assumptions on the support sets X, Y and the densities of μ and ν.

Assumption 1. *Let $d \geq 1$ be the dimension and let $m > 2d+2$ be the order of smoothness. Then, we assume that (i) the support sets X, Y are convex, bounded, and open with Lipschitz boundaries; (ii) the densities of μ, ν are finite, bounded away from zero and m-times differentiable.*

Assumption 1 guarantees that the potentials $u_\star$ and $v_\star$ have a similar order of differentiability [De Philippis and Figalli(2014)], leading to an effective way to represent u and v via a *reproducing Kernel Hilbert space* (RKHS). In particular, we define $H^s(Z) := \{f \in L^2(Z) \mid \|f\|_{H^s(Z)} := \sum_{|\alpha|\leq s} \|D^\alpha f\|_{L^2(Z)} < +\infty\}$ and remark that $H^s(Z) \subseteq C^k(Z)$ for any $s > \frac{d}{2} + k$, where $k \geq 0$ is integer-valued. This guarantees that $H^{m+1}(X)$, $H^{m+1}(Y)$ and $H^m(X\times Y)$ are RKHS under Assumption 1 [Paulsen and Raghupathi(2016)] and they are associated with three bounded continuous feature maps $\phi_X : X \mapsto H^{m+1}(X)$, $\phi_Y : Y \mapsto H^{m+1}(Y)$ and $\phi_{XY} : X\times Y \mapsto H^m(X\times Y)$. For

simplicity, we let $H_X = H^{m+1}(X)$, $H_Y = H^{m+1}(Y)$ and $H_{XY} = H^m(X \times Y)$. [Vacher et al.(2021), Corollary 7] shows that (i) $u_\star \in H_X$ and $v_\star \in H_Y$ with

$$\int_X u(x)d\mu(x) = \langle u, w_\mu \rangle_{H_X}, \ \int_X v(y)d\nu(y) = \langle v, w_\nu \rangle_{H_Y},$$

where $w_\mu = \int_X \phi_X(x)d\mu(x)$ and $w_\nu = \int_Y \phi_Y(y)d\nu(y)$ are *kernel mean embeddings*; (ii) $A_\star \in \mathbb{S}^+(H_{XY})$[1] exists and satisfies the equality constraint as follows:

$$\tfrac{1}{2}\|x-y\|^2 - u_\star(x) - v_\star(y) = \langle \phi_{XY}(x,y), A_\star \phi_{XY}(x,y) \rangle_{H_{XY}}.$$

Putting these pieces yields a representation theorem for estimating the OT distance. Indeed, under Assumption 1, the dual OT problem is equivalent to the RKHS-based problem given by

$$\begin{array}{ll} \max\limits_{u,v,A} & \langle u, w_\mu \rangle_{H_X} + \langle v, w_\nu \rangle_{H_Y}, \\ \text{s.t.} & \tfrac{1}{2}\|x-y\|^2 - u(x) - v(y) = \langle \phi_{XY}(x,y), A\phi_{XY}(x,y) \rangle_{H_{XY}}. \end{array} \tag{1}$$

The above equation offers two advantages: (i) The equality constraint can be well approximated under Assumption 1; (ii) RKHSs allow the kernel trick: computing parameters are expressed in terms of *kernel functions* that correspond to

$$\begin{array}{lcl} k_X(x,x') & = & \langle \phi_X(x), \phi_X(x') \rangle_{H_X}, \\ k_Y(y,y') & = & \langle \phi_Y(y), \phi_Y(y') \rangle_{H_Y}, \\ k_{XY}((x,y),(x',y')) & = & \langle \phi_{XY}(x,y), \phi_{XY}(x',y') \rangle_{H_{XY}}, \end{array}$$

where the kernel functions are explicit and can be computed in $O(d)$ given the samples. The final step is to approximate Eq. (1) using the data $x_1, \ldots, x_{n_{\text{sample}}} \sim \mu$ and $y_1, \ldots, y_{n_{\text{sample}}} \sim \nu$, and the filling points $\{(\tilde{x}_1, \tilde{y}_1), \ldots, (\tilde{x}_n, \tilde{y}_n)\} \subseteq X \times Y$. Indeed, we define $\hat{\mu} = \frac{1}{n_{\text{sample}}} \sum_{i=1}^{n_{\text{sample}}} \delta_{x_i}$ and $\hat{\nu} = \frac{1}{n_{\text{sample}}} \sum_{i=1}^{n_{\text{sample}}} \delta_{y_i}$, and use $\langle u, w_{\hat{\mu}} \rangle_{H_X} + \langle v, w_{\hat{\nu}} \rangle_{H_Y}$ instead of $\langle u, w_\mu \rangle_{H_X} + \langle v, w_\nu \rangle_{H_Y}$ where $w_{\hat{\mu}} = \frac{1}{n_{\text{sample}}} \sum_{i=1}^{n_{\text{sample}}} \phi_X(x_i)$ and $w_{\hat{\nu}} = \frac{1}{n_{\text{sample}}} \sum_{i=1}^{n_{\text{sample}}} \phi_Y(y_i)$. We also impose *the penalization terms* for u, v, and A to alleviate the error induced by sampling the corresponding equality constraints. Then, the resulting problem with regularization parameters $\lambda_1, \lambda_2 > 0$ is summarized as follows:

$$\begin{array}{ll} \max\limits_{u,v,A} & \langle u, w_{\hat{\mu}} \rangle_{H_X} + \langle v, w_{\hat{\nu}} \rangle_{H_Y} - \lambda_1 \mathrm{Tr}(A) - \lambda_2(\|u\|_{H_X}^2 + \|v\|_{H_Y}^2), \\ \text{s.t.} & \tfrac{1}{2}\|\tilde{x}_i - \tilde{y}_i\|^2 - u(\tilde{x}_i) - v(\tilde{y}_i) = \langle \phi_{XY}(\tilde{x}_i, \tilde{y}_i), A\phi_{XY}(\tilde{x}_i, \tilde{y}_i) \rangle_{H_{XY}}. \end{array} \tag{2}$$

Focusing on the case of $n_{\text{sample}} = \Theta(n)$, we let $\hat{u}_\star$ and $\hat{v}_\star$ be the unique maximizers of Eq. (2). Then, the estimator for $\mathrm{OT}(\mu, \nu)$ we consider corresponds to

$$\widehat{\mathrm{OT}}^n = \langle \hat{u}_\star, w_{\hat{\mu}} \rangle_{H_X} + \langle \hat{v}_\star, w_{\hat{\nu}} \rangle_{H_Y}. \tag{3}$$

Remark. It follows from [Vacher et al.(2021), Corollary 3] that the norm of empirical potentials can be controlled using $\lambda_1 = \tilde{\Theta}(n^{-1/2})$ and $\lambda_2 = \tilde{\Theta}(n^{-1/2})$ in high probability and the statistical rate is $\tilde{O}(n^{-1/2})$. Compared with plug-in OT estimators, the kernel-based OT estimators are better when sample size n is small (estimator is still tractable) and dimension d is large (statistical rates are $O(n^{-2/d})$ and $\tilde{O}(n^{-1/2})$ for plug-in and kernel-based estimators, respectively).

[1] We refer to $\mathbb{S}^+(H_{XY})$ as the set of linear, positive and self-adjoint operators on H_{XY}.

Remark. The entropic OT estimators achieve the rate of $\tilde{O}(n^{-1/2})$ for fixed ε [Genevay et al.(2019)]. Such a rate blows up exponentially fast to infinity as $\varepsilon \to 0$ if one wants to approximate non-regularized OT. Hence, entropic OT estimators are only statistically efficient for fixed, and fairly large, values of ε. In contrast, kernel-based OT estimators do not suffer from such a blow-up. While the constants depend exponentially in d, they are fixed, and the rate of $\tilde{O}(n^{-1/2})$ is valid for approximating non-regularized OT.

Eq. (2) is an infinite-dimensional problem and is thus difficult to solve. Thanks to [Vacher et al.(2021), Theorem 15], we have that the dual problem of Eq. (2) can be presented in a finite-dimensional space and strong duality holds true. Indeed, we define $Q \in \mathbb{R}^{n\times n}$ with $Q_{ij} = k_X(\tilde{x}_i, \tilde{x}_j) + k_Y(\tilde{y}_i, \tilde{y}_j)$, and $z \in \mathbb{R}^n$ with $z_i = w_{\hat{\mu}}(\tilde{x}_i) + w_{\hat{\nu}}(\tilde{y}_i) - \lambda_2\|\tilde{x}_i - \tilde{y}_i\|^2$, and $q^2 = \|w_{\hat{\mu}}\|^2_{H_X} + \|w_{\hat{\nu}}\|_{H_Y}$, where we have

$$\begin{array}{rcl} w_{\hat{\mu}}(\tilde{x}_i) & = & \frac{1}{n_{\text{sample}}}\sum_{j=1}^{n_{\text{sample}}} k_X(x_j, \tilde{x}_i), \\ w_{\hat{\nu}}(\tilde{y}_i) & = & \frac{1}{n_{\text{sample}}}\sum_{j=1}^{n_{\text{sample}}} k_Y(y_j, \tilde{y}_i), \\ \|w_{\hat{\mu}}\|^2_{H_X} & = & \frac{1}{n^2_{\text{sample}}}\sum_{1\le i,j\le n_{\text{sample}}} k_X(x_i, x_j), \\ \|w_{\hat{\nu}}\|^2_{H_Y} & = & \frac{1}{n^2_{\text{sample}}}\sum_{1\le i,j\le n_{\text{sample}}} k_Y(y_i, y_j). \end{array}$$

We define $K \in \mathbb{R}^{n\times n}$ with $K_{ij} = k_{XY}((\tilde{x}_i, \tilde{y}_i), (\tilde{x}_j, \tilde{y}_j))$ and R as an upper triangular matrix for the Cholesky decomposition of K. We let Φ_i be the i^{th} column of R. Then, the dual problem of Eq. (2) reads:

$$\begin{array}{ll} \min\limits_{\gamma\in\mathbb{R}^n} & \frac{1}{4\lambda_2}\gamma^\top Q\gamma - \frac{1}{2\lambda_2}\gamma^\top z + \frac{q^2}{4\lambda_2}, \\ \text{s.t.} & \sum_{i=1}^n \gamma_i \Phi_i \Phi_i^\top + \lambda_1 I \succeq 0. \end{array} \tag{4}$$

Suppose that $\hat{\gamma}$ is one such minimizer, we have

$$\widehat{\text{OT}}^n = \frac{q^2}{2\lambda_2} - \frac{1}{2\lambda_2}\sum_{i=1}^n \hat{\gamma}_i(w_{\hat{\mu}}(\tilde{x}_i) + w_{\hat{\nu}}(\tilde{y}_i)).$$

To the best of our knowledge, the only method proposed to solve Eq. (4) is the SSIPM, for which the required number of iterations is known to grow as n grows. To avoid this issue, [Muzellec et al.(2021)] proposed solving an unconstrained relaxation model, which allows for the application of gradient-based methods. However, the estimators obtained from solving such relaxations lack any statistical guarantee.

4 Method and Analysis

In this section, we derive our algorithm and provide a convergence rate analysis. We define first a suitable root function that is optimized by kernel-based OT, and apply the regularized SSN method. We improve the computation of each SSN step by exploring the special structure of the generalized Jacobian of that function. We also safeguard the regularized SSN method using a min-max method to achieve a global rate.

4.1 A nonsmooth equation model for kernel-based OT

We define the operator $\Phi : \mathbb{R}^{n\times n} \mapsto \mathbb{R}^n$ and its adjoint $\Phi^\star : \mathbb{R}^n \mapsto \mathbb{R}^{n\times n}$ as

$$\Phi(X) = \begin{pmatrix} \langle X, \Phi_1\Phi_1^T\rangle \\ \vdots \\ \langle X, \Phi_n\Phi_n^T\rangle \end{pmatrix}, \quad \Phi^\star(\gamma) = \sum_{i=1}^n \gamma_i \Phi_i \Phi_i^T.$$

Clearly, Eq. (4) can be reformulated as the following optimization problem given by

$$\min_{\gamma\in\mathbb{R}^n}\max_{X\in\mathcal{S}_+^n} \quad \tfrac{1}{4\lambda_2}\gamma^T Q\gamma - \tfrac{1}{2\lambda_2}\gamma^T z + \tfrac{q^2}{4\lambda_2} - \langle X, \Phi^\star(\gamma) + \lambda_1 I\rangle. \tag{5}$$

We denote $w = (\gamma, X)$ as a vector-matrix pair and let $R : \mathbb{R}^n \times \mathbb{R}^{n\times n} \to \mathbb{R}^n \times \mathbb{R}^{n\times n}$ be given by

$$R(w) = \begin{pmatrix} \frac{1}{2\lambda_2}Q\gamma - \frac{1}{2\lambda_2}z - \Phi(X) \\ X - \mathrm{proj}_{\mathcal{S}_+^n}(X - (\Phi^\star(\gamma) + \lambda_1 I)) \end{pmatrix}. \tag{6}$$

where $\mathcal{S}_+^n = \{X \in \mathbb{R}^{n\times n} : X \succeq 0, X^T = X\}$. Then, we measure the optimality of w by monitoring $\|R(w)\|$, as supported by the following proposition linking R to minimizers of Eq. (4).

Proposition 1. *A point $\hat{\gamma} \in \mathbb{R}^n$ is an optimal solution of Eq. (4) if and only if $\hat{w} = (\hat{\gamma}, \hat{X})$ satisfies $R(\hat{w}) = 0$ for some $\hat{X} \in \mathcal{S}_+^n$.*

Proposition 1 shows that we can recover a kernel-based OT estimator by solving the nonsmooth equation model $R(w) = 0$.

Regularized SSN method. Since R is Lipschitz, Rademacher's theorem guarantess that R is almost everywhere differentiable. We introduce generalized Jacobians [Clarke(1990)].

Definition 1. *Suppose R is Lipschitz and D_R is the set of differentiable points of R. The B-subdifferential at w is $\partial_B R(w) := \{\lim_{k\to+\infty} \nabla F(w^k) \mid w^k \in D_R, w^k \to w\}$ and the generalized Jacobian at w is $\partial R(w) = \mathrm{conv}(\partial_B R(w))$ where* conv *is the convex hull.*

The regularized SSN method for solving $R(w) = 0$ is as follows: Having the vector w_k, we compute $w_{k+1} = w_k + \Delta w_k$ where Δw_k is obtained by solving

$$(\mathcal{J}_k + \mu_k \mathcal{I})[\Delta w_k] = -r_k, \tag{7}$$

where $\mathcal{J}_k \in \partial R(w_k)$, $r_k = R(w_k)$ and $\mathcal{I}$ is the identity. The parameter is chosen as $\mu_k = \theta_k \|r_k\|$ to stabilize the SSN method in practice. If R is continuously differentiable and $\theta_k = 0$, the regularized SSN method reduces to the classical regularized Newton method which attains a local quadratic rate. Although the regularized SSN method is divergent in general [Kummer(1988)], its local superlinear rate has been proved if R is strongly semi-smooth [Qi and Sun(1993), Zhou and Toh(2005), Xiao et al.(2018)].

4.2 Properties of the nonsmooth map R

Generalized Jacobian. Let us focus on the structure of the generalized Jacobian of $R(w)$. Using the definition of $\mathcal{S}_+^n$, one has $\mathrm{proj}_{\mathcal{S}_+^n}(Z) = P_\alpha \Sigma_\alpha P_\alpha^T$ where

$$Z = P\Sigma P^T = \begin{pmatrix} P_\alpha & P_{\bar{\alpha}} \end{pmatrix} \begin{pmatrix} \Sigma_\alpha & 0 \\ 0 & \Sigma_{\bar{\alpha}} \end{pmatrix} \begin{pmatrix} P_\alpha^T \\ P_{\bar{\alpha}}^T \end{pmatrix}, \tag{8}$$

with $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, with the sets of indices of positive and nonpositive eigenvalues of Z written $\alpha = \{i \mid \sigma_i > 0\}$ and $\bar{\alpha} = \{1, \ldots, n\} \setminus \alpha$.

We define a generalized operator $\mathcal{M}(Z) \in \partial \mathrm{proj}_{\mathcal{S}_+^n}(Z)$ using its application to an $n \times n$ matrix S:

$$\mathcal{M}(Z)[S] = P(\Omega \circ (P^T S P))P^T \text{ for all } S \in \mathcal{S}_+^n,$$

Algorithm 1 Solving Eq. (7) where $r_k = (r_k^1, r_k^2)$

1: $a^1 = -r_k^1 - \frac{1}{\mu_k+1}(\Phi(r_k^2 + \mathcal{T}_k[r_k^2]))$ and $a^2 = -r_k^2$.
2: Solve $(\frac{1}{2\lambda_2}\mathcal{Q} + \mu_k\mathcal{I} + \Phi\mathcal{T}_k\Phi^\star)^{-1}\tilde{a}^1 = a^1$ inexactly and compute $\tilde{a}^2 = \frac{1}{\mu_k+1}(a^2 + \mathcal{T}_k[a^2])$, where $\mathcal{T}_k[\cdot]$ is computed using the trick [Zhao et al.(2010)].
3: Compute the direction $\Delta w_k = (\Delta w_k^1, \Delta w_k^2)$ by $\Delta w_k^1 = \tilde{a}^1$ and $\Delta w_k^2 = \tilde{a}^2 - \mathcal{T}_k[\Phi^\star(\tilde{a}^1)]$.

where the $\circ$ symbol denotes a Hadamard product and $\Omega = \begin{pmatrix} E_{\alpha\alpha} & \eta_{\alpha\bar{\alpha}} \\ \eta_{\alpha\bar{\alpha}}^T & 0 \end{pmatrix}$ with $E_{\alpha\alpha}$ being a matrix of ones and $\eta_{ij} = \frac{\sigma_i}{\sigma_i - \sigma_j}$ for all $(i,j) \in \alpha \times \bar{\alpha}$. Note that all entries of Ω lie in the interval $(0, 1]$. In general, it is nontrivial to characterize the generalized Jacobian $\partial R(w)$ exactly but we can compute an element $\mathcal{J}(w) \in \partial R(w)$ using $\mathcal{M}(\cdot)$ as defined before.

We next introduce the definition of the (strong) semismoothness of an operator.

Definition 2. *Suppose that R is Lipschitz, we say it is (strongly) semismooth at w if (i) R is directionally differentiable at w; and (ii) for any $\mathcal{J} \in \partial R(w + \Delta w)$, we let $\Delta w \to 0$ and have*

$$\begin{aligned} \text{(semismooth)} \quad & \tfrac{\|R(w+\Delta w) - R(w) - \mathcal{J}[\Delta w]\|}{\|\Delta w\|} \to 0, \\ \text{(strongly semismooth)} \quad & \tfrac{\|R(w+\Delta w) - R(w) - \mathcal{J}[\Delta w]\|}{\|\Delta w\|^2} \leq C. \end{aligned}$$

The following proposition characterizes the residual map given in Eq. (6) and guarantees that the SSN method is suitable to solve $R(w) = 0$.

Proposition 2. *The residual map R in Eq.* (6) *is strongly semismooth.*

4.3 Newton updates

We discuss how to compute the Newton direction Δw_k efficiently. From a computational point of view, it is not practical to solve the linear system in Eq. (7) exactly. Thus, we seek an approximation step Δw_k by solving Eq. (7) approximately such that

$$\|(\mathcal{J}_k + \mu_k\mathcal{I})[\Delta w_k] + r_k\| \leq \tau \min\{1, \kappa\|r_k\|\|\Delta w_k\|\}, \tag{9}$$

where $0 < \tau, \kappa < 1$ are some positive constants and $\|\cdot\|$ is defined for a vector-matrix pair $w = (\gamma, X)$ (i.e., $\|w\| = \|\gamma\|_2 + \|X\|_F$ where $\|\cdot\|_2$ is Euclidean norm and $\|\cdot\|_F$ is Frobenius norm). Since $\mathcal{J}_k$ in Eq. (7) is nonsymmetric and its dimension is large, we use the Schur complement formula to transform Eq. (7) into a smaller symmetric system. If we vectorize the vector-matrix pair[2] Δw, the operators $\mathcal{M}(Z)$ and Φ can be expressed as matrices:

$$M(Z) = \tilde{P}\Gamma\tilde{P}^T \in \mathbb{R}^{n^2 \times n^2}, \; A = \begin{pmatrix} \Phi_1^T \otimes \Phi_1^T \\ \vdots \\ \Phi_n^T \otimes \Phi_n^T \end{pmatrix} \in \mathbb{R}^{n \times n^2},$$

where $\tilde{P} = P \otimes P$ and $\Gamma = \mathrm{diag}(\mathrm{vec}(\Omega))$.

We next provide a key lemma on the matrix form of $\mathcal{J}_k + \mu_k I$ at a given iterate $w_k = (\gamma_k, X_k)$.

[2] If $w = (\gamma, X)$ is a vector-matrix pair, we define $\mathrm{vec}(w) = (\gamma; \mathrm{vec}(X))$ as its vectorization.

Lemma 1. *Given $w_k = (\gamma_k, X_k)$, we compute $Z_k = X_k - (\Phi^\star(\gamma_k) + \lambda_1 I)$ and use Eq. (8) to obtain P_k, Σ_k, α_k and $\bar{\alpha}_k$. We then obtain Ω_k, $\tilde{P}_k = P_k \otimes P_k$ and $\Gamma_k = \mathrm{diag}(\mathrm{vec}(\Omega_k))$. Then, the matrix form of $\mathcal{J}_k + \mu_k I$ is given by*

$$
\begin{aligned}
&(J_k + \mu_k I)^{-1} = C_1 B C_2, \text{ where} \\
&C_1 = \begin{pmatrix} I & 0 \\ -T_k A^T & I \end{pmatrix}, \quad C_2 = \begin{pmatrix} I & \frac{1}{\mu_k+1}(A + AT_k) \\ 0 & I \end{pmatrix}, \\
&B = \begin{pmatrix} (\frac{1}{2\lambda_2} Q + \mu_k I + AT_k A^T)^{-1} & 0 \\ 0 & \frac{1}{\mu_k+1}(I + T_k) \end{pmatrix},
\end{aligned}
$$

with $T_k = \tilde{P}_k L_k \tilde{P}_k^T$ where L_k is a diagonal matrix with $(L_k)_{ii} = \frac{(\Gamma_k)ii}{\mu_k+1-(\Gamma_k)_{ii}}$ and $(\Gamma_k)_{ii} \in (0, 1]$ is then denoted as the i^{th} diagonal entry of Γ_k.

As a consequence of Lemma 1, the solution of Eq. (7) can be obtained by solving one certain symmetric linear system with the matrix $\frac{1}{2\lambda_2} Q + \mu_k I + AT_k A^T$. We remark that this system is well-defined since both Q and $AT_k A^T$ are positive semidefinite and the coefficient μ_k is chosen such that $\frac{1}{2\lambda_2} Q + \mu_k I + AT_k A^T$ is invertible. This also shows that Eq. (7) is well-defined.

We define $\mathcal{T}_k$ and $\mathcal{Q}$ as the operator form of $T_k = \tilde{P}_k L_k \tilde{P}_k^T$ and Q and write $r_k = (r_k^1, r_k^2)$ explicitly where $r_k^1 \in \mathbb{R}^n$ and $r_k^2 \in \mathbb{R}^{n \times n}$. Then, we have

$$
\mathrm{vec}(a) = -\begin{pmatrix} I & \frac{1}{\mu_k+1}(A + AT) \\ 0 & I \end{pmatrix} \mathrm{vec}(r_k) \Longrightarrow \begin{cases} a^1 = -r_k^1 - \frac{1}{\mu_k+1}(\Phi(r_k^2 + \mathcal{T}_k[r_k^2])), \\ a^2 = -r_k^2. \end{cases}
$$

The next step consists in solving a new symmetric linear system and is given by

$$
\mathrm{vec}(\tilde{a}) = \begin{pmatrix} \left(\frac{Q}{2\lambda_2} + \mu_k I + AT_k A^T\right)^{-1} & 0 \\ 0 & \frac{1}{1+\mu_k}(I + T_k) \end{pmatrix} \mathrm{vec}(a),
$$

which leads to

$$
\begin{cases} \tilde{a}^1 = (\frac{1}{2\lambda_2}\mathcal{Q} + \mu_k \mathcal{I} + \Phi \mathcal{T}_k \Phi^\star)^{-1} a^1, \\ \tilde{a}^2 = \frac{1}{\mu_k+1}(a^2 + \mathcal{T}_k[a^2]). \end{cases}
$$

Compared to Eq. (7) whose matrix form has size $(n^2+n) \times (n^2+n)$, we remark that the one in the step above is smaller with the size of $n \times n$ and can be efficiently solved using conjugate gradient (CG) or symmetric quasi-minimal residual (QMR) methods [Kelley(1995), Saad(2003)]. The final step is to compute the Newton direction $\Delta w_k = (\Delta w_k^1, \Delta w_k^2)$ as follows,

$$
\mathrm{vec}(\Delta w_k) = \begin{pmatrix} I & 0 \\ -TA^T & I \end{pmatrix} \mathrm{vec}(\tilde{a}) \Longrightarrow \begin{cases} \Delta w_k^1 = \tilde{a}^1, \\ \Delta w_k^2 = \tilde{a}^2 - \mathcal{T}_k[\Phi^\star(\tilde{a}^1)]. \end{cases}
$$

It remains to provide an efficient manner to compute $\mathcal{T}_k[\cdot]$. Since $\mathcal{T}_k$ is defined as the operator form of $T = \tilde{P}_k L_k \tilde{P}_k^T$, we have

$$
\mathcal{T}_k[S] = P_k(\Psi_k \circ (P_k^T S P_k)) P_k^T,
$$

where Ψ_k is determined by μ_k and Ω_k: Indeed,

$$
\Omega_k = \begin{pmatrix} E_{\alpha_k \alpha_k} & \eta_{\alpha_k \bar{\alpha}_k} \\ \eta_{\alpha_k \bar{\alpha}_k}^T & 0 \end{pmatrix} \Longrightarrow \Psi_k = \begin{pmatrix} \frac{1}{\mu_k} E_{\alpha_k \alpha_k} & \xi_{\alpha_k \bar{\alpha}_k} \\ \xi_{\alpha_k \bar{\alpha}_k}^T & 0 \end{pmatrix},
$$

Algorithm 2 Our specialized SSN method

Input: τ, κ, $\alpha_2 \geq \alpha_1 > 0$, $\beta_0, \beta_1 < 1$, $\beta_2 > 1$ and $\underline{\theta}, \overline{\theta} > 0$.
Initialization: $v_0 = w_0 \in \mathbb{R}^n \times \mathcal{S}_+^n$ and $\theta_0 > 0$.
for $k = 0, 1, 2, \ldots$ **do**
  Update v_{k+1} from v_k using one-step EG.
  Select $\mathcal{J}_k \in \partial R(w_k)$.
  Solve the linear system in Eq. (7) approximately such that Δw_k satisfies Eq. (9).
  Compute $\tilde{w}_{k+1} = w_k + \Delta w_k$.
  Update θ_{k+1} in the adaptive manner.
  Set $w_{k+1} = \tilde{w}_{k+1}$ if $\|R(\tilde{w}_{k+1})\| \leq \|R(v_{k+1})\|$ is satisfied. Otherwise, set $w_{k+1} = v_{k+1}$.
end for

where we have $\xi_{ij} = \frac{\eta_{ij}}{\mu_k + 1 - \eta_{ij}}$ for any $(i,j) \in \alpha_k \times \bar{\alpha}_k$. Following [Zhao et al.(2010)], we use the decomposition $\mathcal{T}_k[S] = G + G^T$ where $U = P_k(:, \alpha_k)^T S$ and

$$G = P_k(:, \alpha_k)(\tfrac{1}{2\mu_k}(UP_k(:, \alpha_k))P_k(:, \alpha_k)^\top + \xi_{\alpha_k \bar{\alpha}_k} \circ (UP_k(:, \bar{\alpha}_k))P_k(:, \bar{\alpha}_k)^\top).$$

The number of flops for computing $\mathcal{T}_k[S]$ is $8|\alpha_k|n^2$. If $|\alpha_k| > \bar{\alpha}_k$, we use $\mathcal{T}_k[S] = \frac{1}{\mu_k} S - P_k((\frac{1}{\mu_k} E - \Psi_k) \circ (P_k^\top S P_k))P_k^\top$ with $8|\bar{\alpha}_k|n^2$ flops. Thus, we obtain an inexact solution of Eq. (7) efficiently whenever $|\alpha_k|$ or $|\bar{\alpha}_k|$ is small. We present the scheme for computing an inexact SSN direction in Algorithm 1. We propose a rule for updating θ_k where $\mu_k = \theta_k \|r_k\|$ will be used in Eq. (7). It is summarized as follows:

$$\theta_{k+1} = \begin{cases} \max\{\underline{\theta}, \beta_0 \theta_k\}, & \text{if } \rho_k \geq \alpha_2 \|\Delta w_k\|^2, \\ \beta_1 \theta_k, & \text{if } \alpha_1 \|\Delta w_k\|^2 \leq \rho_k < \alpha_2 \|\Delta w_k\|^2, \\ \min\{\overline{\theta}, \beta_2 \theta_k\}, & \text{otherwise.} \end{cases}$$

where $\rho_k = -\langle R(w_k + \Delta w_k), \Delta w_k \rangle$, $\beta_0 < 1, \beta_1, \beta_2 > 1$ and $\underline{\theta}, \overline{\theta} > 0$. Intuitively, θ_k can control the quality of Δw_k and the larger value of θ_k gives a slow yet stable convergence. The small value of $\frac{\rho_k}{\|\Delta w_k\|^2}$ implies that Δw_k is bad and we shall increase θ_k.

Remark. We see that the per-iteration cost is significantly reduced since we have shown that solving the linear system in Eq. (7) whose matrix form has size $(n^2+n) \times (n^2+n)$ can be equivalently reduced to solving a much smaller linear system whose matrix form has size $n \times n$. Such equivalent reduction is based on Lemma 1 whose proof is summarized in Appendix 5.3.

4.4 Algorithm

We summarize our approach in Algorithm 2. We generate a sequence of iterates by alternating between extragradient (EG) method [Facchinei and Pang(2007), Cai et al.(2022)] and the regularized SSN method.

We maintain an auxiliary sequence of iterates $\{v_k\}_{k \geq 0}$. This sequence is directly generated by the EG method for solving the min-max problem in Eq. (5) and is used to safeguard the regularized SSN method to achieve a global convergence rate. In particular, we start with $v_0 = w_0 \in \mathbb{R}^n \times \mathcal{S}_+^n$ and perform the k^{th} iteration as follows,

1. Update v_{k+1} from v_k via 1-step EG.

2. Update $\tilde{w}_{k+1}$ from w_k via 1-step regularized SSN.

3. Set $w_{k+1} = \tilde{w}_{k+1}$ if $\|R(\tilde{w}_{k+1})\| \leq \|R(v_{k+1})\|$ and $w_{k+1} = v_{k+1}$ otherwise.

Remark. The per-iteration cost would be $O(n^3)$ at worst case but it can be much cheaper in practice. Indeed, the $O(n^3)$ cost comes from exactly solving the $n \times n$ linear system.In contrast, the linear system at each IPM step becomes severely ill-conditioned as the barrier parameter decreases and the matrix factorization has to be done exactly to achieve high precision. Therefore, our method suffers from the same per-iteration cost as IPM at worst case but can be more flexible and efficient from a practical viewpoint.

Remark. Although computing such auxiliary sequence results in extra cost, we can argue that it is not an issue in both theory and practice. Indeed, Theorem 2 guarantees the existence of a local region where 1-step regularized SSN can reduce the residue norm at a quadratic rate. This implies that $\|R(\tilde{w}_{k+1})\| \leq \|R(v_{k+1})\|$ will always hold when k is sufficiently large and $w_{k+1} = v_{k+1}$ will not never hold. This encourages us to stop computing the auxiliary sequence after the iterates enter the local region and only perform the regularized SSN steps.

4.5 Convergence Analysis

We establish the convergence guarantee of Algorithm 2 in the following theorems.

Theorem 1. *Suppose that $\{w_k\}_{k\geq 0}$ is a sequence of iterates generated by Algorithm 2. Then, the residuals of $\{w_k\}_{k\geq 0}$ converge to 0 at a rate of $1/\sqrt{k}$, i.e., $\|R(w_k)\| = O(1/\sqrt{k})$.*

In the context of constrained convex-concave min-max optimization, [Cai et al.(2022)] has proved the $O(1/\sqrt{k})$ last-iterate convergence rate of the EG, matching the lower bounds [Golowich et al.(2020b), Golowich et al.(2020a)]. Since the kernel-based OT estimation can be solved as a min-max problem, the global convergence rate in Theorem 1 demonstrates the efficiency of Algorithm 2. It remains unclear whether or not we can improve these results by exploring special structure of Eq. (5).

Moreover, such global rate depends on the smoothness parameter of Eq. (5) rather than the condition number of original formulation of Eq. (4). The explicit dependence on λ_1 and λ_2 is unknown since the results of [Cai et al.(2022)] does not provide the dependence on these problem parameters.

Theorem 2. *Suppose that $\{w_k\}_{k\geq 0}$ is a sequence of iterates generated by Algorithm 2. Then, the residual norm at $\{w_k\}_{k\geq 0}$ converge to 0 at a quadratic rate, i.e., $\|R(w_{k+1})\| \leq C\|R(w_k)\|^2$ for some constant $C > 0$, if the initial point w_0 is sufficiently close to $w^\star$ with $R(w^\star) = 0$ and every element of $\partial R(w^\star)$ is invertible.*

Similar to classical Newton methods which are key ingredients for IPM, the regularized SSN methods enjoy the weak dependence on problem conditioning; see [Qi and Sun(1993)] for the details.

Remark. Our algorithm becomes inefficient when ϵ is small but has better dependence on n than IPM. This is more desirable since the large n is necessary to ensure good statistical approximation (see [Muzellec et al.(2021), Page 11-12] for details). Such trade-off between n and $1/\epsilon$ has occurred in the computation of plug-in estimators: despite worse dependence on $1/\epsilon$, the Sinkhorn method is recognized as more efficient than IPM in practice since many applications require low-accurate solution ($\epsilon \sim 10^{-2}$) when the sample size n is large. In addition, we remark that our algorithm does not downgrade the value of IPM since the latter one is more suitable when ϵ is small.

5 Deferred Proofs

5.1 Proof of Proposition 1

We first prove that $\hat{\gamma}$ is an optimal solution of Eq. (4) if $\hat{w} = (\hat{\gamma}, \hat{X})$ satisfies $R(\hat{w}) = 0$ for some $\hat{X} \succeq 0$. Indeed, by the definition of R from Eq. (6), we have

$$\tfrac{1}{2\lambda_2} Q\hat{\gamma} - \tfrac{1}{2\lambda_2} z - \Phi(\hat{X}) = 0, \tag{10}$$

and

$$\hat{X} - \mathrm{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) = 0. \tag{11}$$

By the definition of $\mathrm{proj}_{\mathcal{S}_+^n}$, we have

$$\langle X - \mathrm{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)), \mathrm{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X} + (\Phi^\star(\hat{\gamma}) + \lambda_1 I)\rangle \geq 0 \text{ for all } X \succeq 0.$$

Plugging Eq. (11) into the above inequality yields that

$$\langle X - \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0 \text{ for all } X \succeq 0.$$

By setting $X = 0$ and $X = 2\hat{X}$, we have $\langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \leq 0$ and $\langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0$. Thus, we have

$$\langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle = 0, \quad \langle X, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0 \text{ for all } X \succeq 0. \tag{12}$$

Suppose that $\gamma \in \mathbb{R}^n$ satisfies that $\Phi^\star(\gamma) + \lambda_1 I \succeq 0$, we have

$$\begin{aligned}
0 &\overset{(10)}{=} (\gamma - \hat{\gamma})^\top \left(\tfrac{1}{2\lambda_2} Q\hat{\gamma} - \tfrac{1}{2\lambda_2} z - \Phi(\hat{X})\right) \\
&= \left(\tfrac{1}{4\lambda_2}\gamma^\top Q\gamma - \tfrac{1}{2\lambda_2}\gamma^\top z\right) - \left(\tfrac{1}{4\lambda_2}\hat{\gamma}^\top Q\hat{\gamma} - \tfrac{1}{2\lambda_2}\hat{\gamma}^\top z\right) - \tfrac{1}{4\lambda_2}(\gamma - \hat{\gamma})^\top Q(\gamma - \hat{\gamma}) - (\gamma - \hat{\gamma})^\top \Phi(\hat{X}) \\
&\leq \left(\tfrac{1}{4\lambda_2}\gamma^\top Q\gamma - \tfrac{1}{2\lambda_2}\gamma^\top z\right) - \left(\tfrac{1}{4\lambda_2}\hat{\gamma}^\top Q\hat{\gamma} - \tfrac{1}{2\lambda_2}\hat{\gamma}^\top z\right) - (\gamma - \hat{\gamma})^\top \Phi(\hat{X})
\end{aligned}$$

Since $\Phi^\star$ is the adjoint of Φ, we have $(\gamma - \hat{\gamma})^\top \Phi(\hat{X}) = \langle \hat{X}, \Phi^\star(\gamma) - \Phi^\star(\hat{\gamma})\rangle$. By combining this equality with $\Phi^\star(\gamma) + \lambda_1 I \succeq 0$ and the first equality in Eq. (12), we have

$$(\gamma - \hat{\gamma})^\top \Phi(\hat{X}) = \langle \hat{X}, \Phi^\star(\gamma) + \lambda_1 I\rangle - \langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0.$$

Thus, we have

$$0 \leq \left(\tfrac{1}{4\lambda_2}\gamma^\top Q\gamma - \tfrac{1}{2\lambda_2}\gamma^\top z + \tfrac{q^2}{4\lambda_2}\right) - \left(\tfrac{1}{4\lambda_2}\hat{\gamma}^\top Q\hat{\gamma} - \tfrac{1}{2\lambda_2}\hat{\gamma}^\top z + \tfrac{q^2}{4\lambda_2}\right).$$

Combining the above inequality with the second inequality in Eq. (12) yields the desired result.

It suffices to prove that satisfies $R(\hat{w}) = 0$ for some $\hat{X} \succeq 0$ if $\hat{\gamma}$ is an optimal solution of Eq. (4). Indeed, we write that $\sum_{i=1}^n \hat{\gamma}_i \Phi_i \Phi_i^\top + \lambda_1 I \succeq 0$ and

$$\tfrac{1}{4\lambda_2}\hat{\gamma}^\top Q\hat{\gamma} - \tfrac{1}{2\lambda_2}\hat{\gamma}^\top z + \tfrac{q^2}{4\lambda_2} \leq \tfrac{1}{4\lambda_2}\gamma^\top Q\gamma - \tfrac{1}{2\lambda_2}\gamma^\top z + \tfrac{q^2}{4\lambda_2},$$

for all $\gamma \in \mathbb{R}^n$ satisfying that $\sum_{i=1}^n \gamma_i \Phi_i \Phi_i^\top + \lambda_1 I \succeq 0$. Then, the KKT condition guarantees that there exists some $\hat{X} \succeq 0$ satisfying that

$$\begin{aligned}
\textstyle\sum_{i=1}^n \hat{\gamma}_i \Phi_i \Phi_i^\top + \lambda_1 I &\succeq 0, \\
\tfrac{1}{2\lambda_2} Q\hat{\gamma} - \tfrac{1}{2\lambda_2} z - \Phi(\hat{X}) &= 0, \\
\langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle &= 0.
\end{aligned} \tag{13}$$

The first and third inequalities guarantee that

$$\langle X - \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I \rangle \geq 0 \text{ for all } X \succeq 0.$$

By letting $X = \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I))$, we have

$$\langle \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I \rangle \geq 0. \tag{14}$$

Recall that the definition of $\text{proj}_{\mathcal{S}_+^n}$ implies that

$$\langle X - \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)), \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X} + (\Phi^\star(\hat{\gamma}) + \lambda_1 I) \rangle \geq 0 \text{ for all } X \succeq 0.$$

By letting $X = \hat{X}$, we have

$$\|\text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X}\|^2 \leq \langle \hat{X} - \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)), \Phi^\star(\hat{\gamma}) + \lambda_1 I \rangle \overset{(14)}{\leq} 0.$$

Combining the above inequality with the second equality in Eq. (13) yields that

$$\tfrac{1}{2\lambda_2} Q\hat{\gamma} - \tfrac{1}{2\lambda_2} z - \Phi(\hat{X}) = 0, \qquad \hat{X} - \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) = 0.$$

Combining these inequalities with the definition of R implies $R(\hat{w}) = 0$ and hence the desired result.

5.2 Proof of Proposition 2

The strong semismoothness of R follows from the derivation given in [Sun and Sun(2002)] to establish the semismoothness of projection operators. Indeed, the projection over a positive semidefinite cone is guaranteed to be strongly semismooth [Sun and Sun(2002), Corollary 4.15]. Thus, we have that $\text{proj}_{\mathcal{S}_+^n}(\cdot)$ is strongly semismooth. Since the strong semismoothness is closed under scalar multiplication, summation and composition, the residual map R is strongly semismooth.

5.3 Proof of Lemma 1

As stated in Lemma 1, we compute $Z_k = X_k - (\Phi^\star(\gamma_k) + \lambda_1 I)$ and the spectral decomposition of Z_k (cf. Eq. (8)) to obtain P_k, Σ_k and the sets of the indices of positive and nonpositive eigenvalues α_k and $\bar{\alpha}_k$. We then compute Ω_k using Σ_k, α_k and $\bar{\alpha}_k$ and finally obtain that $\tilde{P}_k = P_k \otimes P_k$ and $\Gamma_k = \text{diag}(\text{vec}(\Omega_k))$. Thus, we can write the matrix form of $\mathcal{J}_k + \mu_k I$ as

$$J_k + \mu_k I = \begin{pmatrix} \frac{1}{2\lambda_2} Q + \mu_k I & -A \\ \tilde{P}_k \Gamma_k \tilde{P}_k^\top A^\top & \tilde{P}_k((\mu_k + 1)I - \Gamma_k)\tilde{P}_k^\top \end{pmatrix}.$$

For simplicity, we let $W_k = \tilde{P}_k \Gamma_k \tilde{P}_k^\top$ and $D_k = \tilde{P}_k((\mu_k + 1)I - \Gamma_k)\tilde{P}_k^\top$. Then, the Schur complement trick implies that

$$\begin{aligned} (J_k + \mu_k I)^{-1} &= \begin{pmatrix} \frac{1}{2\lambda_2} Q + \mu_k I & -A \\ W_k A^\top & D_k \end{pmatrix}^{-1} \\ &= \begin{pmatrix} I & 0 \\ -D_k^{-1} W_k A^\top & I \end{pmatrix} \begin{pmatrix} (\frac{1}{2\lambda_2} Q + \mu_k I + A D_k^{-1} W_k A^\top)^{-1} & 0 \\ 0 & D_k^{-1} \end{pmatrix} \begin{pmatrix} I & A D_k^{-1} \\ 0 & I \end{pmatrix}. \end{aligned}$$

Define $T_k = \tilde{P}_k L_k \tilde{P}_k^\top$ where L_k is a diagonal matrix with $(L_k)_{ii} = \frac{(\Gamma_k)_{ii}}{\mu_k + 1 - (\Gamma_k)_{ii}}$ and $(\Gamma_k)_{ii} \in (0, 1]$ is the i^{th} diagonal entry of Γ_k. By the definition of W_k and D_k, we have $D_k^{-1} = \frac{1}{\mu_k + 1}(I + T_k)$ and $D_k^{-1} W = T_k$. Using these two identities, we can further obtain that

$$(J_k + \mu_k I)^{-1} = \begin{pmatrix} I & 0 \\ -T_k A^\top & I \end{pmatrix} \begin{pmatrix} (\frac{1}{2\lambda_2} Q + \mu_k I + A T_k A^\top)^{-1} & 0 \\ 0 & \frac{1}{\mu_k + 1}(I + T_k) \end{pmatrix} \begin{pmatrix} I & \frac{1}{\mu_k + 1}(A + A T_k) \\ 0 & I \end{pmatrix}.$$

This completes the proof.

5.4 Proof of Theorem 1

We can see from the scheme of Algorithm 2 that

$$\|R(w_k)\| \leq \|R(v_k)\| \quad \text{for all } k \geq 0,$$

where the iterates $\{v_k\}_{k \geq 0}$ are generated by applying the extragradient (EG) method for solving the min-max optimization problem in Eq. (5). We also have that [Cai et al.(2022), Theorem 3] guarantees that $\|R(v_k)\| = O(1/\sqrt{k})$. Putting these pieces together yields that

$$\|R(w_k)\| = O(1/\sqrt{k}).$$

This completes the proof.

5.5 Proof of Theorem 2

We analyze the convergence property for one-step SSN step as follows,

$$w_{k+1} = w_k + \Delta w_k,$$

where $\mu_k = \theta_k \|R(w_k)\|$ and

$$\|(\mathcal{J}_k + \mu_k \mathcal{I})[\Delta w_k] + R(w_k)\| \leq \tau \min\{1, \kappa \|R(w_k)\| \|\Delta w_k\|\}. \tag{15}$$

Since R is strongly smooth (cf. Proposition 2), we have

$$\frac{\|R(w + \Delta w) - R(w) - \mathcal{J}[\Delta w]\|}{\|\Delta w\|^2} \leq C, \quad \text{as } \Delta w \to 0.$$

Since w_0 is sufficiently close to $w^\star$ with $R(w^\star) = 0$ and the global convergence guarantee holds (cf. Theorem 1), we have

$$\|R(w_k + \Delta w_k) - R(w_k) - \mathcal{J}_k[\Delta w_k]\| \leq 2C \|\Delta w_k\|^2.$$

which implies that

$$\|R(w_{k+1})\| = \|R(w_k + \Delta w_k)\| \leq \|R(w_k) + \mathcal{J}_k[\Delta w_k]\| + 2C \|\Delta w_k\|^2. \tag{16}$$

Plugging Eq. (15) into Eq. (16) yields that

$$\begin{aligned} \|R(w_{k+1})\| &\leq 2C \|\Delta w_k\|^2 + \mu_k \|\Delta w_k\| + \tau\kappa \|R(w_k)\| \|\Delta w_k\| \\ &\leq 2C \|\Delta w_k\|^2 + (\theta_k + \tau\kappa) \|R(w_k)\| \|\Delta w_k\|. \end{aligned} \tag{17}$$

Since w_0 is sufficiently close to $w^\star$ with $R(w^\star) = 0$ and every element of $\partial R(w^\star)$ is invertible, we have that there exists some $\delta > 0$ such that

$$\|(\mathcal{J}_k + \mu_k \mathcal{I})[\Delta w_k]\| \geq \delta \|\Delta w_k\|.$$

The above equation together with Eq. (15) yields that

$$\|\Delta w_k\| \leq \tfrac{1}{\delta}\|(\mathcal{J}_k + \mu_k \mathcal{I})[\Delta w_k]\| \leq \tfrac{1}{\delta}\left(1 + \tau\kappa\|\Delta w_k\|\right)\|R(w_k)\|. \tag{18}$$

Plugging Eq. (18) into Eq. (17) yields that

$$\|R(w_{k+1})\| \leq \|R(w_k)\|^2 \left(\tfrac{2C}{\delta^2}\left(1 + \tau\kappa\|\Delta w_k\|\right)^2 + \tfrac{\theta_k + \tau\kappa}{\delta}\left(1 + \tau\kappa\|\Delta w_k\|\right)\right)$$

Note that $\|\Delta w_k\| \to 0$ and θ_k is bounded. Thus, we have $\|R(w_{k+1})\| = O(\|R(w_k)\|^2)$. From the above arguments, we see that the quadratic convergence rate can be achieved if Algorithm 2 performs the SSN step when the initial iterate x_0 is sufficiently close to $w^\star$ with $R(w^\star) = 0$. This implies that the safeguarding steps will never affect in local sense where Algorithm 2 generates $\{w_k\}_{k\geq 0}$ by performing the SSN steps only. So Algorithm 2 achieves the local quadratic convergence. This completes the proof.

6 Concluding Remarks

We propose a nonsmooth equation model for computing kernel-based OT estimators and show that its special problem structure allows it to be solved in an efficient manner using a SSN method. Specifically, we propose a specialized SSN method that achieves low per-iteration cost by exploiting such structure, and prove a global sublinear rate and a local quadratic rate under standard regularity conditions. We hope this progress can motivate further improvements and/or modifications of kernel-based OT approaches.

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