A Further Related Works on Semismooth Newton Method

Semismooth Newton methods [58] are a modern class of remarkably powerful and versatile algorithms for solving constrained optimization problems with partial differential equations, variational inequalities, and related problems.

The notion of semi-smoothness was originally introduced by Mifflin [37] for real-valued functions and later extended to vector-valued mappings by Qi and Sun [47]. A pioneering work on the semismooth Newton method was due to Solodov and Svaiter [54], 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 [69] to the setting where the generalized Jacobian is not necessarily nonsingular.

Recently, the semismooth Newton method has 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 [68, 67], LASSO [30], nearest correlation matrix estimation [45], clustering [61], sparse inverse covariance selection [65] and composite convex minimization [64]. The closest works to ours is Liu et al. [33], who developed a fast semismooth Newton method to compute the plug-in optimal transport estimator by exploring the sparsity and multiscale structure of its linear programming formulation. To the best of our knowledge, this paper is the first to apply the semismooth Newton method to computing the kernel-based optimal transport estimator and prove the convergence rate guarantees.

B Proof of Proposition 2.3

We first prove that $\hat{\gamma}$ is an optimal solution of Eq. (2.4) 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. (2.6), we have

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

and

$$\hat{X} - \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) = 0. \tag{B.2}$$

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

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

Plugging Eq. (B.2) 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

$$\langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle = 0, \quad \langle X, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0 \text{ for all } X \succeq 0. \tag{B.3}$$

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

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

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. (B.3), 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. (B.3) 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. (2.4). Indeed, we follow Definition 2.1 and 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

$$\begin{array}{rcl} \sum_{i=1}^n \hat{\gamma}_i \Phi_i \Phi_i^\top + \lambda_1 I & \succeq & 0, \\ \frac{1}{2\lambda_2} Q\hat{\gamma} - \frac{1}{2\lambda_2} z - \Phi(\hat{X}) & = & 0, \\ \langle \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle & = & 0. \end{array} \tag{B.4}$$

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

$$\langle \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X}, \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \geq 0. \tag{B.5}$$

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

$$\|\text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)) - \hat{X}\|^2 \leq \langle \hat{X} - \text{proj}_{\mathcal{S}_+^n}(\hat{X} - (\Phi^\star(\hat{\gamma}) + \lambda_1 I)), \Phi^\star(\hat{\gamma}) + \lambda_1 I\rangle \overset{\text{(B.5)}}{\leq} 0.$$

Combining the above inequality with the second equality in Eq. (B.4) 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.

C Proof of Proposition 3.1

The strong semismoothness of R follows from the derivation given in Sun and Sun [56] to establish the semismoothness of projection operators. Indeed, the projection over a positive semidefinite cone is guaranteed to be strongly semismooth [56, 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.

D Proof of Lemma 3.2

As stated in Lemma 3.2, we compute $Z_k = X_k - (\Phi^\star(\gamma_k) + \lambda_1 I)$ and the spectral decomposition of Z_k (cf. Eq. (3.1)) 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

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

This completes the proof.

E Proof of Theorem 3.3

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. (2.5). We also have that Cai et al. [6, 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.

F Proof of Theorem 3.4

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

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

Since R is strongly smooth (cf. Proposition 3.1), 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 3.3), 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

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

Plugging Eq. (F.1) into Eq. (F.2) yields that

$$\begin{aligned}\|R(w_{k+1})\| &\leq 2C\|\Delta w_k\|^2 + \mu_k\|\Delta w_k\| + \tau\kappa\|R(w_k)\|\|\Delta w_k\| \\ &\leq 2C\|\Delta w_k\|^2 + (\theta_k + \tau\kappa)\|R(w_k)\|\|\Delta w_k\|.\end{aligned} \tag{F.3}$$

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. (F.1) yields that

$$\|\Delta w_k\| \leq \tfrac{1}{\delta}\|(\mathcal{J}_k + \mu_k\mathcal{I})[\Delta w_k]\| \leq \tfrac{1}{\delta}\left(1 + \tau\kappa\|\Delta w_k\|\right)\|R(w_k)\|. \tag{F.4}$$

Plugging Eq. (F.4) into Eq. (F.3) 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.

G Additional Experimental Results

We describe our setup for the experiment on the real-world 4i datasets from Bunne et al. [5]. Indeed, we draw the unperturbed/perturbed samples for training from 15 cell datasets as follows,

$$x_1, \ldots, x_{n_{\text{sample}}} \sim \mu_{\text{unperturb}}, \quad y_1, \ldots, y_{n_{\text{sample}}} \sim \nu^k_{\text{perturb}} \text{ for } 1 \leq k \leq 15.$$

where $x_i, y_i \in \mathbb{R}^{48}$ and $\mu_{\text{unperturb}}, \nu^k_{\text{perturb}}$ represent the unperturbed cells and k^{th} perturbed cells. For our algorithm, we generate 256 filling points and compare our method with the default implementation in `OTT` package [13]. Both our algorithm and `OTT` capture the OT map T from training samples. Then, we fix the number of test samples as $m = 200$ and use the OT distance to measure the differences between $\frac{1}{m}\sum_{j=1}^m \delta_{T(\hat{x}_j)}$ and $\frac{1}{m}\sum_{j=1}^m \delta_{\hat{y}_j}$, where $\hat{x}_1, \ldots, \hat{x}_m \sim \mu_{\text{unperturb}}$ and $\hat{y}_1, \ldots, \hat{y}_m \sim \nu^k_{\text{perturb}}$ are unperturbed/perturbed samples for testing. Figure 4 reports the results on 15 single-cell datasets.

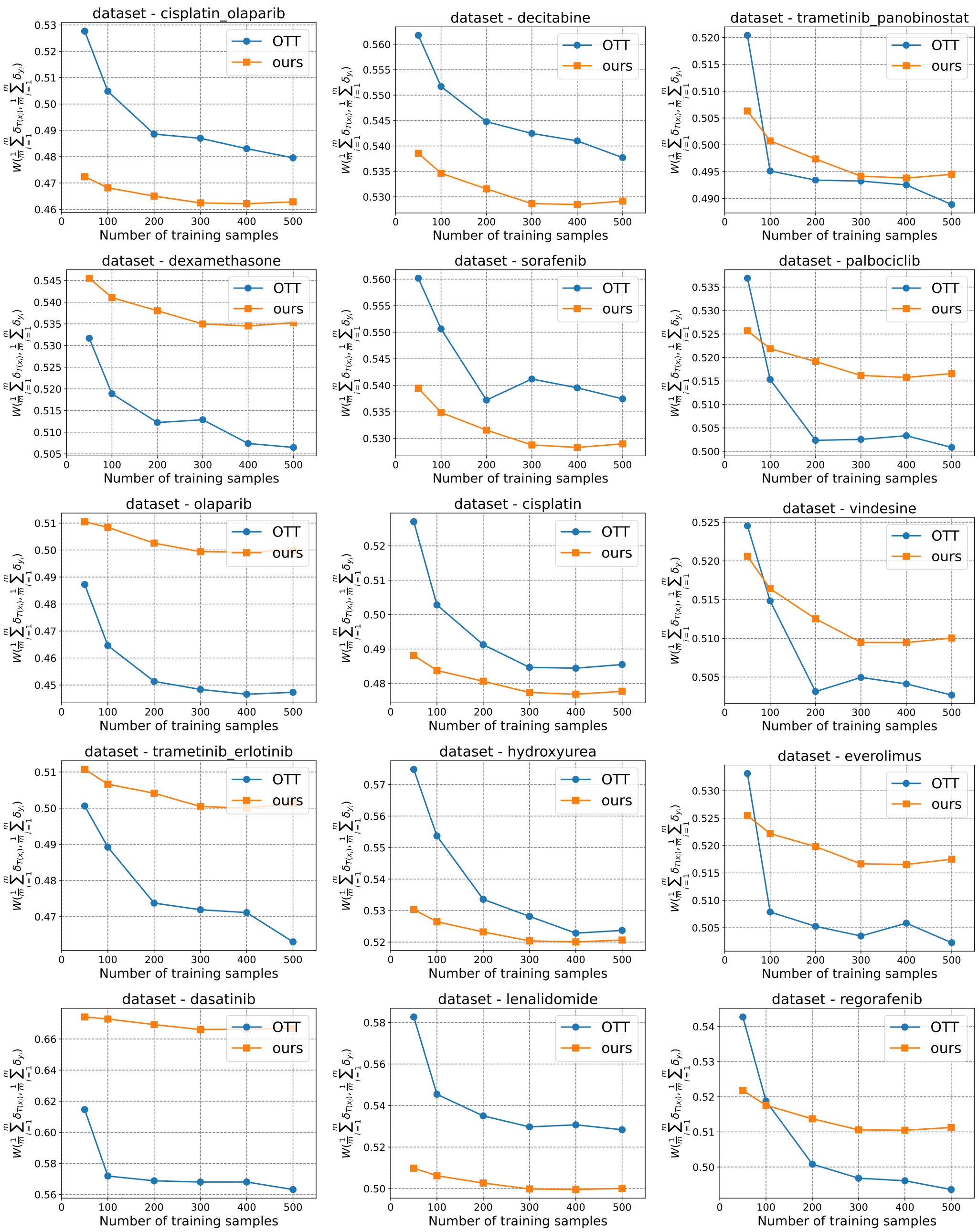

Figure 4: Performance of OTT and kernel-based OT estimators computed by our algorithm on 15 drug perturbation datasets. X-axis represent the number of training samples and Y-axis represents the error induced by OT map T on test samples in terms of OT distance.