A GLOBAL OPTIMIZATION APPROACH FOR MULTI-MARGINAL OPTIMAL TRANSPORT PROBLEMS WITH COULOMB COST

YUKUAN HU†, HUAJIE CHEN‡, AND XIN LIU†§

Abstract. In this work, we construct a novel numerical method for solving the multi-marginal optimal transport problems with Coulomb cost. This type of optimal transport problems arises in quantum physics and plays an important role in understanding the strongly correlated quantum systems. With a Monge-like ansatz, the original high-dimensional problems are transferred into mathematical programmings with generalized complementarity constraints, and thus the curse of dimensionality is surmounted. However, the latter ones are themselves hard to deal with from both theoretical and practical perspective. Moreover in the presence of nonconvexity, brute-force searching for global solutions becomes prohibitive as the problem size grows large. To this end, we propose a global optimization approach for solving the nonconvex optimization problems, by exploiting an efficient proximal block coordinate descent local solver and an initialization subroutine based on hierarchical grid refinements. We provide numerical simulations on some typical physical systems to show the efficiency of our approach. The results match well with both theoretical predictions and physical intuitions, and give the first visualization of optimal transport maps for some two dimensional systems.

Key words. Multi-marginal optimal transport; Coulomb cost; mathematical programming with generalized complementarity constraints; global optimization; grid refinement; optimal transport maps

AMS subject classifications. 49M37, 65K05, 81V05, 90C26, 90C30

1. Introduction. The aim of this paper is to provide an optimization method for the multi-marginal optimal transport (MMOT) problems [37, 44] arising in many-electron physics [11, 13, 42]. Let $d \in \{1, 2, 3\}$ be the dimension of system, $\Omega \subseteq \mathbb{R}^d$ be a bounded domain where the electrons are located, $N \in \mathbb{N}$ with $N \geq 2$ be the number of electrons and $\mathbf{r}_i \in \Omega \ (i \in \{1, \ldots, N\})$ be the position of the $i$-th electron. For the many-electron system, the MMOT problem with Coulomb cost reads

$$
\begin{align*}
\min_{\gamma} & \quad \int_{\Omega^N} c(\mathbf{r}_1, \ldots, \mathbf{r}_N) \gamma(\mathbf{r}_1, \ldots, \mathbf{r}_N) \, d\mathbf{r}_1 \cdots d\mathbf{r}_N \\
\text{subject to} & \quad (s. \ t. \ \Pi_i \gamma(\mathbf{r}) = \frac{1}{N} \rho(\mathbf{r}), \ \ i = 1, \ldots, N, \ \ \forall \mathbf{r} \in \Omega,
\end{align*}
$$

where the cost function $c(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is determined by the electron-electron Coulomb interaction

$$
c(\mathbf{r}_1, \ldots, \mathbf{r}_N) := \sum_{i<j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|},
$$

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†State Key Laboratory of Scientific and Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, and University of Chinese Academy of Sciences, China (email: ykh@lsec.cc.ac.cn, liuxin@lsec.cc.ac.cn).

‡School of Mathematical Sciences, Beijing Normal University, China (email: chen.huajie@bnu.edu.cn).

§Corresponding author.
\( \gamma(r_1, \ldots, r_N) \) is an \( N \)-point probability measure on \( \Omega^N \), with the single-electron density \( \rho : \Omega \to \mathbb{R} \) being the \( i \)-th marginal \( \Pi_i \gamma \), i.e. for any \( r \in \Omega \), \( \frac{1}{|r_i - r_j|} \) equals

\[
\Pi_i \gamma(r) := \int_{\Omega^{N-1}} \gamma(r_1, \ldots, r_{i-1}, r, r_{i+1}, \ldots, r_N) \, dr_1 \cdots dr_{i-1} \, dr_{i+1} \cdots dr_N.
\]

Note that the Coulomb interaction \( 1/|r_i - r_j| \) between the electrons in (1.2) can be approximated or regularized, especially in the simulations of systems with \( d < 3 \) [4, 19]. Nevertheless, the approach constructed in this paper will make no essential difference as long as the interaction between the electrons is repulsive (i.e. the cost decreases with respect to \( |r_i - r_j| \)). Therefore in this paper, we will focus ourselves on the Coulomb interaction of the form (1.2).

The MMOT problem (1.1) with Coulomb cost (1.2) arises as the strictly correlated electrons limit in the density functional theory (DFT). DFT has been most widely used for electronic structure calculations in physics, chemistry, and material sciences (see [3] for a review). The strictly correlated electrons limit was first introduced in [41], later noticed in [7, 12] that the limit problem is an optimal transport problem. The strictly correlated electrons limit provides an alternative route to derive the DFT energy functionals and has been exploited to extend the capability of DFT to treat strongly correlated quantum systems [9, 10, 21, 32, 34].

Direct discretization of the MMOT problem (1.1) leads to a linear programming, with the size increasing exponentially fast with respect to \( N \) (the number of electrons/marginals). There are several works devoted to numerical methods that try to circumvent the curse of dimensionality. In [5], the Sinkhorn scaling algorithm based on iterative Bregman projections was applied to an entropy-regularized discretized MMOT problem of 1D systems. In [7, 33], the numerical methods based on Kantorovich dual of the MMOT problem were proposed, while there are exponentially many constraints in the dual problem. In [29, 30], a convex relaxation approach was proposed by imposing certain necessary constraints satisfied by the two-marginal, and the relaxed problem was then solved by semidefinite programming to obtain tight lower bounds for the optimal cost. In [1, 2], the existence of sparse global solutions was established and a constrained overdamped Langevin process was proposed to solve the moment constrained relaxations. In [19, 20], the sparsity of optimal solution was rigorously justified and an efficient numerical method was proposed based on column generation and machine learning.

The starting point of this work is to approximate the \( N \)-point measure \( \gamma \) by the following ansatz

\[
\gamma(r_1, \ldots, r_N) = \frac{\rho(r_1)}{N} \gamma_2(r_1, r_2) \cdots \gamma_N(r_1, r_N),
\]

where \( \gamma_i : \Omega^2 \to \mathbb{R} \) (\( i \in \{2, \ldots, N\} \)) satisfies

\[
\gamma_i(r, r') \geq 0, \quad \int_{\Omega} \gamma_i(r, r') \, dr' = 1, \quad \text{and} \quad \int_{\Omega} \rho(r) \gamma_i(r, r') \, dr = \rho(r').
\]

Here we do not have \( \gamma_1 \) since \( \gamma_1(r, r') = \delta(r - r') \) by convention, where \( \delta \) is the Dirac delta function. The condition (1.5) is derived from the multi-marginal constraints (1.3). From a physical point of view, \( \gamma_i(r, r') \) represents the correlation between the first and the \( i \)-th electron, which gives the probability of finding the \( i \)-th electron at \( r' \) while the first electron is located at \( r \). Under ansatz (1.4), the MMOT problem (1.1) (with \( N > 2 \)) can be rewritten as
subsection 1.3 includes the Monge state into some finite dimensional Appendix A amounts to a spectacular dimension reduction, in that the unknowns $s_{42}^{10} = 2^{i}$ we can approximate the map. The Monge formulation gives significant information on the MMOT problem note the volumes of elements. Second, we approximate the marginal/electron mass on the space of non-overlapping elements, i.e. for any $j, k \in \{1, \ldots, K\}$, 
\begin{align}
    c_{jk} := \frac{1}{|e_j| \cdot |e_k|} \int_{e_j} \int_{e_k} \frac{1}{|r - r'|} \, dr \, dr' \\
    \text{and} \\
    x_{i,j,k} := \frac{1}{|e_j| \cdot |e_k|} \int_{e_j} \int_{e_k} \gamma_i(r, r') \, dr \, dr',
\end{align}
respectively, leading to $K \times K$ matrices $C := ((1 - a_{jk})c_{jk})_{jk}$ and $X_i = (x_{i,j,k})_{jk}$ for $i = 2, \ldots, N$. Here $a_{jk}$ equals 1 if $j = k$ and 0 otherwise. With this discretization, we can approximate (1.6) using the following optimization problem with unknowns \{$X_i\}_{i=2}^N$:
\begin{align}
    \min_{x_2, \ldots, x_N} \quad & f(x_2, \ldots, x_N) := \sum_{2 \leq i \leq N} \langle X_i, \Lambda \Xi C \Xi \rangle + \sum_{2 \leq i < j \leq N} \langle X_i, \Xi \Lambda X_j \Xi C \Xi \rangle \\
    \text{s. t.} \quad & X_i e = 1, \quad X_i^\top \Xi \varrho = \varrho, \quad \text{Tr}(X_i) = 0, \quad X_i \geq 0, \quad i = 2, \ldots, N, \\
    & \langle X_i, X_j \rangle = 0, \quad \forall \ i \neq j,
\end{align}
where $1$ is the all-one vector in $\mathbb{R}^K$, $\Lambda = \text{Diag}(\varrho)$, $\Xi = \text{Diag}(e)$ are $K \times K$ diagonal matrices formed by entries in $\varrho$ and $e$, respectively. More detailed derivation of (1.8) is given in Appendix A. Note that the diagonal elements in matrix $C$ are removed due to integral divergence in (1.7). The extra constraints
\begin{align}
    \text{Tr}(X_i) = 0, \quad i = 2, \ldots, N, \quad \text{and} \quad \langle X_i, X_j \rangle = 0, \quad \forall \ i \neq j
\end{align}
are hence accordingly added. From a physical point of view, this constraint can keep the electrons spatially away from each other in the case of Coulomb repulsion, so that unfavorable particle clustering can be avoided.
In the case of \( N = 3 \), (1.8) is a mathematical programming with complementarity constraints (MPCC) in view of nonnegative constraints and \( \langle X_2, X_3 \rangle = 0 \). Due to the disjunctive nature of feasible set, a general MPCC violates commonly used constraint qualifications at any feasible point [15]. As a result, the well-known Karush-Kuhn-Tucker conditions are no longer certificate for feasible points to be local minimizers. When \( N > 3 \), the formulation of the constraints in (1.8) is more complicated than that of the complementarity constraints. Since \( \langle X_i, X_j \rangle, \forall i \neq j \) impose the requirements that, for each \( i \in \{2, \ldots, N\} \), the block variable \( X_i \) complements all the other blocks, we call (1.8) a mathematical programming with generalized complementarity constraints (MPGCC).

In addition to its intrinsic difficulty, we are in quest for global solutions of (1.8). This is a hard matter because both the repulsive energy \( f \) and the feasible set are nonconvex in variables \((X_i)_{i=2}^N\). Since the degrees of freedom \((N-1)K^2\) grow quickly as the meshes become finer, the state-of-art global optimization solvers cannot be our last resort.

1.1. Optimization Background. Although little is known about MPGCC, there exists rich literature on MPCC. To overcome the intrinsic difficulties mentioned above, several MPCC-tailored constraint qualifications have been provided for MPCC. Under these constraint qualifications, points satisfying certain stationary systems are shown to be proper candidates of local minimizers. The related notions and theoretical results are gathered in \([38, 47]\) and the references within.

With these in place, researchers have proposed various numerical approaches, wherein those based on the original MPCC formulation rank top choices; they employ the modified nonlinear programming solvers. For example, the authors in [17] solved MPCCs using sequential quadratic programming algorithm with filter techniques [16]; the software introduced in [8, 45] incorporates a suite of nonlinear programming algorithms to tackle MPCCs, including interior-point methods and sequential quadratic programming algorithm, together with globalization techniques such as line search and trust region.

Owing to the troubles when coping with complementarity constraints, methods based on penalty functions gain popularity as well. Among others, we confine our attention to the \( \ell_1 \) (complementarity) penalty function, which favours direct extension to MPGCC (1.8) as

\[
(1.9) \quad f(X_2, \ldots, X_N) + \beta \sum_{i<j} \langle X_i, X_j \rangle,
\]

namely, penalizing merely the complementarity violation in \( \ell_1 \) form. Here \( f \) is the repulsive energy defined in (1.8), \( \beta > 0 \) is the penalty parameter. Apart from algorithmic benefit, with \( N = 3 \), it can be verified under certain conditions that the global solutions of (1.8) coincide with those globally minimizing (1.9) over \( S^{N-1} \), where

\[
(1.10) \quad S := \{ W \in \mathbb{R}^{K \times K} : We = 1, \ W^T \Xi q = q, \ \text{Tr}(W) = 0, \ W \geq 0 \}.
\]

A direct consequence is that, if the global solutions of (1.8) are required, one can in turn minimize (1.9) over \( S^{N-1} \) starting with proper initialization. However, we are not aware of any existing method that fully exploits the special structure of (1.9). A customized algorithm is thus needed, particularly in the large-scale context.

In addition, methods based on approximation (smoothing or regularization), augmented Lagrangian functions and full penalization are available as well. We refer interested readers to \([14, 25, 26, 27, 39, 40]\) and the references therein. Compared with
methods using modified nonlinear programming solvers or penalty functions, other approaches suffer from an obvious drawback: for a specific MPGCC, the latter ones require solving a sequence of subproblems in the same size to stationarity or even optimality [28]. This weakness excludes them from our choices, particularly when the number of grid points $K$ is tremendously large.

1.2. Contributions. Our contributions are three-fold:

1. A global optimization approach, equipped with a local solver and a hierarchical initialization subroutine, is constructed for solving (1.8).

   The initialization subroutine (Algorithm 2.2), derived from hierarchical grid refinements, helps the local solver locate good approximations of global solutions, and hence serves as the core of the proposed global optimization approach (Framework 2.1). The proposed approach saves one from brute-force solving large-scale (1.8) via plain global optimization methods. Remarkably in Framework 2.1, the optimal transport maps can be directly evaluated by the solutions, which is usually difficult in the context of Coulomb cost.

2. An inexact proximal block coordinate descent (PBCD) algorithm is proposed for locally minimizing (1.9) over $S^{N-1}$.

   The PBCD algorithm (Algorithm 2.3) acts as the local solver in Framework 2.1 and enjoys global convergence guarantee in the presence of iterate infeasibility (Theorem 3.3), which is not covered by existing works.

3. Simulations of optimal transport maps for some typical 1D and 2D systems.

   We consider systems with the number of electrons up to 7, and discretization with the number of grid points up to $1.6 \times 10^4$. The results are in line with both theoretical predictions and physical intuitions (section 4). We also give the first visualization of optimal transport maps for some 2D systems.

1.3. Further Remarks.

Monge formulations. It is unknown whether the MMOT problem (1.1) with Coulomb cost has a solution of the form (1.4). However, the ansatz (1.4) includes the Monge solutions, which are most widely studied in physics. The Monge formulation makes the ansatz

$$\gamma(r_1, \ldots, r_N) = \frac{\rho(r_1)}{N} \theta(r_2 - T_2(r_1)) \cdots \theta(r_N - T_N(r_1)),$$

where $\theta$ is the Dirac delta function, the transport map $T_i : \Omega \to \Omega$ ($i \in \{2, \ldots, N\}$) (we can prescribe $T_1(r) = r$ for completeness of notations) preserves the single-electron density $\rho$. The Monge solution has a simple physical interpretation: the many-electron repulsive energy is minimized at a state such that one electron at position $r$ can determine the positions of all other $N - 1$ electrons via $\{T_i\}_{i=2}^N$. It is known that for 1D systems, the Monge formulation gives the global solution of the MMOT problems [11, 12]. But in the general $d > 1$ and $N > 2$ cases, it is unknown whether there exists a minimizer of (1.1) in the form (1.4). Nevertheless, the Monge solution involves a lot of physical information of the many-electron system and can give rise to the Kantorovich potential (which is needed in applications for electronic structure); see [42, 43]. Therefore, the Monge solution is crucial for the MMOT problems in DFT, which is though still difficult to evaluate in the context of Coulomb cost. In our Framework 2.1, however, the optimal transport maps $\{T_i\}_{i=2}^N$ can be approximated by the transportation between elements in mesh. More precisely, let $a_j$ be the barycenter of the element $e_j$, then $T_i(a_j)$ ($i = 2, \cdots, N$) can be approximated by solution $(X_i)_{i=2}^N$.
as

\begin{equation}
T^K_i(a_j) := \frac{\sum_{1 \leq k \leq K} a_k x_{i,jk}}{\sum_{1 \leq l \leq K} x_{i,jl}}, \quad j = 1, \ldots, K, \quad i = 2, \ldots, N.
\end{equation}

**Symmetric constraints.** In physics, one is only interested in the measures that are symmetric with respect to \(\{r_i\}\) (as \(\gamma(r_1, \ldots, r_N)\) represents \(N\)-point position density of electrons, which is symmetric by the laws of quantum theory). More precisely, one requires that for any permutation \(\mathcal{P}\) on \(\{1, \ldots, N\}\), \(\gamma(r_1, \ldots, r_N) = \gamma(r_{\mathcal{P}(1)}, \ldots, r_{\mathcal{P}(N)})\). Although we do not have this symmetric restriction in the MMOT problem (1.1) and the ansatz (1.11) is in general not symmetric, dropping the restriction does not alter the minimum value. This is because we have a symmetric cost function \(c\) in (1.2) and equal marginal for any \(\Pi_i\gamma\) in (1.3). Hence each nonsymmetric \(\gamma\) can give a symmetric one with the same energy value by symmetrization \(\frac{1}{N!} \sum_{\mathcal{P}} \gamma(r_{\mathcal{P}(1)}, \ldots, r_{\mathcal{P}(N)})\). We do not have to impose the symmetric constraints in the optimization formulation (1.8).

**Discretization.** Most of the existing works discretize the MMOT problems with real space methods [5, 10]. Particularly, this paper discretizes (1.6) into (1.8) by representing the marginal \(\rho\) with piecewise finite elements and using effective cost coefficients obtained by integrating the continuous cost functions with respect to these elements. To further reduce the computational cost (i.e. use less grid points where the marginal is small), we choose the elements adaptively such that each element carries approximately the same marginal mass.

1.4. Outline. The rest of this paper is organized as follows. We introduce the global optimization approach in section 2, where the initialization subroutine (subsection 2.1) and the local solver (subsection 2.2) are detailed in order. Section 3 is dedicated to the rough statements of the convergence property of PBCD. We corroborate the proposed approach with numerical simulations on several typical systems in section 4. Finally, conclusions and discussions are drawn in section 5.

1.5. Notations. The image of a linear operator \(A\) is denoted by \(\text{Im}(A)\). The notation \(\|X\|_p\) gives the \(p\)-norm of matrix \(X\), while \(\|X\|_F\) yields its Frobenius norm. The components of matrices or vectors are indicated by subscripts, e.g. \(x_{ij}\). The inequality \(X \geq 0\) means \(x_{ij} \geq 0, \quad \forall \ i, j\).

The notation \(\delta_S\) represents the indicator function of set \(S\), namely \(\delta_S(x) = 0\) if \(x \in S\) otherwise \(\infty\). For the multi-block objective functions referred in this work (such as (1.8)), we occasionally adopt abbreviations in brackets. For example, \(f(X_{<i}, X_i, X_{>i})\) means \(f(X_2, \ldots, X_{i-1}, X_i, X_{i+1}, \ldots, X_N)\); abbreviations like \(X_{<i}\), \(X_{(i,j)}, X_{>j}\) represent aggregation of blocks with certain subscripts.

Regarding algorithm, we use (double) superscripts within bracket for iterates in outer (inner) loop; for instance, \(X^{(l)}\) is the iterate in the \(l\)-th outer iteration, \(X^{(l,k)}\) is the iterate in the \(k\)-th inner iteration of the \((l + 1)\)-th outer iteration.

2. A Global Optimization Approach for Solving (1.8). In light of ansatz (1.4), the original MMOT problem with Coulomb cost (1.1) is approximated by MPGCC (1.8). Violating commonly used constraint qualifications, MPGCC (1.8) itself is a hard nut to crack from both algorithmic design and theoretical analysis.
Rather, we concentrate on the $\ell_1$ penalized MPGCC (1.8), i.e.

$$
\begin{align*}
\min_{X_2, \ldots, X_N} & \quad f_\beta(X_2, \ldots, X_N) := f(X_2, \ldots, X_N) + \beta \sum_{i<j} \langle X_i, X_j \rangle \\
\text{s. t.} & \quad X_i \in \mathcal{S}, \ i = 2, \ldots, N,
\end{align*}
$$

where $f$ is the repulsive energy defined in (1.8), $\mathcal{S}$, defined in (1.10), stands for a section of feasible region. Problem (2.1) is a nonconvex quadratic programming problem, still NP-hard [36]. In the sequel, when we reference (2.1) and its solution in space $(\mathbb{R}^{K \times K})^{N-1}$, we simply say (2.1) and its solution with size $K$.

For practical purposes, a global solution of (2.1) is always required. Meanwhile, we notice that the degrees of freedom in (2.1), $(N - 1)K^2$, grow fast w.r.t. $K$. This prevents us from brute-force solving (2.1) by state-of-art global optimization methods (e.g. branch-and-bound and cutting plane algorithm) due to exponentially increasing running time.

Motivated by [5], we propose a global optimization approach GGR; see Framework 2.1. Here, “G” and “GR” stand for global optimization and the GR initialization subroutine based on hierarchical grid refinement, respectively. **GGR_Init** and **GGR_LS** are in turn referred to as the initial step invoking a global solver, and the subsequent step invoking a local solver. Framework 2.1 progresses step by step along with the process of mesh refinements.

**Framework 2.1** The GGR approach

**Require:** Oracle returning $R, e, \varrho$ in proper dimensions; global solver; local solver; the GR subroutine; initial mesh with $K^{(0)}$ elements $\{e_j^{(0)}\}$.

1: Set $l := 0$.

2: **GGR_Init:** use global solver to solve (2.1) with size $K^{(0)}$ and get $(X_i^{(0)})_{i=2}^N$.

3: **while** certain stopping criteria are not satisfied **do**

4: Refine the last mesh $\{e_j^{(l)}\}$ to $\{e_j^{(l+1)}\}$ with $K^{(l+1)}$ elements.

5: Modify $(X_i^{(l)})_{i=2}^N$ using the GR subroutine to obtain $(X_i^{(l,0)})_{i=2}^N$.

6: **GGR_LS**(l + 1): start local solver from $(X_i^{(l,0)})_{i=2}^N$ to solve (2.1) with size $K^{(l+1)}$ and get $(X_i^{(l+1)})_{i=2}^N$.

7: $l := l + 1$.

8: **end while**

9: **return** $(X_i^{(l)})_{i=2}^N \in (\mathbb{R}^{K^{(l)} \times K^{(l)}})^{N-1}$.

Justification on the usage of global solver in the initial step (**line 2 in Framework 2.1**) is in order. From the point of applicability, given initial size $K^{(0)}$ of moderate magnitude, globally solving (2.1) is amenable to state-of-art global optimization methods. Considering the necessity, the quality of constructed initial points largely depends on the solutions in the previous step. Hence it is a natural choice for us to invoke a global solver in the initial step. For our choices in implementation, please refer to subsection 4.1.

Without specification, the mesh refinements (**line 4 in Framework 2.1**) are done such that the coarse meshes are always embedded into the refined meshes. For more remarks, see subsection 1.3. Although the refinements are uniform in the numerical simulations of present work (subsections 4.2 and 4.3), practical implementations focus on the region where marginals vary violently. Nevertheless in the latter circumstances, our GGR approach still works.
In what follows, we leave the initialization subroutine part to subsection 2.1 and the local solver part to subsection 2.2, respectively.

2.1. Initialization Subroutine based on Grid Refinement. Brute-force global optimization of (2.1) becomes impracticable once $K$ grows large. One treatment for this is arming a local solver with good initialization. Roughly speaking, if the energy surface forms a basin around the global solution $(X_i)^{N}_{i=2}$, the local solver is able to find $(X_i)^{N}_{i=2}$ provided the initial point lies inside the basin near $(X_i)^{N}_{i=2}$. This subsection is devoted to the development of the GR subroutine for initialization (line 5 in Framework 2.1). In words, the GR subroutine passes the solution information of previous step on to the current one such that good initialization can be anticipated. Without this process, the located point by local solver is very likely not a global minimizer, resulting in bad solution afterwards.

We derive the GR subroutine from some 1D numerical experience: for a particular problem (given oracle of $R, e, \varrho$, the solutions with different sizes share “similar” patterns. This phenomenon suggests that we can construct an initial point based on the pattern reflected in the solution with a small size $K$. This point was also observed in [5], where the authors supplied a refinement strategy to meet the accuracy demand with relatively low cost for discretized 1D (1.1). Their strategy, however, remains to be explained rigorously and quantitatively. More importantly, they did not discuss the treatment in higher-dimensional context. In the following, we try to understand the “similarity” standing at optimal transport and then introduce the GR subroutine.

Basically, the proposed subroutine is applicable under any space dimension $d$.

Let us begin with 1D setting. Suppose we already have a finite elements mesh $\{e_j\}$ and a global solution $(X_i)^{N}_{i=2}$ of (2.1) with $X_i = (x_{i,jk})_{jk}$. Then for any $i \in \{2, \ldots, N\}$, $x_{i,jk} > 0$ means that mass of $x_{i,jk}$ is transported from $e_j$ to $e_k$ by transport $X_i$. For the problem with a doubly refined mesh $\{e_k\}$, the original $e_j, e_k$ correspond to $\tilde{e}_{2j-1}$ and $\tilde{e}_{2j}, \tilde{e}_{2k-1}$ and $\tilde{e}_{2k}$, respectively. Let $j_1 = 2j - 1$, $j_2 = 2j$, $k_1 = 2k - 1$, $k_2 = 2k$. A reasonable speculation is that there also exists certain mass transported from $\tilde{e}_{2j-1}, \tilde{e}_{2j}$ to $\tilde{e}_{2k-1}, \tilde{e}_{2k}$ by the new $\tilde{X}_i = (\tilde{x}_{i,mn})_{mn}$, i.e. $\tilde{x}_{i,jt,ku} > 0$, $t, u \in \{1, 2\}$, which happens to explain the similarity observed in [5]. See Figure 2.1 for illustration.

The above reasoning applies to any $d \in \mathbb{N}$. Suppose a finite elements mesh $\{e_j\}$ and a global solution $(X_i)^{N}_{i=2}$ are at hand, with $X_i = (x_{i,jk})_{jk}$. Then for any $i \in \{2, \ldots, N\}$, $x_{i,jk} > 0$ means that mass of $x_{i,jk}$ is transported from element $e_j$ to $e_k$ by transport $X_i$. After mesh refinement, the original $\{e_j\}$ becomes $\{\tilde{e}_j\}$; for each $j$, the original element $e_j$ is divided into $s_j$ parts: $e_j = \bigcup_{i=1}^{s_j} \tilde{e}_i$, and $\tilde{e}_j \bigcap \tilde{e}_{j'} = \emptyset$ when $j_1 \neq j_2$. A reasonable speculation is that there also exists certain mass transported from $\tilde{e}_{j_t}$ to $\tilde{e}_{k_u}$, where $t \in \{1, \ldots, s_j\}$, $u \in \{1, \ldots, s_k\}$. Accordingly in $\tilde{X}_i = (\tilde{x}_{i,mn})_{mn}$, there should be $\tilde{x}_{i,j_t,ku} > 0$, $s_j \times s_k$ positive entries in total. We make illustration for 2D case in Figure 2.2. Note that the coordinates in transport are rearranged from the 2D coordinates in mesh.

Based upon the above arguments, we derive the GR subroutine for initialization; see Algorithm 2.2.

2.2. Local Solver. The global solver and the GR subroutine make brute-force globally solving large-scale (2.1) unnecessary. Instead, we only need to provide a local solver (see line 6 in Framework 2.1). We assume the procedure is in the $(l+1)$-th iteration of Framework 2.1. This is the same in the sequel whenever talking about local solver.

Regarding algorithm design, the block structure of (2.1) reminds us of using splitting type methods. One natural choice is an $(N - 1)$-block cyclic PBCD; see
Algorithm 2.3. In PBCD, the $i$-th block problem merely depends on the $i$-th block variable $X_i$, while keeping other block variables their latest values, where $f_{\beta(l+1)}$ is defined in (2.1). Moreover, proximal term $\|X_i - X_{i}^{(l,k)}\|_F^2$ is added to the objective function such that the block problem admits unique global solution. Here $\sigma > 0$ is the proximal parameter.
```
Algorithm 2.2 The GR initialization subroutine

Require: Coarse mesh with $K$ elements $\{e_j\}$ and refined mesh with $\tilde{K}$ elements $\{\tilde{e}_k\}$; Solution of the previous step $(X_{i})^N_{i=2}$; scaling factor $r > 0$.

1: for $i = 2, \ldots, N$ do
2:   for $j = 1, \ldots, K$ do
3:     for $k = 1, \ldots, \tilde{K}$ do
4:       if $x_{i,jk} > 0$ then
5:         Find $\tilde{e}_{j,t}$, $t = 1, \ldots, s_j$ such that $e_j = \bigcup_{t=1}^{s_j} \tilde{e}_{j,t}$.
6:         Find $\tilde{e}_{k,u}$, $u = 1, \ldots, s_k$ such that $e_k = \bigcup_{u=1}^{s_k} \tilde{e}_{k,u}$.
7:         Set $\tilde{x}_{i,j,t,u} = r \cdot x_{i,jk}$ for $t \in \{1, \ldots, s_j\}$, $u \in \{1, \ldots, s_k\}$.
8:       end if
9:     end for
10:   end for
11: end for
12: return $(\tilde{X}_{i})^N_{i=2} \in (\mathbb{R}^{\tilde{K} \times K})^{N-1}$, where for any $i$, $\tilde{X}_i = (\tilde{x}_{i,mn})_{mn}$.

Algorithm 2.3 PBCD for (2.1)

Require: $R^{(l+1)}(X_{i}^{(l,0)}) \in \mathbb{R}^{K^{(l+1)} \times K^{(l+1)}}$, $i = 2, \ldots, N$; $e^{(l+1)}$, $\varrho^{(l+1)} \in \mathbb{R}^{K^{(l+1)}}$; $\beta^{(l+1)}$, $\sigma > 0$.

1: Set $k := 0$.
2: while certain stopping criteria are not satisfied do
3:   For $i = 2, \ldots, N$, inexactly solve
4:   \begin{equation}
   \min_{X^{\tilde{X}_{i}^{(l,k+1)}} \in S^{(l+1)}} f_{\beta^{(l+1)}}(X^{(l,k+1)}_{<i}, X^{(l,k)}_{i}, X^{(l,k)}_{>i}) + \frac{\sigma}{2} \|X_i - X_i^{(l,k)}\|_F^2
   \end{equation}
5:   to obtain $X_i^{(l,k+1)}$.
6:   $k := k + 1$.
7: end while
8: return $(X_{i}^{(l+1)})^N_{i=2} := (X_{i}^{(l,k)})^N_{i=2} \in (\mathbb{R}^{K^{(l+1)} \times K^{(l+1)}})^{N-1}$.
```

Zooming in on (2.2) in Algorithm 2.3, we find that the block problems are essentially strongly convex quadratic programmings, or more precisely, projecting a point onto $S^{(l+1)}$. Since the projection does not possess a closed-form expression, iterate infeasibility w.r.t. $(S^{(l+1)})^{N-1}$ is inevitable in Algorithm 2.3. On the one hand, this brings difficulties in analyzing the convergence; see section 3. On the other hand, there exist abundant algorithm resources for solving (2.2). For instance, we can extend the semismooth Newton-CG method proposed in [31] to tackle (2.2); see more discussions in subsection 4.1.

3. Convergence Analysis. In this section, we show the convergence of the PBCD algorithm (Algorithm 2.3) to first-order stationary points (Karush-Kuhn-Tucker (KKT) points) or global solutions of (2.1) in different settings. The definition of KKT points for (2.1) can be found in the supplementary material.

Since the convergence results are independent of the skeleton of the GGR approach (Framework 2.1), we omit outer iteration index in the superscripts as well as the specification on the problem size; e.g., use $X_i^{(k)}$ instead of $X_i^{(l,k)}$. For the sake of brevity,
we adopt the abbreviation \( Z^{(k)} := (X^{(k)}_i)_{i=2}^N \) and \( F(Z) := f_\beta(Z) + \sum_{i=2}^N \delta s_i(X_i) \), where \( f_\beta \) is defined in (2.1).

When the block problems are exactly solved, we can directly follow the results in [46] and obtain the following theorem.

**Theorem 3.1** (Global Convergence of Algorithm 2.3 – Exact Version). Let \( \sigma > 0 \), and \{Z^{(k)}\} be the sequence generated by Algorithm 2.3 where block problems are exactly solved. Then \{Z^{(k)}\} converges to a KKT point of (2.1). Moreover, \{Z^{(k)}\} converges to a global minimizer of (2.1) if the initial point \( Z^{(0)} \in S^{N-1} \) is sufficiently close to some global minimizer.

Since block exact solutions are not available in our case, we turn to study the global convergence property of Algorithm 2.3 allowing block problems to be solved inexactly; in particular, the iterates are permitted to be infeasible w.r.t. \( S^{N-1} \).

In the nonconvex context, existing convergence analyses of the PBCD algorithm restrict the iterates to be feasible, regardless of the complicate feasible set [6, 22]. Limitations as they have, their analyses pave way for our study. Before presenting the results, we define the block optimal sequence \{(X^{(k)}_i)_{i=2}^N\} as follows: for any \( i \in \{2, \ldots, N\} \),

\[
\bar{X}^{(k+1)}_i := \arg \min_{X_i \in S} f_\beta(X^{(k+1)}_i, X_{<i}^{(k)}, X_{>i}^{(k)}) + \frac{\sigma}{2} \|X_i - X^{(k)}_i\|_F^2.
\]

In other words, \( \bar{X}^{(k+1)}_i \) is the unique global solution of the \( i \)-th block problems (2.2) in Algorithm 2.3. For any \( k \), let \( \bar{Z}^{(k)} := (\bar{X}^{(k)}_i)_{i=2}^N \). To facilitate analysis, we need assumptions on the local solver and energy value sequence.

**Assumption 3.2** (Assumptions on the Local Solver and Energy Sequence).

1. \( \{F(\bar{Z}^{(k)})\} \) is non-increasing;
2. \( \sum_{k=1}^\infty \|\bar{Z}^{(k)} - Z^{(k)}\|_F < \infty \).

Since \( F \) is continuous over the compact \( S^{N-1} \), \( F \) must attains its infimum in \( S^{N-1} \). Hence Assumption 3.2 (1) actually yields that the sequence \{F(\bar{Z}^{(k)})\} converges to some \( \overline{F} \geq 0 \). Assumption 3.2 (2) lays restrictions on the local solver, in that the block problems (2.2) are solved more and more accurately.

Since the analysis is rather involved, we give a rough statement of the convergence result for the PBCD algorithm below. The formal statement and proof are left to the supplementary material.

**Theorem 3.3** (Convergence Property of Algorithm 2.3 – Inexact Version). Suppose Assumption 3.2 holds and \( \sigma \) is sufficiently large. Let \{Z^{(k)}\} be the sequence generated by Algorithm 2.3, \{\bar{Z}^{(k)}\} be the sequence defined in (3.1). Assume also that \( F(Z^{(k)}) > \overline{F}, \forall k \geq 1 \). Then

1. the sequence \{Z^{(k)}\} converges to a KKT point of (2.1);
2. if further \( \sum_{k=1}^\infty \|\bar{Z}^{(k)} - Z^{(k)}\|_F \) is small enough, \( Z^{(0)} \) is feasible and sufficiently close to some global minimizer, then \{Z^{(k)}\} converges to a global minimizer of (2.1).

4. Numerical Experiments. In this section, we validate the proposed GGR approach via numerical simulations on several typical systems, including both 1D and 2D systems. During the experiments, we mainly monitor the repulsive energy \( f \) in (1.8) (denoted by \( E \)). We also calculate the approximated transport maps \{T^{(k)}_i\}_{i=2}^N \) as in (1.12), and in turn evaluate the quality of solution through the average error
(denoted by err)

$$\text{err}(K, \Omega) := \frac{1}{K |\Omega|} \sum_{i=1}^{K} \sum_{j=2}^{N} |T_j(a_i) - T^K_j(a_i)|,$$

if the optimal transport maps \( \{T_i\}_{i=2}^{N} \) are already available. We refer interested readers to supplementary material for the numerical comparison among local solvers proposed in [8, 17, 45] and PBCD.

All the numerical experiments presented here are run in a platform with Intel(R) Xeon(R) Gold 6242R CPU @ 3.10GHz and 510GB RAM running MATLAB R2018b under Ubuntu 20.04.

4.1. Default Settings.

Global solver. Considering the applicability and efficiency, we take the stochastic method, random multi-start, as global solver for 1D systems, and employ software BARON for 2D systems. The implementation of random multi-start follows [24]. The software BARON invokes efficient random multi-start procedures initially, and then carries out branch-and-bound and cutting plane algorithm for global optimization. Version 21.1.13 of BARON is available in the downloadable AMPL system [18].

Details in PBCD. We adapt the semi-smooth Newton-CG (SSNCG) method in [31] to solve the dual block problems. A general iteration in SSNCG consists of approximately solving a sparse symmetric positive definite linear system of the form

$$(\mathcal{V}^{(l+1)} + \varepsilon I) d + r^{(l+1)} = 0, \quad d \in \text{Im}(\mathcal{B}^{(l+1)}),$$

and then performing line searches along direction \( d \) for a sufficient reduction on dual objective. Here \( \mathcal{B}^{(l+1)} \) is a linear operator defined as

$$\mathcal{B}^{(l+1)}(W) = [(\mathcal{E}^{(l+1)})^\top W^\top (\mathcal{G}^{(l+1)})^\top \mathcal{X}^{(l+1)}W \quad \text{Tr}(W)],$$

\( \mathcal{V}^{(l+1)} \) is a positive semidefinite operator associated with \( \mathcal{B}^{(l+1)} \), \( \varepsilon > 0 \), \( I \) stands for an identity matrix in proper dimension for convenience, and \( r^{(l+1)} \) is the residual vector. In our context, the linear system can be solved quickly to desirability by the preconditioned conjugate gradient method equipped with block Jacobi preconditioner.

Parameter setting. In the GR subroutine, we set scaling value \( r = 1 \). In all experiments, we fix \( \sigma = 10^{-3} \), \( \text{maxit} = 10^6 \) in PBCD. For different \( K \), we choose \( \beta \) according to Table 4.1. We invoke SSNCG for block problems in PBCD. The maximum

| \( K \)          | (0, 10) | (10, 36) | (36, 80) | (80, 160) | (160, 320) |
|-----------------|--------|---------|---------|----------|-----------|
| \( \beta \)     | 2\(^2\) | 2\(^1\) | 2\(^0\) | 2\(^{-2}\) | 2\(^{-3}\) |

| \( K \)          | (320, 640) | (640, 1280) | (1280, 2560) | (2560, 5120) | (5120, \( \infty \)) |
|-----------------|-----------|-------------|-------------|-------------|----------------|
| \( \beta \)     | 2\(^{-4}\) | 2\(^{-5}\) | 2\(^{-6}\) | 2\(^{-7}\) | 2\(^{-8}\) |

SSNCG iteration number is set to \( \text{maxitSSN} = 10^5 \). We start SSNCG from zero point in the first call; after that, we perform \text{walt start}. 


Stopping criteria. We terminate SSNCG if feasibility violation

\begin{equation}
\text{Feas}(Z) = \sum_{i=2}^{N} \|B^{(l+1)}(X_i) - y^{(l+1)}\|_2
\end{equation}

is smaller than \( \varepsilon_{\text{inner}} = 10^{-9} \) in all cases, where \( B^{(l+1)} \) is the linear operator defined in (4.1) and \( b^{(l+1)} = [1^T (\phi^{(l+1)})^T 0]^T \). We stop PBCD when the scaled difference of two consecutive iterate \( \sqrt{\pi} \|Z^{(l,k+1)} - Z^{(l,k)}\|_F \) is less than a prescribed value \( \varepsilon_{\text{outer}} \), which is chosen as

\begin{equation}
\varepsilon_{\text{outer}} = \begin{cases} 
10^{-8}, & K^{(l+1)} \in (0, 200], \\
10^{-6}, & K^{(l+1)} \in (200, 2000], \\
10^{-5}, & K^{(l+1)} \in (2000, 10000], \\
10^{-4}, & K^{(l+1)} \in (10000, \infty),
\end{cases}
\end{equation}

or, when the absolute value of the difference between two consecutive energies is less than \( 10^{-8} \).

4.2. Numerical Results on 1D Systems. We first consider some typical 1D systems with our GGR approach. In the simulations, we use “equal-mass” discretization of the marginal for the initial mesh, in that each element in mesh carries the same marginal mass. This can be achieved cheaply and exactly for 1D systems. The meshes are refined uniformly afterwards.

The first three systems under consideration all consist of 3 particles \( (N = 3) \), whose single-electron densities (marginals) are given by

\begin{align*}
\rho_1(x) &= c_1 (\cos(\pi x) + 1), & \Omega = [-1, 1], \\
\rho_2(x) &= c_2 (2e^{-6(x+0.5)^2} + 1.5e^{-4(x-0.5)^2}), & \Omega = [-1, 1], \\
\rho_3(x) &= c_3 e^{-|x|}, & \Omega = [-5, 5],
\end{align*}

respectively, with \( c_i, \ i = 1, 2, 3 \), the normalization constants such that \( \int_\Omega \rho_i(x) \, dx = 3 \). The number of grid points used for the initial meshes is \( K^{(0)} = 12 \) for all three systems. The single-electron densities (marginals) and the approximated transport maps \( \{T_i^k\} \) (1.12) are shown in Figure 4.1. The convergence of the GGR approach can be observed as the meshes being refined. Note that explicit solutions of the original MMOT problems are known for 1D systems [42], our results can match the theory perfectly. We also list the output energies and the calculated average errors (the “\text{err}_{\text{e}}” column) at each step in Table 4.2 (a), supporting the efficiency of our approach.

The second set includes three systems, each of which contains 7 particles \( (N = 7) \). Note that this particle number is already intractable if one tries to solve the original MMOT problem (1.1) directly. The single-electron densities (marginals) are given by

\begin{align*}
\rho_4(x) &= c_4 e^{-x^2}, & \Omega = [-2, 2], \\
\rho_5(x) &= c_5 (e^{-3(x+3)^2} + e^{-3(x+2)^2} + e^{-2(x+1)^2} + e^{-x^2} + e^{-2(x-1)^2} + e^{-3(x-2)^2} + e^{-3(x-3)^2}), & \Omega = [-4, 4], \\
\rho_6(x) &= c_6 (e^{-8(x+2.7)^2} + e^{-8(x+2.025)^2} + e^{-8(x+1.35)^2} + e^{-8(x+0.675)^2} + e^{-5(x-0.5)^2} + e^{-5(x-1.5)^2} + e^{-5(x-2.5)^2}), & \Omega = [-3, 3],
\end{align*}
respectively, with $c_i$, $i = 4, 5, 6$, the normalization constants such that $\int_{\Omega} \rho_i(x) \, dx = 7$. The last two examples can be viewed as systems with localized electrons, where each Gaussian represents the distribution of an electron. The number of grid points used for the initial meshes is $K^{(0)} = 14$ for these three systems.

We show the single-electron densities (marginals) and the convergence of the GGR approach during the mesh refinements in Figure 4.2. We also list the output energies and the calculated average errors at each step in Table 4.2 (b). We observe from the numerical results that the iterates given by our GGR approach converge well to the correct solutions.
Fig. 4.2. Marginals (the first row) and approximated transport maps (the remaining four rows) in 1D $N = 7$ systems; left to right: systems with $\rho_4, \rho_5, \rho_6$. The maps in the last four rows correspond to rows in Table 4.2 (b) where $K = 14, 56, 224, 896$. The blue, red, black, green, brown and purple dots are images of $T^K_i, i = 2, \ldots, 7$ over grid barycenters, respectively.

To show that the GR subroutine yields high-quality initialization, we compute the average errors of the initial points (the “err_s” column) as well; the notation “-” in the GGR_Init step indicates no initial point is fed to global solver. The decreasing err_s’s underline the efficacy of the GR subroutine, which boosts the GGR approach and helps us find global solutions. Incidentally, the comparison between err_s and err_e in the same row highlights the improvements due to the local solver PBCD. Meanwhile, one can see that err_e is sometimes slightly larger than err_s. In these cases, PBCD eliminates infeasibility while inheriting the high quality of initial points.
4.3. Numerical results on 2D systems. We then consider some 2D systems with the GGR approach. We use the finite elements package FreeFEM [23] to generate the initial meshes for the marginal discretization. The meshes are non-uniform such that every element carries almost the same mass. In the later loops of the GGR approach, each element is refined in the same manner.

The two systems under consideration both consist of 3 particles ($N = 3$), whose single-electron densities (marginals) are given by

\[
\rho_{\tau}(x, y) = c_{7}\left(e^{-2.5((x, y)-(1.5, 0))^2} + 0.5e^{-2.5((x, y)-(1.5, 0))^2}\right), \quad \Omega = [-3, 3] \times [-2, 2],
\]

\[
\rho_{\delta}(x, y) = c_{8}\left(e^{-2.5((x, y)-(0, 0.96))^2} + e^{-2.5((x, y)-(0, 0.96))^2}\right), \quad \Omega = [-2.5, 2.5]^2,
\]

respectively, with $c_i$, $i = 7, 8$, the normalizing factors such that $\int_{\Omega} \rho_{\tau}(x, y) \, dx \, dy = 7$. For the first 2D system, $\rho_{\tau}$ corresponds to a system that has two electrons located on the left part of $\Omega$ (represented by the first Gaussian centered at $(-1.5, 0)$), and the third electron located on the right part (represented by the second Gaussian centered at $(1.5, 0)$). For the second 2D system, $\rho_{\delta}$ corresponds to a system that has three electrons concentrated on three different sites $(-1.032, -0.84)$, $(0, 0.96)$ and $(1.032, -0.84)$ (represented by three Gaussians), respectively. The electron densities (marginals) and the corresponding initial meshes (obtained by FreeFEM) are shown in the first two rows of Figure 4.3. The numbers of grid points used for the initial meshes are $K^{(0)} = 240$ for $\rho_{\tau}$ and $K^{(0)} = 170$ for $\rho_{\delta}$, respectively. After three steps in Framework 2.1, we reach $K^{(3)} = 15360$ for $\rho_{\tau}$ and $K^{(3)} = 10880$ for $\rho_{\delta}$, respectively.

To show our results on the 2D systems, in the remaining three rows of Figure 4.3, we plot the images of the barycenters of triangular elements within some given regions $\omega \subset \Omega$, where $T_{3}^{K}$ and $T_{3}^{K}$ are the approximated transport maps (1.12) given by the GGR approach. For the two-Gaussian system $\rho_{\tau}$, the pictures show that: if the first electron is around the left Gaussian center, then the third electron will go to the region near the right Gaussian center, and the second electron will lie in the left part.
In system 7-8, we calculated $K$ to 15360 and 10880, respectively. The gray, blue and green circles are pre-images $\omega \subseteq \Omega$, $T_2^K(\omega)$ and $T_3^K(\omega)$, respectively.

**Table 4.3**

| Step     | System 7 |   | System 8 |   |
|----------|----------|---|----------|---|
|          | $K$      | E |          | $K$| E  |
| GGR_{Init} | 240 | 9.503 | 170 | 9.491 |
| GGR_{LS(1)} | 960 | 9.577 | 680 | 9.533 |
| GGR_{LS(2)} | 3840 | 9.598 | 2720 | 9.543 |
| GGR_{LS(3)} | 15360 | 9.604 | 10880 | 9.546 |

**Fig. 4.3.** Contours of marginals (the first row), initial meshes (the second row) and slices of approximated transport maps (the third-fifth row) in 2D systems; left to right: systems with $\rho_7, \rho_8$. In system 7-8, we calculated $K$ to 15360 and 10880, respectively. The gray, blue and green circles are pre-images $\omega \subseteq \Omega$, $T_2^K(\omega)$ and $T_3^K(\omega)$, respectively.
(to satisfy the marginal constraints) but stay away from the first one \((\omega \text{ and } T_2^K(\omega))\) lie in two different regions around the left Gaussian center); if one electron is located around the right Gaussian center, then the other two electrons will be around the left Gaussian center while keeping distance away from each other. For the three-Gaussian system \(\rho_8\), we can see that if one electron is located around one of the Gaussian centers, then the other two electrons go to the other two Gaussian centers, respectively. We also list the output energies at each step in Table 4.3. Though there are no theoretical results for comparison, our simulations match physical intuitions quite well and can support the reliability of our approach.

5. Conclusions. In the present work, we consider the MMOT problem with Coulomb cost arising in quantum physics. The Monge-like ansatz tides us over curse of dimensionality, in that the number of unknowns scales linearly w.r.t. the number of electrons, however resulting in MPGCC. In quest for global solutions, we propose a global optimization approach GGR for dealing with the derived MPGCC. The GGR approach solves the problem step by step along with the process of mesh refinement, and is equipped with an initialization subroutine such that global solutions are amenable to the proposed local solver PBCD. The convergence property of PBCD is established in the presence of iterate infeasibility. We corroborate the merits of the GGR approach with numerical simulations on several typical 1D and 2D physical systems. Notably, we obtain solutions with high resolution in the 1D cases, and visualize the optimal transport maps in the 2D context.

Appendix A. Discretization of (1.6).

For the repulsive energy in (1.6), we have for any \(i \in \{2, \ldots, N\}\),

\[
\int_{\Omega} \int_{\Omega} \frac{\rho(r) \gamma_i(r, r')}{|r - r'|} \, dr \, dr' = \sum_{j,k} \int_{e_k} \int_{e_j} \frac{\rho(r) \gamma_i(r, r')}{|r - r'|} \, dr \, dr'.
\]

Note when \(k = j\), the integral explodes and hence we impose \(x_{i,k}^j = 0\), \(\forall k\) as extra constraints to avoid numerical instability. In the sequel derivation, we take \(\gamma_i(r, r') = 0\) whenever \(r\) and \(r'\) belong to the same element:

\[
\int_{\Omega} \int_{\Omega} \frac{\rho(r) \gamma_i(r, r')}{|r - r'|} \, dr \, dr' = \sum_{j \neq k} \int_{e_k} \int_{e_j} \frac{\rho(r) \gamma_i(r, r')}{|r - r'|} \, dr \, dr' \\
= \sum_{j \neq k} q_j x_{i,j} \int_{e_k} \int_{e_j} \frac{1}{|r - r'|} \, dr \, dr' + O(h) \\
(A.1)
= \sum_{j \neq k} q_j x_{i,j} k r_{j} |e_j| |e_k| + O(h) = \langle X_i, \Lambda \Xi C \Xi \rangle + O(h),
\]

where \(h := \|e\|_{\infty}\) represents the size of the largest element. By similar reasoning, we can write for any \(i, j \in \{2, \ldots, N\} : i \neq j\),

\[
\int_{\Omega} \int_{\Omega} \int_{\Omega} \frac{\rho(r) \gamma_i(r, r') \gamma_i(r, r''')}{|r - r'''|} \, dr \, dr' \, dr'' \\
= \sum_{m,n,t \neq \ell} q_m x_{i,mn} x_{j,mt} |e_m| |e_n| |e_t| + O(h) \\
(A.2)
= \langle X_i, \Lambda \Xi X_j \Xi C \Xi \rangle + O(h).
\]
Note that we have excluded \( n = t \) cases and impose \( \langle X_i, X_j \rangle = 0 \) as extra complementarity constraints. By (A.1) and (A.2), the repulsive energy in (1.6) can be approximated by
\[
\sum_{2 \leq i \leq N} \langle X_i, \Lambda \Xi C \Xi \rangle + \sum_{i<j} \langle X_i, \Xi \Lambda X_j \Xi C \Xi \rangle,
\]
with error depending on the size of the largest element.

Regarding normalizing and marginal constraints in (1.5), we can see from similar derivation that, for any \( i \in \{2, \ldots, N\} \),
\[
1 = \frac{1}{|e_j|} \int_{e_j} 1 \, dr = \frac{1}{|e_j|} \int \int_{\Omega} \gamma_i(r, r') \, dr \, dr' = \sum_{k=1}^{K} x_{i,jk} |e_k|, \quad \forall j,
\]
\[
g_k = \frac{1}{|e_k|} \int_{e_k} \rho(r') \, dr' = \frac{1}{|e_k|} \int \int_{\Omega} \rho(r) \gamma_i(r, r') \, dr \, dr' = \sum_{j=1}^{K} g_{j,x_{i,jk}} |e_j| + O(h), \quad \forall k.
\]
Consequently, the constraints in (1.5) can be approximated using
\[
X_i e = 1, \quad X_i^T \Xi \rho = \rho, \quad \forall i \in \{2, \ldots, N\}.
\]

REFERENCES

[1] A. Alfonsi, R. Coyaud, and V. Ehrlacher, Constrained overdamped Langevin dynamics for symmetric multimarginal optimal transportation, Feb. 2021, https://arxiv.org/abs/2102.03091.

[2] A. Alfonsi, R. Coyaud, V. Ehrlacher, and D. Lombardi, Approximation of optimal transport problems with marginal moments constraints, Math. Comp., 90 (2021), pp. 689–737, https://doi.org/10.1090/mcom/3568.

[3] A. Becke, Perspective: fifty years of density-functional theory in chemical physics, J. Chem. Phys., 140 (2014), 18A301 (18 pages), https://doi.org/10.1063/1.4869598.

[4] S. Bednarek, B. Szafran, T. Chwiej, and J. Adamowski, Effective interaction for charge carriers confined in quasi-one-dimensional nanostructures, Phys. Rev. B, 68 (2003), 045328 (9 pages), https://doi.org/10.1103/PhysRevB.68.045328.

[5] J.-D. Benamou, G. Carlier, and L. Nenna, A numerical method to solve multi-marginal optimal transport problems with Coulomb cost, in Splitting Methods in Communication, Imaging, Science, and Engineering, Springer, Cham, 2016, p. 577–601, https://doi.org/10.1007/978-3-319-41589-5_17.

[6] J. Bolte, S. Sabach, and M. Teboulle, Proximal alternating linearized minimization for nonconvex and nonsmooth problems, Math. Program., 146 (2014), pp. 459–494, https://doi.org/10.1007/s10107-013-0701-9.

[7] G. Buttazzo, L. Pascale, and P. Gori-Giorgi, Optimal-transport formulation of electronic density-functional theory, Phys. Rev. A, 85 (2012), 062502 (11 pages), https://doi.org/10.1103/PhysRevA.85.062502.

[8] R. Byrd, J. Nocedal, and R. Waltz, Knitro: an integrated package for nonlinear optimization, in Large-Scale Nonlinear Optimization, Springer, Boston, MA, 2006, pp. 35–59, https://doi.org/10.1007/0-387-30065-1_4.

[9] H. Chen and G. Friesecke, Pair densities in density functional theory, Multiscale Model. Simul., 13 (2015), pp. 1259–1289, https://doi.org/10.1137/15M1014024.

[10] H. Chen, G. Friesecke, and C. Mendl, Numerical methods for a Kohn-Sham density functional model based on optimal transport, J. Chem. Theory Comput., 10 (2014), pp. 4360–4368, https://doi.org/10.1021/ct400585q.

[11] M. Colombo, L. Pascale, and S. Marino, Multimarginal optimal transport maps for one-dimensional repulsive costs, Can. J. Math., 67 (2015), pp. 350–368, https://doi.org/10.4153/CJM-2014-011-x.

[12] C. Cotar, G. Friesecke, and C. Klüppelberg, Density functional theory and optimal transport with Coulomb cost, Commun. Pure Appl. Math., 66 (2013), pp. 548–599, https://doi.org/10.1002/cpa.21437.
[13] C. Cotar, G. Friesecke, and B. Pass, Infinite-body optimal transport with Coulomb cost, Calc. Var., 54 (2015), pp. 717–742, https://doi.org/10.1007/s00526-014-0803-0.

[14] F. Facchinei, H. Jiang, and L. Qi, A smoothing method for mathematical programs with equilibrium constraints, Math. Program., 85 (1999), pp. 107–134, https://doi.org/10.1007/s10107990015a.

[15] M. Flegel and C. Kanzow, On the Guignard constraint qualification for mathematical programs with equilibrium constraints, Optimization, 54 (2005), pp. 517–534, https://doi.org/10.1080/02331930500342591.

[16] R. Fletcher and S. Leyffer, Nonlinear programming without a penalty function, Math. Program., 91 (2002), pp. 239–269, https://doi.org/10.1007/s101070100244.

[17] R. Fletcher and S. Leyffer, Solving mathematical programs with complementarity constraints as nonlinear programs, Optim. Methods Softw., 19 (2004), pp. 15–40, https://doi.org/10.1080/10556780410001654241.

[18] R. Fourer, D. Gay, and B. Kernighan, A modeling language for mathematical programming, Manage. Sci., 36 (1990), pp. 519–641, https://doi.org/10.1287/mnsc.36.5.519.

[19] G. Friesecke, A. Schulz, and D. Vögler, Genetic column generation: fast computation of high-dimensional multi-marginal optimal transport problems, Mar. 2021, https://arxiv.org/abs/2103.12624.

[20] G. Friesecke and D. Vögler, Breaking the curse of dimension in multi-marginal Kantorovich optimal transport on finite state spaces, SIAM J. Math. Anal., 50 (2018), pp. 3996–4019, https://doi.org/10.1137/17M1150025.

[21] J. Grossi, D. Kooi, K. Giesbertz, M. Seidl, A. Cohen, P. Mori-Sánchez, and P. Gori-Giorgi, Fermionic statistics in the strongly correlated limit of density functional theory, J. Chem. Theory Comput., 13 (2017), pp. 6089–6100, https://doi.org/10.1021/acs.jctc.7b00998.

[22] E. Gur, S. Sabach, and S. Sibert, Convergent nested alternating minimization algorithms for non-convex optimization problems. https://ssabach.net.technion.ac.il/files/2020/11/GSS2020-1.pdf, 2020.

[23] F. Hecht, New development in freefem++, J. Numer. Math., 20 (2012), pp. 251–265, https://doi.org/10.1515/jnum-2012-0013, https://freefem.org/.

[24] F. Hickernell and Y. Yuan, A simple multistart algorithm for global optimization, Operations Research Transactions (China), 1 (1997), pp. 1–12, http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.46.1346.

[25] T. Hoheisel, C. Kanzow, and A. Schwartz, Theoretical and numerical comparison of relaxation methods for mathematical programs with complementarity constraints, Math. Program., 137 (2013), pp. 257–288, https://doi.org/10.1007/s10107-011-0488-5.

[26] X. Hu and D. Ralph, Convergence of a penalty method for mathematical programming with complementarity constraints, J. Optim. Theory Appl., 123 (2004), pp. 365–390, https://doi.org/10.1023/B:JOTA.0000027044.47565.0f.

[27] X. Jia, C. Kanzow, P. Mehitz, and G. Wachsmuth, An augmented Lagrangian method for optimization problems with structured geometric constraints, May 2021, https://arxiv.org/abs/2105.08217.

[28] C. Kanzow and A. Schwartz, The price of inexactness: convergence properties of relaxation methods for mathematical programs with complementarity constraints revisited, Math. Oper. Res., 40 (2015), pp. 253–275, https://doi.org/10.1287/moor.2014.0667.

[29] Y. Khoo, L. Lin, M. Lindsey, and L. Ying, Semidefinite relaxation of multimarginal optimal transport for strictly correlated electrons in second quantization, SIAM J. Comput., 42 (2020), pp. B1462–B1489, https://doi.org/10.1137/20M1310977.

[30] Y. Khoo and L. Ying, Convex relaxation approaches for strictly correlated density functional theory, SIAM J. Sci. Comput., 41 (2019), pp. B773–B795, https://doi.org/10.1137/18M1207478.

[31] X. Li, D. Sun, and K.-C. Toh, On the efficient computation of a generalized Jacobian of the projector over the Birkhoff polytope, Math. Program., 179 (2020), pp. 419–446, https://doi.org/10.1007/s10107-018-1342-9.

[32] F. Malet and P. Gori-Giorgi, Strong correlation in Kohn-Sham density functional theory, Phys. Rev. Lett., 109 (2012), 246402 (5 pages), https://doi.org/10.1103/PhysRevLett.109.246402.

[33] C. Mendl and L. Lin, Kantorovich dual solution for strictly correlated electrons in atoms and molecules, Phys. Rev. B, 87 (2013), 125106 (6 pages), https://doi.org/10.1103/PhysRevB.87.125106.

[34] C. Mendl, F. Malet, and P. Gori-Giorgi, Wigner localization in quantum dots from Kohn-Sham density functional theory without symmetry breaking, Phys. Rev. B, 89 (2014),
A GLOBAL OPTIMIZATION APPROACH FOR MMOT

125106 (8 pages), https://doi.org/10.1103/PhysRevB.89.125106.

[35] G. Monge, Mémoire sur la Théorie des Déblais et des Remblais, Histoire Acad. Sciences, 1781.

[36] P. Pardalos and S. Vavasis, Quadratic programming with one negative eigenvalue is NP-hard, J. Glob. Optim., 1 (1991), pp. 15–22, https://doi.org/10.1007/BF00120662.

[37] F. Santambrogio, Optimal Transport for Applied Mathematicians, Birkhäuser, Cham, 2015, https://doi.org/10.1007/978-3-319-20828-2.

[38] H. Schöel and S. Scholtes, Mathematical programs with complementarity constraints: stationarity, optimality, and sensitivity, Math. Oper. Res., 25 (2000), pp. 1–22, https://doi.org/10.1287/moor.25.1.15213.

[39] S. Scholtes, Convergence properties of a regularization scheme for mathematical programs with complementarity constraints, SIAM J. Optim., 11 (2001), pp. 918–936, https://doi.org/10.1137/S1052623499361233.

[40] S. Scholtes and M. Stöhr, Exact penalization of mathematical programs with equilibrium constraints, SIAM J. Control Optim., 37 (1999), pp. 617–652, https://doi.org/10.1137/S0363012996300121.

[41] M. Seidl, Strong-interaction limit of density-functional theory, Phys. Rev. A, 60 (1999), pp. 4387–4395, https://doi.org/10.1103/PhysRevA.60.4387.

[42] M. Seidl, P. Gori-Giorgi, and A. Savin, Strictly correlated electrons in density-functional theory: a general formulation with applications to spherical densities, Phys. Rev. A, 75 (2007), 042511 (12 pages), https://doi.org/10.1103/PhysRevA.75.042511.

[43] M. Seidl, S. Marino, A. Gerolin, L. Nenna, K. Giesbertz, and P. Gori-Giorgi, The strictly-correlated electron functional for spherically symmetric systems revisited, Feb. 2017, https://arxiv.org/abs/1702.05022.

[44] C. Villani, Optimal Transport: Old and New, vol. 338, Springer, Berlin, Heidelberg, 2009, https://doi.org/10.1007/978-3-540-71050-9.

[45] R. Waltz, J. Morales, J. Nocedal, and D. Orban, An interior algorithm for nonlinear optimization that combines line search and trust region steps, Math. Program., 107 (2006), pp. 391–408, https://doi.org/10.1007/s10107-004-0560-5.

[46] Y. Xu and W. Yin, A block coordinate descent method for regularized multiconvex optimization with applications to nonnegative tensor factorization and completion, SIAM J. Imaging Sci., 6 (2013), pp. 1758–1789, https://doi.org/10.1137/120887795.

[47] J. Ye, Necessary and sufficient optimality conditions for mathematical programs with equilibrium constraints, J. Math. Anal. Appl., 307 (2005), pp. 350–369, https://doi.org/10.1016/j.jmaa.2004.10.032.
We provide technical results on \textbf{PBCD} in sections SM1 to SM3. Section SM1 is dedicated to some preliminaries, containing optimality conditions of the problem to be solved, some necessary definitions and key tools for convergence analysis. The proof ingredients and main results are detailed in sections SM2 and SM3, respectively.

Section SM4 is devoted to the numerical comparison among local solvers, Knitro, \texttt{filtermpec} and our proposed \textbf{PBCD}. The former two are nonlinear programming based solvers whose performance comparison on a benchmark is available online\(^1\).

The analysis and description hereinafter are irrelevant to the skeleton of the GGR approach. Therefore we make abbreviations on the superscripts and omit specification on size $K$. For example, we replace $Z_{(l,k)}$ with $Z^{(k)}$.

For better readability, we restate some frequently referenced things. The problem to be solved by local solver \textbf{PBCD} is

\begin{equation}
\begin{aligned}
\min_{X_2, \ldots, X_N} f_\beta(X_2, \ldots, X_N) \quad \text{s. t. } B(X_i) &= b, X_i \geq 0, \ i = 2, \ldots, N, \\
\end{aligned}
\end{equation}

where the repulsive energy

\begin{equation}
f_\beta(X_2, \ldots, X_N) = \sum_{2 \leq i \leq N} \langle X_i, \Lambda \Xi C \Xi \rangle + \sum_{i < j} \langle X_i, \Xi \Lambda X_j \Xi \rangle + \beta \sum_{i < j} \langle X_i, X_j \rangle,
\end{equation}

the linear operator $B : \mathbb{R}^{K \times K} \rightarrow \mathbb{R}^{2K+1}$ is defined as

\begin{equation}
B(W) = \left[ e^\top W^\top \quad \varrho^\top \Xi W \quad \text{Tr}(W) \right]^\top, \quad \forall \ W \in \mathbb{R}^{K \times K},
\end{equation}

and the vector $b = [1^\top \varrho^\top 0]^\top \in \mathbb{R}^{2K+1}$.

The \textbf{PBCD} algorithm solves (SM0.1) iteratively in a Gauss-Seidel style, i.e. in each cycle inexactly solves the block problem

\begin{equation}
\begin{aligned}
\min_{X_i \in S} f_\beta(X_i^{(k+1)}; X_i, X_{\neq i}^{(k)}) + \frac{\sigma}{2} \| X_i - X_i^{(k)} \|^2_F \\
\end{aligned}
\end{equation}

to obtain $X_i^{(k+1)}$ for $i = 2, \ldots, N$, where $S := \{ W \in \mathbb{R}^{K \times K} : B(W) = b, W \geq 0 \}$.

The block optimal sequence \( \{ Z^{(k)} := (X_i^{(k)})_{i=2}^N \} \) is cast as

\begin{equation}
\bar{X}_i^{(k+1)} := \arg \min_{X_i \in S} f_\beta(X_i^{(k+1)}; X_i, X_{\neq i}^{(k)}) + \frac{\sigma}{2} \| X_i - X_i^{(k)} \|^2_F, \quad \forall \ i = 2, \ldots, N.
\end{equation}

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\item [†] State Key Laboratory of Scientific and Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, and University of Chinese Academy of Sciences, Beijing (email: ykhu@lsec.cc.ac.cn, liuxin@lsec.cc.ac.cn).
\item [‡] School of Mathematical Sciences, Beijing Normal University, China (email: chen.huajie@bnu.edu.cn).
\item [§] Corresponding author.
\item [1] See \url{http://plato.asu.edu/ftp/mpec.html}.
\end{itemize}
To facilitate the convergence analysis on PBCD, we make assumptions on energy value and local solver below.

**Assumption SM0.1** (Assumptions on the Local Solver and Energy Sequence).

1. \(\{F(Z^{(k)})\}\) is non-increasing and hence converges to some \(F > 0\);
2. \(\sum_{k=1}^{\infty} \|Z^{(k)} - Z^{(k)}\|_F < \infty\).

**SM1. Preliminaries.** In what follows, we briefly go through the first-order stationary conditions of \(\text{(SM0.1)}\) (Lemma SM1.1) together with some notions and tools concerning the convergence analysis (e.g. Lemma SM1.7).

Since in \(\text{(SM0.1)}\), the feasible set \(S^{N-1}\) is a polyhedron, we naturally have the necessity of Karush-Kuhn-Tucker (KKT) conditions.

**Lemma SM1.1** (KKT Conditions of \(\text{(SM0.1)}\)). If \(\{X_i\}_{i=2}^N\) is a local minimizer of \(\text{(SM0.1)}\), there exist multipliers \(\lambda_i \in \mathbb{R}^{2K+1}, \Phi_i \in \mathbb{R}^{K \times K}, i = 2, \ldots, N\) such that for any \(i \in \{2, \ldots, N\}\),

\[
\Lambda \Xi C \Xi + \Xi A \left( \sum_{j \neq i} X_j \right) \Xi C \Xi + \beta \left( \sum_{j \neq i} X_j \right) - B^*(\lambda_i) - \Phi_i = 0,
\]
\[
B(X_i) = b, \quad X_i, \Phi_i \geq 0, \quad \Phi_i \circ X_i = 0,
\]

where “\(\circ\)” denotes the Kronecker product between two matrices. The tuple \(\{X_i\}_{i=2}^N\) satisfying the above relations is called a KKT point of \(\text{(SM0.1)}\).

The convergence analysis involves some definitions about subdifferentials and the well-known Kurdyka-Lojasiewicz property.

**Definition SM1.2** (Subdifferentials). Let \(G : V \rightarrow (-\infty, \infty]\) be a proper and lower semi-continuous function, where \(V\) is an Euclidean space with \((.,.)_V\) as its inner product and \(\|\cdot\|_V = \sqrt{(.,.)_V}\) as its norm.

1. For a given \(x \in \text{dom}(G) := \{y : G(y) < \infty\}\), the Fréchet subdifferential of \(G\) at \(x\), denoted by \(\partial G(x)\), is the set consisting of all vectors \(u \in V\) satisfying

\[
\liminf_{y \neq x, y \to x} \frac{G(y) - G(x) - \langle u, y - x \rangle_V}{\|y - x\|_V} \geq 0.
\]

When \(x \notin \text{dom}(G)\), we simply set \(\partial G(x) = \emptyset\).

2. The limiting-sudifferential of \(G\) at \(x \in V\), denoted by \(\partial G(x)\), is defined as

\[
\partial G(x) := \left\{ u \in V : \exists x^{(k)} \rightarrow x, G(x^{(k)}) \rightarrow G(x), u^{(k)} \in \partial G(x^{(k)}) \rightarrow u \right\}.
\]

**Remark SM1.3.**

1. Let \(\{(x^{(k)}, u^{(k)})\} \subseteq \text{graph}(\partial G)\) be a sequence converging to \((x, u)\). Here \(\text{graph}(\partial G)\) is the graph of set-valued map \(\partial G\) defined as \(\text{graph}(\partial G) := \{ (x, u) : u \in \partial G(x) \}\). By the definition of \(\partial G(x)\), if \(G(x^{(k)})\) converges to \(G(x)\), then \((x, u) \in \text{graph}(\partial G)\).

2. If \(x \in V\) is a local minimizer of \(G\), then \(0 \in \partial G(x)\); the point \(x\) satisfying \(0 \in \partial G(x)\) is called a critical point of \(G\).

3. For the extended-value function

\[
F(X_2, \ldots, X_N) := f_\beta(X_2, \ldots, X_N) + \sum_{i=2}^N \delta_S(X_i),
\]

a tuple \(\{X_i\}_{i=2}^N\) is a critical point of \(F\) if and only if it is a KKT point of \(\text{(SM0.1)}\); see [SM9, Proposition 6.6].
**Definition SM1.4 (Function class \( \Phi_\eta \)).** Let \( \eta \in (0, \infty] \). \( \Phi_\eta \) is the class of all concave and continuous functions \( \varphi : [0, \eta] \to \mathbb{R}_+ \) satisfying (i) \( \varphi(0) = 0 \); (ii) \( \varphi \in C^1((0, \eta)) \) and is continuous at 0; (iii) \( \varphi'(s) > 0, \ \forall \ s \in (0, \eta) \).

With the definition of limiting-subdifferential (Definition SM1.2) and function class \( \Phi_\eta \) (Definition SM1.4), we can state the Kurdyka-Lojasiewicz (KL) property as follows.

**Definition SM1.5 (KL property).** Let \( G : V \to (-\infty, \infty] \) be proper and lower semi-continuous, where \( V \) is an Euclidean space with \( \langle \cdot, \cdot \rangle_V \) as its inner product and \( \| \cdot \|_V = \sqrt{\langle \cdot, \cdot \rangle_V} \) as its norm.

(1) \( G \) is said to have the KL property at \( \bar{x} \in \text{dom}(\partial G) := \{x \in V : \partial G(x) \neq \emptyset\} \) if there exist a scalar \( \eta \in (0, \infty] \), a neighborhood \( U \) of \( \bar{x} \), and \( \varphi \in \Phi_\eta \), such that for all \( x \in U \cap \{y : G(y) < G(\bar{x}) < G(\bar{x}) + \eta\} \), the following inequality holds:

\[
\varphi'(G(x) - G(\bar{x})) \cdot \text{dist}(0, \partial G(x)) \geq 1,
\]

where \( \text{dist}(u, S) := \inf\{\|u - v\| : v \in S\} \).

(2) If \( G \) satisfies the KL property at each point of \( \text{dom}(\partial G) \), then \( G \) is called a KL function.

**Remark SM1.6.** It is hard to tell whether the KL property holds for a function (at some point) by the very Definition SM1.5. Nevertheless, extensive works have revealed some special cases. For example, in [SM12, section 2.2], the authors mentioned, among others, real analytic functions, locally strongly convex functions and semi-algebraic functions. They also noted that the finite sum of real analytic and semi-algebraic functions also enjoys this property.

In [SM1], Bolte et al. proved the following uniformized version of the KL property, which will be used for our convergence analysis.

**Lemma SM1.7 (Uniformized KL property).** Let \( \Omega \subseteq V \) be a compact set and \( G : V \to (-\infty, \infty] \) be a proper and lower semi-continuous function, where \( V \) is an Euclidean space with \( \langle \cdot, \cdot \rangle_V \) as its inner product and \( \| \cdot \|_V = \sqrt{\langle \cdot, \cdot \rangle_V} \) as its norm. Assume that \( G \) is constant on \( \Omega \) and satisfies the KL property at each point of \( \Omega \). Then, there exist \( \varepsilon > 0, \ \eta > 0 \) and \( \varphi \in \Phi_\eta \) such that for all \( \bar{x} \in \Omega \) and all \( x \) in \( \{x \in V : \text{dist}(x, \Omega) < \varepsilon\} \cap \{y : G(y) < G(\bar{x}) < G(\bar{x}) + \eta\} \), we have

\[
\varphi'(G(x) - G(\bar{x})) \cdot \text{dist}(0, \partial G(x)) \geq 1.
\]

**SM2. Auxiliary Lemmas.** In this section, we elaborate some ingredients that are useful in the later section SM3, including

- approximate sufficient reduction of energy value at \( \bar{Z}^{(k)} \) (Corollary SM2.2);
- approximate subgradient norm lower bound for “iterate gap” \( \|\bar{Z}^{(k+1)} - \bar{Z}^{(k)}\|_V \) (Lemma SM2.3); and
- properties of accumulation point set of \( \{\bar{Z}^{(k)}\} \) (Lemma SM2.4).

We shall mention beforehand that the sequence \( \{\bar{Z}^{(k)}\} \) closes the gap caused by infeasibility of the real iterate sequence \( \{Z^{(k)}\} \). Thus it is not surprising that most ingredients listed above revolve around \( \{\bar{Z}^{(k)}\} \). In the sequel, we assume \( N \geq 3 \) by default.

We list below constants that will be used. Note that if \( \sigma > 2M(N - 2) \), all of them are positive.

\[
M = \|\varrho\|_\infty \|e\|_\infty^3 \|C\|_2 + \beta, \quad C_0 = \frac{\sigma}{2} - M(N - 2), \quad C_1 = \frac{\sigma + 3MN}{2} - 2M, \\
C_2 = (N - 1)C_1, \quad C_3 = (\sigma + M(N - 1))\sqrt{N - 1}.
\]
One can verify that function $f_\beta$ is $M$-Lipschitz continuously differentiable: for any $j \in \{2, \ldots, N\}$ and $Z_1, Z_2 \in (\mathbb{R}^{K \times K})^{N-1}$,

$$\| \nabla X_j f_\beta(Z_1) - \nabla X_j f_\beta(Z_2) \|_F \leq M \| Z_1 - Z_2 \|_F. \tag{SM2.1}$$

In addition, we use notation “$\Delta$” for the difference between optimal iterate (SM0.3) and real iterate. For instance,

$$\Delta X_j^{(k+1)} := \bar{X}_j^{(k+1)} - X_j^{(k+1)}, \quad Z^{(k+1)} := \bar{Z}^{(k+1)} - Z^{(k+1)}.$$

**Lemma SM2.1.** Let $\{Z^{(k)}\}$ be the sequence generated by PBCD, $\{\bar{Z}^{(k)}\}$ be the sequence defined in (SM0.3). Then for each $i \in \{2, \ldots, N\}$, $\forall k \geq 1$,

$$f_\beta \left( \bar{X}_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)} \right) - f_\beta \left( \bar{X}_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)} \right) \geq C_0 \| \bar{X}_i^{(k+1)} - X_i^{(k+1)} \|_F^2 - C_1 \left( \| \Delta Z^{(k+1)} \|_F^2 + \| \Delta Z^{(k)} \|_F^2 \right). \tag{SM2.2}$$

**Proof.** The proof mainly leverages the bilinearity of $f_\beta$ and the optimality of $\bar{X}_i^{(k+1)}$. We first note that the expression in the left-hand side (LHS) of (SM2.3) can be split into five parts of summations of differences below:

1. **Part 1** $\sum_{j=1}^{i-1} f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k)}, \bar{X}_{>i}^{(k+1)})$;
2. **Part 2** $\sum_{j=i+1}^{N} f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k)}, \bar{X}_{>i}^{(k+1)})$;
3. **Part 3** $f_\beta(X_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<i}^{(k+1)}, \bar{X}_i^{(k)}, \bar{X}_{>i}^{(k+1)})$;
4. **Part 4** $\sum_{j=1}^{i-1} f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k)}, \bar{X}_{>i}^{(k+1)})$;
5. **Part 5** $\sum_{j=i+1}^{N} f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k)}, \bar{X}_{>i}^{(k+1)})$.

By the optimality of $\bar{X}_i^{(k+1)}$ in (SM0.3) and recalling (SM2.2), we readily have a lower bound for Part 3:

$$f_\beta(X_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)}) - f_\beta(X_{<i}^{(k+1)}, \bar{X}_i^{(k)}, \bar{X}_{>i}^{(k+1)}) \geq \frac{\sigma}{2} \left( \| \bar{X}_i^{(k+1)} - X_i^{(k)} \|_F^2 - \| \Delta X_i^{(k)} \|_F^2 \right).$$

Since the analysis for the remaining differences is very similar, we merely demonstrate in detail for Part 1 and Part 4. Recall (SM2.2),

$$\text{Part 1} = \sum_{j=2}^{i-1} \left( \nabla X_j f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}), \Delta X_j^{(k+1)} \right),$$

$$\text{Part 4} = \sum_{j=2}^{i-1} \left( \nabla X_j f_\beta(X_{<j}^{(k+1)}, \bar{X}_j^{(k+1)}, \bar{X}_{>i}^{(k+1)}), \Delta X_j^{(k+1)} \right).$$

Hence using the fact that for any $a, b, c \geq 0$, $ab \leq (a^2 + b^2)/2$, $(a + b)^2 \leq 2(a^2 + b^2)$ and recalling (SM2.1), we have

$$\text{Part 1} + \text{Part 4} \geq -\sum_{j=2}^{i-1} M \left( \| \bar{X}_i^{(k+1)} - \bar{X}_i^{(k)} \|_F + \sum_{j \neq l < i} \| \Delta X_l^{(k+1)} \|_F + \sum_{l > i} \| \Delta X_l^{(k)} \|_F \right) \| \Delta X_j^{(k+1)} \|_F.$$
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\begin{align*}
\geq & - \sum_{j=2}^{i-1} \frac{M}{2} \left( 3 \|\Delta X_j^{(k+1)}\|_F^2 + \sum_{j \neq i, j < i} \|\Delta X_{i,j}^{(k+1)}\|_F^2 + \sum_{j > i} \|\Delta X_{i,j}^{(k)}\|_F^2 \right) \\
& - \sum_{j=2}^{i-1} M \left( \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 + \|\Delta X_i^{(k)}\|_F^2 \right) \\
& = - \frac{M}{2} \left[ (i-3) \sum_{j=2}^{i-1} \|\Delta X_j^{(k+1)}\|_F^2 + (i-2) \sum_{j=i+1}^N \|\Delta X_j^{(k)}\|_F^2 \right] \\
& - \frac{3M}{2} \sum_{j=2}^{i-1} \|\Delta X_j^{(k+1)}\|_F^2 - M(i-2) \left( \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 + \|\Delta X_i^{(k)}\|_F^2 \right) .
\end{align*}

Similar arguments yield a lower bound for Part 2 + Part 5:

\[(SM2.6) \quad \text{Part 2 + Part 5} \]

\begin{align*}
\geq & - \frac{M}{2} \left[ (N-i) \sum_{j=2}^{i-1} \|\Delta X_j^{(k+1)}\|_F^2 + (N-1-i) \sum_{j=i+1}^N \|\Delta X_j^{(k)}\|_F^2 \right] \\
& - \frac{3M}{2} \sum_{j=i+1}^N \|\Delta X_j^{(k)}\|_F^2 - M(N-i) \left( \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 + \|\Delta X_i^{(k)}\|_F^2 \right) .
\end{align*}

Combining (SM2.4), (SM2.5) and (SM2.6), we have

\begin{align*}
f_\beta \left( \bar{X}_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)} \right) - f_\beta \left( \bar{X}_{<i}^{(k+1)}, \bar{X}_i^{(k+1)}, \bar{X}_{>i}^{(k+1)} \right) \\
\geq & [\sigma/2 - M(N-2)] \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 - [\sigma/2 + M(N-2)] \|\Delta X_i^{(k)}\|_F^2 \\
& - \frac{3M}{2} \sum_{j<i} \|\Delta X_j^{(k+1)}\|_F^2 - \frac{M}{2} \left[ (i-3) \sum_{j<i} \|\Delta X_j^{(k+1)}\|_F^2 + (i-2) \sum_{j>i} \|\Delta X_j^{(k)}\|_F^2 \right] \\
& - \frac{3M}{2} \sum_{j>i} \|\Delta X_j^{(k)}\|_F^2 - \frac{M}{2} \left[ (N-i) \sum_{j<i} \|\Delta X_j^{(k+1)}\|_F^2 + (N-1-i) \sum_{j>i} \|\Delta X_j^{(k)}\|_F^2 \right] \\
= & [\sigma/2 - M(N-2)] \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 - [\sigma/2 + M(N-2)] \|\Delta X_i^{(k)}\|_F^2 \\
& - \frac{MN}{2} \left( \sum_{j<i} \|\Delta X_j^{(k+1)}\|_F^2 + \sum_{j>i} \|\Delta X_j^{(k)}\|_F^2 \right) \\
\geq & [\sigma/2 - M(N-2)] \|\bar{X}_i^{(k+1)} - X_i^{(k)}\|_F^2 - [\sigma/2 + M(N-2)] \|\Delta X_i^{(k)}\|_F^2 \\
& - \frac{MN}{2} \left( \|\Delta Z^{(k+1)}\|_F^2 + \|\Delta Z^{(k)}\|_F^2 \right) ,
\end{align*}

which completes the proof by noticing the definition of $C_0, C_1$. \(\blacksquare\)

The following approximate sufficient reduction is then a direct corollary of the above lemma. We omit the proof.

**Corollary SM2.2 (Approximate Sufficient Reduction).** Let \(\{Z^{(k)}\}\) be the sequence generated by PBOD, \(\{\bar{Z}^{(k)}\}\) be the sequence defined in (SM0.3). Then \(\forall k \geq 1,\)

\[f_\beta(\bar{Z}^{(k)}) - f_\beta(\bar{Z}^{(k+1)}) \geq C_0 \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F^2 - C_2 \left( \|\Delta Z^{(k)}\|_F^2 + \|\Delta Z^{(k+1)}\|_F^2 \right) .\]
LEMMA SM2.3 (Approximate Subgradient Lower Bound). Let \( \{Z^{(k)}\} \) be the sequence generated by PBCD, \( \{\bar{Z}^{(k)}\} \) be the sequence defined in (SM0.3). Then for any \( k \geq 0 \), there exists \( W^{(k+1)} \in \partial F(\bar{Z}^{(k+1)}) \) such that,

\[
\|W^{(k+1)}\|_F \leq C_3 \left( \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F + \|\Delta Z^{(k+1)}\|_F \right).
\]

Proof. For each \( i \in \{2, \ldots, N\} \), it follows from the optimality of \( \bar{X}^{(k+1)}_i \) that there exists \( A^{(k+1)}_i \in \bar{\partial}_S(\bar{X}^{(k+1)}_i) \) such that

\[
0 = \nabla X, f_\beta \left( X^{(k+1)}_{\leq i}, \bar{X}^{(k+1)}_i, X^{(k)}_{>i} \right) + \sigma \left( \bar{X}^{(k+1)}_i - X^{(k)}_i \right) + A^{(k+1)}_i.
\]

Using (SM2.8) and the calculus of subdifferential (e.g. see [SM10]), we have

\[
\partial F(\bar{Z}^{(k+1)}) \ni \nabla X, f_\beta (\bar{Z}^{(k+1)}) + \left( A^{(k+1)}_i \right)_{i=2}^N = \left( \nabla X, f_\beta (\bar{Z}^{(k+1)}) - \nabla X, f_\beta (X^{(k+1)}_{\leq i}, \bar{X}^{(k+1)}_i, X^{(k)}_{>i}) - \sigma (\bar{X}^{(k+1)}_i - X^{(k)}_i) \right)_{i=2}^N.
\]

Let \( W^{(k+1)} \) be the subgradient defined above. We have for any \( i \in \{2, \ldots, N\} \)

\[
\|\nabla X, f_\beta (\bar{Z}^{(k+1)}) - \nabla X, f_\beta (X^{(k+1)}_{\leq i}, \bar{X}^{(k+1)}_i, X^{(k)}_{>i}) - \sigma (\bar{X}^{(k+1)}_i - X^{(k)}_i)\|_F \leq M \left( \sum_{j<i} \|\Delta X^{(k+1)}_j\|_F + \sum_{j>i} \|\bar{X}^{(k+1)}_j - X^{(k)}_j\|_F \right) + \sigma \|\bar{X}^{(k+1)}_i - X^{(k)}_i\|_F
\]

\[
\leq M \left( \sum_{j=2}^N \|\Delta X^{(k+1)}_j\|_F + \|\bar{X}^{(k+1)}_j - X^{(k)}_j\|_F \right) + \sigma \|\bar{X}^{(k+1)}_i - X^{(k)}_i\|_F
\]

\[
\leq M \sqrt{N-1} \left( \|\Delta Z^{(k+1)}\|_F + \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F \right) + \sigma \|\bar{X}^{(k+1)}_i - X^{(k)}_i\|_F.
\]

Therefore, it follows that

\[
\|W^{(k+1)}\|_F \leq (\sigma + M(N-1))\sqrt{N-1}\|\bar{Z}^{(k+1)} - Z^{(k)}\|_F + M(N-1)\sqrt{N-1}\|\Delta Z^{(k+1)}\|_F,
\]

which completes the proof by recalling the definition of \( C_3 \).

In the following lemma, we gather several properties of the accumulation point set \( \omega(Z^{(0)}) \) defined as

\[
\omega(Z^{(0)}) := \left\{ \mathbf{Z} = (\mathbf{X})_{i=2}^N : \exists \text{ a subsequence } \{\bar{Z}^{(k)}\}_{k \in K}, \text{ s. t. } \bar{Z}^{(k)} \to \mathbf{Z} \text{ in } K \right\}.
\]

LEMMA SM2.4 (Properties of Accumulation Point Set). Suppose \( \sigma > 2M(N-2) \) and Assumption SM0.1 holds. Let \( \{Z^{(k)}\} \) be the sequence generated by PBCD, \( \{\bar{Z}^{(k)}\} \) be the sequence defined in (SM0.3). Then we have that

1. \( \omega(Z^{(0)}) \subseteq S^{N-1} \) is nonempty compact and \( \text{dist}(\bar{Z}^{(k)}, \omega(Z^{(0)})) \to 0 \);
2. \( F \) is finite and constant on \( \omega(Z^{(0)}) \);
3. all the elements in \( \omega(Z^{(0)}) \) are KKT points of (SM0.1).
Proof. (1) Since \( \{Z^{(k)}\} \subseteq S^{N-1} \) and \( S \) is bounded, there exist a subsequence \( \{\tilde{Z}^{(k)}\}_{k \in K} \) and \( \tilde{Z} \) such that \( \tilde{Z}^{(k)} \to \tilde{Z} \) in \( K \), which gives \( \omega(Z^{(0)}) \neq \emptyset \). Also note that \( S^{N-1} \) is closed, thus \( \tilde{Z} \in S^{N-1} \) and hence \( \omega(Z^{(0)}) \subseteq S^{N-1} \). To prove the compactness, we only need to verify the closedness. Let \( \omega(Z^{(0)}) \ni Z_j \to \tilde{Z} \). For any \( j \), there exists a subsequence \( K_j \subseteq \mathbb{N} \) so that \( Z^{(k)} \to Z_j \) in \( K_j \). Hence for each \( j \), we can pick an integer \( k_j \in K_j \) such that \( \{k_j\}_j \) is a sequence increasing to \( \infty \), and \( \|Z^{(k_j)} - Z_j\|_F \leq \frac{1}{j} \). Therefore, the sequence \( \{Z^{(k_j)}\}_j \) satisfies
\[
\|Z^{(k_j)} - Z\|_F \leq \|Z^{(k_j)} - Z_j\|_F + \|Z_j - Z\|_F \leq \frac{1}{j} + \|Z_j - Z\|_F.
\]
Based on \( Z_j \to \tilde{Z} \) and the definition (SM2.9) of \( \omega(Z^{(0)}) \), we obtain \( \tilde{Z} \in \omega(Z^{(0)}) \), and hence the closedness of \( \omega(Z^{(0)}) \).

The latter part of this item follows directly from the definition (SM2.9) of the nonempty \( \omega(Z^{(0)}) \).

(2) By (1), \( F \) must be finite on \( \omega(Z^{(0)}) \subseteq S^{N-1} \). Now for any \( \tilde{Z} \in \omega(Z^{(0)}) \), there exists a subsequence \( \{\tilde{Z}^{(k)}\}_{k \in K} \) converging to \( \tilde{Z} \). The monotonicity of \( \{F(\tilde{Z}^{(k)})\} \) (Assumption SM0.1 (1)) and the continuity of \( F \) in \( S^{N-1} \) imply \( F(\tilde{Z}) = \tilde{F} \). By the arbitrariness of \( \tilde{Z}, F = \tilde{F} \) on \( \omega(Z^{(0)}) \).

(3) From Corollary SM2.2, we get for \( \forall \ k \geq 1 \),
\[
C_0\|\tilde{Z}^{(k+1)} - Z^{(k)}\|_F^2 \leq f_{\beta}(\tilde{Z}^{(k)}) - f_{\beta}(\tilde{Z}^{(k+1)}) + C_2 \left( \|\Delta Z^{(k)}\|_F^2 + \|\Delta Z^{(k+1)}\|_F^2 \right).
\]

Summing the above inequality over \( k \) from \( r \) to \( s \) \((s \geq r > 1)\), we have
\[
C_0 \sum_{k=r}^{s} \|\tilde{Z}^{(k+1)} - Z^{(k)}\|_F^2 \leq \sum_{k=r}^{s} \left( f_{\beta}(\tilde{Z}^{(k)}) - f_{\beta}(\tilde{Z}^{(k+1)}) \right) + 2C_2 \sum_{k=r-1}^{s} \|\Delta Z^{(k)}\|_F^2
\]
\[(SM2.10) \quad = f_{\beta}(\tilde{Z}^{(r)}) - f_{\beta}(\tilde{Z}^{(s+1)}) + 2C_2 \sum_{k=r-1}^{s} \|\Delta Z^{(k)}\|_F^2.
\]

Assumption SM0.1 (1) and \( \sigma > 2M(N-2) \) (hence \( C_0 > 0 \)) imply
\[
\sum_{k=r}^{s} \|\tilde{Z}^{(k+1)} - Z^{(k)}\|_F^2 \leq C_0^{-1} \left( f_{\beta}(\tilde{Z}^{(r)}) - \tilde{F} + 2C_2 \sum_{k=1}^{\infty} \|\Delta Z^{(k)}\|_F^2 \right) < \infty, \ \forall \ s \geq r > 1.
\]

Therefore \( \|\tilde{Z}^{(k+1)} - Z^{(k)}\|_F \to 0 \). By Lemma SM2.3 and Assumption SM0.1 (2), we further derive \( W^{(k+1)} \to 0 \).

Now pick \( \tilde{Z} \in \omega(Z^{(0)}) \) and the associated converging subsequence \( \{\tilde{Z}^{(k)}\}_{k \in K} \). Since \( \{\tilde{Z}^{(k)}, W^{(k+1)}\}_{k \in K} \) converges to \( (\tilde{Z}, 0) \), \( (\tilde{Z}^{(k+1)}, W^{(k+1)}) \in \text{graph}(\partial F) \) and \( F(\tilde{Z}^{(k+1)}) \to \tilde{F} = F(\tilde{Z}) \) (by (2)), from Remark SM1.3 (1), we deduce \( (\tilde{Z}, 0) \in \partial F(\tilde{Z}) \). In view of Remark SM1.3 (3), \( \tilde{Z} \) is a KKT point of (SM0.1). We complete the proof by the arbitrariness of \( \tilde{Z} \).

**SM3. Formal Statement and Proof of Theorem 3.3.** Thus far, we have established three auxiliary ingredients and are ready to prove Theorem 3.3 using the uniformized KL property (Lemma SM1.7). Beforehand, we shall mention that \( f_{\beta} \) is a real analytic function, and \( \partial S \) is semi-algebraic since \( S \) is apparently a semi-algebraic set. According to Remark SM1.6, \( F \) is a KL function, which is the premise for applying Lemma SM1.7.
For a global minimizer $\mathbf{Z}$, since $F$ is a KL function, we have the related scalar $\bar{\eta} > 0$, neighborhood $\mathcal{U}$ of $\mathbf{Z}$ and function $\bar{\varphi} \in \Phi_{\bar{\eta}}$ as in Definition SM1.5, which will be used in the sequel. Additionally, we define the following constants.

$$\tilde{C}_0 = \sqrt{C_0} - \frac{1}{2p}, \quad \tilde{C}_1 = \frac{pC_0}{C_0},$$

$$\tilde{C}_2 = \left( \frac{1}{2pC_0} + 1 \right) \frac{1}{\sqrt{C_0}}, \quad \tilde{C}_4 = \frac{1}{C_0} \left( \frac{1}{2p} + 2\sqrt{C_2} \right) + \sqrt{C_2} \tilde{C}_2 + 1.$$

Here constant $p$ satisfies

$$p > \frac{1}{2\sqrt{C_0}}.$$

As a result, all the constants listed above are positive.

In what follows, we give the formal statement of Theorem 3.3 and its complete proof.

**Theorem SM3.1** (Convergence Property of Algorithm 2.3 – Inexact Version). Suppose $\sigma > 2M(N - 2)$ and Assumption SM0.1 holds. Let $\{Z^{(k)}\}$ be the sequence generated by Algorithm 2.3, $\{\bar{Z}^{(k)}\}$ be the sequence defined in (SM0.3). Assume also that $F(\bar{Z}^{(k)}) > \mathcal{T}$, $\forall \; k \geq 1$. Then

1. the sequence $\{Z^{(k)}\}$ converges to a KKT point of (SM0.1);
2. if further $Z^{(0)} \in \{Z : F(\mathbf{Z}) < F(Z) < F(\mathbf{Z}) + \bar{\eta}\}$ and

$$\tilde{C}_1 \bar{\varphi} \left( F(Z^{(0)}) - F(\mathbf{Z}) \right) + \tilde{C}_2 \sqrt{F(Z^{(0)}) - F(\mathbf{Z})} + \sum_{k=1}^{\infty} \|\Delta Z^{(k)}\|_F + \|Z^{(0)} - \mathbf{Z}\|_F \leq \epsilon,$$

where $\mathbf{Z}$ is a global minimizer of (SM0.1) and $r$ is a positive scalar such that the closed ball $B_r(\mathbf{Z}) := \{Z : \|Z - \mathbf{Z}\|_F \leq r\} \subseteq \mathcal{U}$. Then $\{Z^{(k)}\}$ converges to a global minimizer of (SM0.1).

**Proof.** (1) Let $Z_* \in \omega(Z^{(0)})$ and $\varphi \in \Phi_{\bar{\eta}}$, $\varepsilon, \eta > 0$ be defined in Lemma SM1.7, where $G := F$, $\Omega := \omega(Z^{(0)})$. Since $F(Z^{(k)}) > \mathcal{T} = F(Z_*)$ and $\{F(Z^{(k)})\}$ converges monotonically to $\mathcal{F}$ (Assumption SM0.1 (1)), there exists an integer $k_0$, such that $F(Z_*) < F(Z^{(k)}) < F(Z_*) + \eta$, $\forall \; k \geq k_0$. Then $\varphi'(F(Z^{(k)}) - F(Z_*))$ is well-defined for any $k \geq k_0$. On the other, by Lemma SM2.4 (1), there exists an integer $k_1$, such that $\|\Delta Z^{(k)}(\omega(Z^{(0)}))\| < \varepsilon, \forall \; k \geq k_1$. Let $s = \max(k_0, k_1)$. By Lemma SM1.7, for $\forall \; k \geq s$,

$$\varphi' \left( F(Z^{(k)}) - F(Z_*) \right) \cdot \text{dist} \left( 0, \partial F(Z^{(k)}) \right) \geq 1,$$

which, combined with Lemma SM2.3, further gives

$$\varphi' \left( F(Z^{(k)}) - F(Z_*) \right) \geq \frac{1}{\text{dist}(0, \partial F(Z^{(k)}))} \geq \frac{1}{\|W^{(k)}\|_F},$$

where

$$\varphi' \left( F(Z^{(k)}) - F(Z_*) \right) \geq \frac{1}{C_3(\|Z^{(k)} - Z^{(k-1)}\|_F + \|\Delta Z^{(k)}\|_F)},$$

Let $D^{(k,k+1)} := \varphi \left( F(Z^{(k)}) - F(Z_*) \right) - \varphi \left( F(Z^{(k+1)}) - F(Z_*) \right)$.
By the concavity of $\varphi$, Assumption SM0.1 (1), Corollary SM2.2 and (SM3.3), we obtain
\[
D^{(k,k+1)} \geq \varphi' \left( F(Z^{(k)}) - F(Z_s) \right) \cdot \left( F(Z^{(k)}) - F(Z^{(k+1)}) \right) \\
\geq \frac{F(Z^{(k)}) - F(Z^{(k+1)})}{C3(\|Z^{(k)} - Z^{(k-1)}\|_F + \|\Delta Z(k)\|_F)} \\
\geq \frac{C0\|Z^{(k+1)} - Z^{(k)}\|_F^2 - C2(\|\Delta Z(k)\|_F^2 + \|\Delta Z^{(k+1)}\|_F^2)}{C3(\|Z^{(k)} - Z^{(k-1)}\|_F + \|\Delta Z(k)\|_F)}.
\]

An upper bound for $\|\bar{Z}^{(k+1)} - Z^{(k)}\|_F$ follows from some algebraic manipulations:
\[
\sqrt{C0} \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F \leq \sqrt{C3D^{(k,k+1)}} \|\bar{Z}^{(k)} - Z^{(k-1)}\|_F + \sqrt{C3D^{(k,k+1)} \|\Delta Z^{(k)}\|_F} \\
+ \sqrt{C2}\|\Delta Z^{(k)}\|_F + \sqrt{C2}\|\Delta Z^{(k+1)}\|_F \\
\leq pC3D^{(k,k+1)} + \frac{1}{2p} \left( \|\bar{Z}^{(k)} - Z^{(k-1)}\|_F + \|\Delta Z^{(k)}\|_F \right) \\
+ \sqrt{C2}\|\Delta Z^{(k)}\|_F + \sqrt{C2}\|\Delta Z^{(k+1)}\|_F,
\]

where the first inequality uses $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$, $\forall a, b \geq 0$, while the second one uses $\sqrt{ab} \leq pa/2 + b/(2p)$, $\forall a, b \geq 0$, $p > 0$. Here $p$ is chosen as in (SM3.1). Summing (SM3.4) over $k$ from $s$ to some $t \geq s$ gives
\[
\sqrt{C0} \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F \\
\leq pC3 \sum_{k=s}^{t} D^{(k,k+1)} + \frac{1}{2p} \left( \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F + \|\bar{Z}^{(s)} - Z^{(s-1)}\|_F \right) \\
+ \left( \frac{1}{2p} + \sqrt{C2} \right) \sum_{k=s}^{t} \|\Delta Z^{(k)}\|_F + \sqrt{C2} \sum_{k=s+1}^{t+1} \|\Delta Z^{(k)}\|_F \\
\leq pC3D^{(s,t+1)} + \frac{1}{2p} \left( \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F + \|\bar{Z}^{(s)} - Z^{(s-1)}\|_F \right) \\
+ \left( \frac{1}{2p} + 2\sqrt{C2} \right) \sum_{k=s}^{t+1} \|\Delta Z^{(k)}\|_F.
\]

Since
\[
D^{(s,t+1)} = \varphi \left( F(Z^{(s)}) - F(Z_s) \right) - \varphi \left( F(Z^{(t+1)}) - F(Z_s) \right) \leq \varphi \left( F(Z^{(s)}) - F(Z_s) \right),
\]
we further derive that
\[
\left( \sqrt{C0} - \frac{1}{2p} \right) \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F \leq pC3\varphi \left( F(Z^{(s)}) - F(Z_s) \right) + \frac{1}{2p} \|\bar{Z}^{(s)} - Z^{(s-1)}\|_F \\
+ \left( \frac{1}{2p} + 2\sqrt{C2} \right) \sum_{k=s}^{t+1} \|\Delta Z^{(k)}\|_F.
\]

(SM3.6)
Passing $t \to \infty$ in (SM3.6), and recalling (SM3.1) and the summability of $\{\|\Delta Z^{(k)}\|_F\}$ (Assumption SM0.1 (2)), we conclude that $\{\bar{Z}^{(k+1)} - Z^{(k)}\}$ is summable. Again using the summability of $\{\|\Delta Z^{(k)}\|_F\}$, we have the convergence of $\{Z^{(k)}\}$: for any $t \geq s$,

$$\sum_{k=s}^{t} \|Z^{(k+1)} - Z^{(k)}\| \leq \sum_{k=s}^{t} \|\Delta Z^{(k+1)}\|_F + \sum_{k=s}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F.$$ 

By Lemma SM2.4 (3), $Z_* \in \omega(Z^{(0)})$ is a KKT point of (SM0.1). Since $\|\Delta Z^{(k)}\|_F \to 0$, $\{\bar{Z}^{(k)}\}$ and $\{Z^{(k)}\}$ converge to the same point. Therefore, $\omega(Z^{(0)}) = \{z_*\}$ and $Z^{(k)} \to Z_*$. 

(2) We first assume the following claim holds:

**Claim SM3.2.** Under the assumptions made in (2), we have

$$\bar{Z}^{(k)} \in B_r(\bar{Z}) \cap \{Z : F(\bar{Z}) < F(Z) < F(\bar{Z}) + \bar{\eta}, \quad \forall k \geq 0.$$ 

By (1), we derive that $\{\bar{Z}^{(k)}\}$ (and hence $\{Z^{(k)}\}$) converges to some $Z_* \in B_r(\bar{Z})$ and $0 \in \partial F(Z_*)$. If $F(Z_*) > F(\bar{Z})$, then the KL property at $\bar{Z}$ indicates

$$\varphi' (F(Z_*) - F(\bar{Z})) \cdot \text{dist}(0, \partial F(Z_*)) \geq 1,$$

which contradicts with $0 \in \partial F(Z_*).$ Therefore, we must have $F(Z_*) = F(\bar{Z}).$

Now we turn to prove Claim SM3.2 by induction. Denote $\bar{Z}^{(0)} = Z^{(0)}$. The Claim SM3.2 holds trivially for $k = 0$. Next let $k = 1$. Since $Z^{(0)}$ is feasible, by Corollary SM2.2, we have

$$F(\bar{Z}^{(0)}) - F(\bar{Z}^{(1)}) = F(\bar{Z}^{(0)}) - F(\bar{Z}^{(1)}) \geq C_0\|\bar{Z}^{(1)} - Z^{(0)}\|^2_F - C_2\|\Delta Z^{(1)}\|^2_F,$$

which, together with $\sigma > 2M(N - 2)$, yield

$$\|\bar{Z}^{(1)} - Z^{(0)}\|^2_F \leq \frac{1}{\sqrt{C_0}} \sqrt{F(\bar{Z}^{(0)}) - F(\bar{Z}^{(1)}) + C_2\|\Delta Z^{(1)}\|^2_F} \tag{SM3.7} \leq \frac{1}{\sqrt{C_0}} \sqrt{\|F(\bar{Z}^{(0)}) - F(\bar{Z}^{(1)})\|_F + \sqrt{C_2\|\Delta Z^{(1)}\|_F}}.$$ 

Combining (SM3.7), triangle inequality of Frobenius norm and (SM3.2), we deduce

$$\|\bar{Z}^{(1)} - \bar{Z}\|_F \leq \|\bar{Z}^{(1)} - Z^{(0)}\|_F + \|Z^{(0)} - \bar{Z}\|_F \leq \frac{1}{\sqrt{C_0}} \sqrt{F(\bar{Z}^{(0)}) - F(\bar{Z}) + \sqrt{C_2\|\Delta Z^{(1)}\|_F} + \|Z^{(0)} - \bar{Z}\|_F \leq r.$$ 

Hence $\bar{Z}^{(1)} \in B_r(\bar{Z})$, and Claim SM3.2 holds for $k = 1$ by noting $F(\bar{Z}) < F(\bar{Z}^{(1)}) \leq F(Z^{(0)}) = F(\bar{Z}) + \bar{\eta}.$

Now suppose Claim SM3.2 holds for some $t \geq 1$. From (SM3.6) in the proof of (1), we get

$$C_0 \sum_{k=1}^{t} \|\bar{Z}^{(k+1)} - Z^{(k)}\|_F \leq \rho C_3 \varphi \left( F(\bar{Z}^{(1)}) - F(\bar{Z}) \right) + \frac{1}{2p} \|\bar{Z}^{(1)} - Z^{(0)}\|_F.$$
Claim SM3.2 holds for any \( \bar{\psi} \). Again, Claim SM3.2 holds for \( (\text{SM3.8}) \). Hence \( \bar{\psi} \) and \( \text{triangle inequality} \), we derive that
\[
\|Z^{(t+1)} - Z\|_F \leq \sum_{k=1}^{t} \left( \|Z^{(k+1)} - Z^{(k)}\|_F + \|\Delta Z^{(k)}\|_F \right) + \|\bar{Z}^{(1)} - Z^{(0)}\|_F + \|Z^{(0)} - Z\|_F
\]
\[
\leq pC_3\bar{\psi} \left( F(Z^{(0)}) - F(\bar{Z}) \right) + \frac{1}{C_0} \left( \frac{1}{2p} + 2\sqrt{C_2} \right) \sum_{k=1}^{t+1} \|\Delta Z^{(k)}\|_F + \|\bar{Z}^{(1)} - Z^{(0)}\|_F + \|Z^{(0)} - Z\|_F
\]
\[
\leq \frac{pC_3}{C_0} \bar{\psi} \left( F(Z^{(0)}) - F(\bar{Z}) \right) + \frac{1}{2pC_0} \sum_{k=1}^{t} \|\Delta Z^{(k)}\|_F + \|\bar{Z}^{(1)} - Z^{(0)}\|_F + \|Z^{(0)} - Z\|_F
\]
\[
\leq \frac{pC_3}{C_0} \bar{\psi} \left( F(Z^{(0)}) - F(\bar{Z}) \right) + \left( \frac{1}{2pC_0} + 1 \right) \|\bar{Z}^{(1)} - Z^{(0)}\|_F
\]
\[
\leq \frac{pC_3}{C_0} \bar{\psi} \left( F(Z^{(0)}) - F(\bar{Z}) \right) + \tilde{C}_1\bar{\psi} \left( F(Z^{(0)}) - F(\bar{Z}) \right) + \tilde{C}_2\sqrt{F(Z^{(0)}) - F(\bar{Z})}
\]
\[
\leq \tilde{C}_3 \sum_{k=1}^{\infty} \|\Delta Z^{(k)}\|_F + \|Z^{(0)} - Z\|_F \leq r.
\]

Hence \( \bar{Z}^{(t+1)} \in B_r(\bar{Z}) \), and Claim SM3.2 holds for \( t+1 \) by noting \( F(\bar{Z}) < F(\bar{Z}^{(t+1)}) \leq F(Z^{(0)}) = F(\bar{Z}) \). By induction, Claim SM3.2 holds for any \( k \geq 0 \). We complete the proof. \( \square \)

**Remark SM3.3.**
1. The results in this section recover those established in [SM1] if \( Z^{(k)} = \bar{Z}^{(k)} \), \( \forall \ k \).
2. The results in this section still hold if \( f \) is Lipschitz continuously differentiable and PBCD performs proximal linearized minimization for each block.

**SM4. Numerical Comparison among Local Solvers.** Since few methods are known for MPGCC, we consider (1.8) with \( N = 3 \) (hence an MPCC), and compare our local algorithm PBCD with some modified nonlinear programming solvers, including Knitro [SM2, SM11] and filtermpec [SM5, SM6]. Version 12.4.0 of Knitro is available in the downloadable AMPL system [SM7], and filtermpec has an interface to the online NEOS Server [SM3, SM4, SM8].

We investigate the performance of Knitro, filtermpec and PBCD on three 1D \( N = 3 \) systems in subsection 4.2, starting from the initial points provided by the GR subroutine (see Table 4.2 (a)). Additionally in virtue of the high-quality initial points, we set \( \text{alg} = 4 \) for Knitro so as to invoke sequential quadratic programming.
algorithm\(^2\). We use up to 40 cores for computation involving Knitro and PBCD and use AMPL input for Knitro and filtermpec. We monitor the repulsive energy (denoted by \(E\)), the average error (denoted by \(err\)) and the wall clock time in seconds (denoted by \(CPU\)) of all the three solvers. Note the CPU time reported by filtermpec is based on the computational resources on the NEOS Server. We need to point out that the formulation fed to Knitro and filtermpec is the original MPCC (1.8) rather than the \(\ell_1\) penalty form (SM0.1).

We terminate these solvers according to optimality violation. For PBCD, the sub-solver SSNCG stops if primal infeasibility (defined in (4.2)) is smaller than \(\varepsilon_{\text{inner}} = 10^{-9}\), and the outer loop terminates when KKT violation

\[(SM4.1) \sum_{i=2}^{N} \sum_{j>i} [\Xi \Lambda (X_j^{(k-1)} - X_j^{(k)}) \Xi C \Xi + \beta (X_j^{(k-1)} - X_j^{(k)}) + \sigma (X_i^{(k)} - X_i^{(k-1)})]^T\]

is smaller than a prescribed value \(\varepsilon_{\text{outer}}\), chosen as in (4.3). In Knitro, we specify stopping criteria \(\text{feastol}_{\text{abs}} = \text{opttol}_{\text{abs}} = \varepsilon_{\text{outer}}\); in filtermpec, we set \(\varepsilon_{\text{eps}} = \varepsilon_{\text{outer}}\). Other parameters of these two solvers are left unchanged as default.

The results on three 1D \(N = 3\) examples are gathered in Table SM4.1, where the best energies, average errors and CPUs are marked out in bold. The average errors in the brackets are the those of the corresponding initial points (see also the “err\(_s\)” column in Table 4.2 (a)).

| Table SM4.1 | Comparison among local solvers |
|-------------|-------------------------------|
|              | Example 1                     |
| Alg.        | \(K = 24\) (err = 0.049)     | \(K = 48\) (err = 0.022) | \(K = 96\) (err = 0.014) | \(K = 192\) (err = 0.007) |
| E           | 18.911                        | 19.004                      | 19.019                      | 19.021                      |
| err         | 0.013                         | 0.009                       | 0.004                       | 0.003                       |
| CPU         | 4.11                          | 9.33                        | 393.41                      | 7487.25                     |
| Knitro      | 19.035                        | 19.019                      | 19.021                      | 19.021                      |
| E           | 0.071                         | 0.004                       | 0.004                       | 0.003                       |
| err         | 7.06                          | 2.74                        | 29.90                       | 531.72                      |
| filtermpec  | 19.011                        | 19.004                      | 19.019                      | 19.021                      |
| E           | 0.013                         | 0.009                       | 0.004                       | 0.003                       |
| err         | 1.67                          | 1.67                        | 8.83                        | 110.58                      |
| PBCD        | 18.911                        | 19.004                      | 19.019                      | 19.021                      |
|              | Example 2                     |
| Alg.        | \(K = 24\) (err = 0.041)     | \(K = 48\) (err = 0.026) | \(K = 96\) (err = 0.017) | \(K = 192\) (err = 0.010) |
| E           | 12.372                        | 12.360                      | 12.360                      | 12.358                      |
| err         | 0.011                         | 0.009                       | 0.009                       | 0.003                       |
| CPU         | 5.30                          | 1.36                        | 18.37                       | 11199.66                    |
| Knitro      | 12.405                        | 12.360                      | 12.358                      | 12.358                      |
| E           | 0.060                         | 0.015                       | 0.004                       | 0.004                       |
| err         | 7.06                          | 2.40                        | 30.54                       | 523.86                      |
| filtermpec  | 12.372                        | 12.360                      | 12.358                      | 12.358                      |
| E           | 0.011                         | 0.009                       | 0.009                       | 0.003                       |
| err         | 1.41                          | 0.59                        | 3.16                        | 25.82                       |
| PBCD        | 12.367                        | 12.360                      | 12.358                      | 12.358                      |
|              | Example 3                     |
| Alg.        | \(K = 24\) (err = 0.053)     | \(K = 48\) (err = 0.027) | \(K = 96\) (err = 0.028) | \(K = 192\) (err = 0.033) |
| E           | 6.318                         | 6.400                       | 6.400                       | 6.403                       |
| err         | 0.018                         | 0.011                       | 0.011                       | 0.011                       |
| CPU         | 5.55                          | 17.53                       | 37.94                       | 504.53                      |
| Knitro      | 6.389                         | 6.400                       | 6.403                       | 6.403                       |
| E           | 0.013                         | 0.011                       | 0.011                       | 0.011                       |
| err         | 17.53                         | 37.94                       | 504.53                      | 504.53                      |
| filtermpec  | 6.389                         | 6.389                       | 6.389                       | 6.389                       |
| E           | 0.013                         | 0.013                       | 0.013                       | 0.013                       |
| err         | 1.97                          | 3.63                        | 3.63                        | 3.63                        |
| PBCD        | 6.318                         | 6.318                       | 6.318                       | 58.19                       |

The results in Table SM4.1 demonstrate that PBCD is comparable to both Knitro and filtermpec, the two state-of-art solvers for MPCC, in view of converged energies and solution errors, and meanwhile, underscore the incredible superiority of PBCD over

\(^2\)For reasons, please refer to https://www.artelys.com/docs/knitro/2_userGuide/algorithms.html#sec-algorithms.

\(^3\)The expression of KKT violation can be derived by comparing the iterative scheme of PBCD (SM0.2) and KKT condition in Lemma SM1.1. Note we actually omit \(\text{Feas}(X_i^{(k)})\) in (SM4.1) due to its tiny magnitude.

\(^4\)Actually, Knitro stops as well in default setting if stepsize is smaller than \(10^{-15}\) for 3 consecutive iterations. We keep this for less running time of Knitro.
the other two in terms of CPU time. This is not surprising, because both of them need to handle an $O(K^4)$ sparse Hessian, whose number of non-zeros is of $O(K^3)$. Indeed though not listed, the online interface of filtermpec fails to handle (1.8) with size $K = 384$ owing to the explosion of memory. Moreover according to our numerical experience, the proximal parameter $\sigma$ can be tuned for better performance of PBCD. To conclude, our proposed PBCD is a nice alternative in solving (1.8) when $N = 3$, and emerges as a novel and efficient tool for $N > 3$ cases.

REFERENCES

[SM1] J. Bolte, S. Sabach, and M. Teboulle, Proximal alternating linearized minimization for nonconvex and nonsmooth problems, Math. Program., 146 (2014), pp. 459–494, https://doi.org/10.1007/s10107-013-0701-9.

[SM2] R. Byrd, J. Nocedal, and R. Waltz, Knitro: an integrated package for nonlinear optimization, in Large-Scale Nonlinear Optimization, Springer, Boston, MA, 2006, pp. 35–59, https://doi.org/10.1007/0-387-30065-1.

[SM3] J. Czyzyk, M. Messier, and J. Moré, The NEOS server, IEEE Journal on Computational Science and Engineering, 5 (1998), pp. 68–75, https://doi.org/10.1109/99.714603.

[SM4] E. Dolan, The NEOS server 4.0 administrative guide, Technical Memorandum ANL/MCS- TM-250, Mathematics and Computer Science Division, Argonne National Laboratory, 2001, https://doi.org/10.2172/822567.

[SM5] R. Fletcher and S. Leyffer, Solving mathematical programs with complementarity constraints as nonlinear programs, Optim. Methods Softw., 19 (2004), pp. 15–40, https://doi.org/10.1080/10556780410001654241.

[SM6] R. Fletcher, S. Leyffer, D. Ralph, and S. Scholtes, Local convergence of SQP methods for mathematical programs with equilibrium constraints, SIAM J. Optim., 17 (2006), pp. 259–286, https://doi.org/10.1137/S1052623402407382.

[SM7] R. Fourer, D. Gay, and B. Kernighan, A modeling language for mathematical programming, Manage. Sci., 36 (1990), pp. 519–641, https://doi.org/10.1287/mnsc.36.5.519.

[SM8] W. Gropp and J. Moré, Optimization environments and the NEOS server, in Approximation Theory and Optimization, Cambridge University Press, 1997, pp. 167–182, https://doi.org/10.1.1.649.6743.

[SM9] J.-P. Penot, Calculus without Derivatives, vol. 266, Springer, New York, NY, 2013, https://doi.org/10.1007/978-1-4614-4538-8.

[SM10] R. Rockafellar and R. Wets, Variational Analysis, vol. 317, Springer-Verlag Berlin Heidelberg, 1998, https://doi.org/10.1007/978-3-642-02431-3.

[SM11] R. Waltz, J. Morales, J. Nocedal, and D. Orban, An interior algorithm for nonlinear optimization that combines line search and trust region steps, Math. Program., 107 (2006), pp. 391–408, https://doi.org/10.1007/s10107-004-0560-5.

[SM12] Y. Xu and W. Yin, A block coordinate descent method for regularized multiconvex optimization with applications to nonnegative tensor factorization and completion, SIAM J. Imaging Sci., 6 (2013), pp. 1758–1789, https://doi.org/10.1137/120887795.