This paper proposes a new variant of Frank-Wolfe (FW), called $k$FW. Standard FW suffers from slow convergence: iterates often zig-zag as update directions oscillate around extreme points of the constraint set. The new variant, $k$FW, overcomes this problem by using two stronger subproblem oracles in each iteration. The first is a $k$ linear optimization oracle ($k$LOO) that computes the $k$ best update directions (rather than just one). The second is a $k$ direction search ($k$DS) that minimizes the objective over a constraint set represented by the $k$ best update directions and the previous iterate. When the problem solution admits a sparse representation, both oracles are easy to compute, and $k$FW converges quickly for smooth convex objectives and several interesting constraint sets: $k$FW achieves finite $\frac{4L_f D_1^4}{\gamma \delta^2}$ convergence on polytopes and group norm balls, and linear convergence on spectrahedra and nuclear norm balls. Numerical experiments validate the effectiveness of $k$FW and demonstrate an order-of-magnitude speedup over existing approaches.

1 Introduction

We consider the following optimization problem with decision variable $x$:

$$\begin{align*}
\text{minimize} & \quad f(x) := g(Ax) + \langle c, x \rangle \\
\text{subject to} & \quad x \in \Omega.
\end{align*}$$

The constraint set $\Omega \subseteq \mathbb{E}$ is a convex and compact subset of a finite dimensional Euclidean space $\mathbb{E}$ and has diameter $D_1^1$. The map $A : \mathbb{E} \to \mathbb{F}$ is linear, where $\mathbb{F}$ is another finite dimensional Euclidean space. We equip both spaces $\mathbb{E}$ and $\mathbb{F}$ with real inner products denoted as $\langle \cdot, \cdot \rangle$. The vector $c$ is in $\mathbb{E}$. The function $g : \mathbb{F} \to \mathbb{R}$ is convex and $L_g$-smooth. The smoothness of $g$ implies that $f$ is $L_f$-smooth for some $L_f > 0$. For ease of exposition, we assume Problem (1) admits a unique solution.

Applications. The optimization problem (1) appears in a wide variety of applications, such as sparse vector recovery [CDS01], group-sparse vector recovery [YL06], combinatorial problems [JTPF14], submodular optimization [B+13, ZGU18], and low rank matrix recovery problems [RFP10, JS10, YUTC17, DU18].
Frank-Wolfe and two subproblems. In many modern high-dimensional applications, Euclidean projection onto the set $\Omega$ is challenging. Hence the well-known projected gradient (PG) method and its acceleration version (APG) are not well suited for (1). Instead, researchers have turned to projection-free methods, such as the Frank-Wolfe algorithm (FW) \cite{FW56}, also known as the conditional gradient method \cite[Section 6]{LP66}. As stated in Algorithm 1, FW operates in two computational steps:

1. **Linear Optimization Oracle (LOO):** Find a direction $v_t$ that solves $\min_v \langle \nabla f(x_t), v \rangle$.

2. **Line Search:** Find $x_{t+1}$ that solves $\min_{x = \eta v_t + (1-\eta)x_t, \eta \in [0,1]} f(x)$.

The linear optimization oracle can be computed efficiently for many interesting constraint sets $\Omega$ even when projection is prohibitively expensive. These sets include the probability simplex, the $\ell_1$ norm ball, and many more polytopes arising from combinatorial optimization, the spectrahedron $SP^n = \{ X \in S^n_+ \mid \text{tr}(X) = 1 \}$, and the unit nuclear norm ball $B_{\| \cdot \| \text{nuc}} = \{ X \mid \| X \| \text{nuc} \leq 1 \}$. We refer the reader to \cite{Jag13,LJJ15} for further examples. Line search is easy to implement using a closed formula for quadratic $f$, or bisection in general.

Slow convergence of FW and the Zigzag. However, FW is known to be slow in both theory and practice, reaching an accuracy of $O\left(\frac{1}{t}\right)$ after $t$ iterations. This slow convergence is often described pictorially by the Zigzag phenomenon depicted in Figure 1a. The Zigzag phenomenon occurs when the optimal solution $x_*$ of (1) lies on the boundary of $\Omega$ and is a convex combination of $r_*$ many extreme points $v_1^*, \ldots, v_{r_*}^* \in \Omega$. (In Figure 1a $r_* = 2$.)

$$x_* = \sum_{i=1}^{r_*} \lambda_i^* v_i^*, \quad \lambda_i^* > 0, \text{ and } \sum_{i=1}^{r_*} \lambda_i^* = 1. \quad (2)$$

When $\Omega$ is a polytope, the LOO will alternate between the extreme points $v_i^*$s and the line search updates the estimate of $\lambda_i^*$ slowly as the iterate approaches to $x_*$. A similar Zigzag occurs for other sets such as the spectrahedron and nuclear norm ball. A long line of work has explored methods to reduce the complexity of FW using LOO and line search alone \cite{GM86,LJJ13,LJJ15,GH15,GM16,FGM17}.

Our key insight: overcoming zigzags with kFW. Our first observation is that the sparsity $r_*$ is expected to be small for most large scale applications mentioned. For example, the sparsity is the number of nonzeros in sparse vector recovery, the number of nonzero groups in group-sparse vector recovery, and the rank in low rank matrix recovery. Next, note that from the optimality condition (also see Figure 1b), the gradient $\nabla f(x_*)$ in this case has the smallest inner product with $v_1^*, \ldots, v_{r_*}^*$, among all $v \in \Omega$. Also, for small $r_*$, we can solve $\min_{x \in \text{conv}(x_t, v_1^*, \ldots, v_{r_*}^*)} f(x)$ efficiently\footnote{Here $\text{conv}(v_1^*, \ldots, v_{r_*}^*)$ is the convex hull of $v_1, \ldots, v_{r_*}$.} to obtain the solution $x_*$. Hence, our key insight to overcome the Zigzag is simply

Compute all extreme points $v_i^*$ that minimize $\langle \nabla f(x_*), v \rangle$ and solve the smaller problem $\min_{x \in \text{conv}(x_t, v_1^*, \ldots, v_{r_*}^*)} f(x)$.  


This insight leads us to define a new algorithmic ways to choose extreme points and define a smaller convex search set, which we call $k$LOO and $k$DS. For polytope $\Omega$, they are defined as

- $k$ linear optimization oracle ($k$LOO): for any $y \in \mathbb{R}^n$, compute the $k$ extreme points $v_1, \ldots, v_k$ ($k$ best directions) with the smallest $k$ inner products $\langle v, y \rangle$ among all extreme points $v$ of $\Omega$.
- $k$ direction search ($k$DS): given input directions $w, v_1, \ldots, v_k \in \Omega$, output $x_{k\text{DS}} = \arg \min_{x \in \text{conv}(w, v_1, \ldots, v_k)} f(x)$.

Combining the two subproblem oracles, we arrive at a new variant of the Frank-Wolfe algorithm: $k$FW, presented in Algorithm 2. In Section 2, we show that the two subproblems can actually be efficiently solved over many polytopes (for small $k$). Moreover, we redefine $k$LOO and $k$DS to incorporate the situation where $k$ best extreme points are not well-defined for sets such as group norm ball, spectrahedron, and nuclear norm ball, yet sparsity structure still persists. Finally, we note that with our terminology, $1$FW is the same as FW. Hence our main results, Theorem 6, 7, and 10, give new insight into the fast convergence of FW when $r_\star = 1$.

**Computational efficiency of $k$FW.** Here we summarize the computational efficiency of $k$FW in terms of its per iteration cost, iteration complexity, and storage for polytopes:

- **Per iteration cost:** For many important cases displayed in Section 2, $k$FW admits efficient subproblem oracles.
- **Iteration complexity:** $k$FW achieves the same $O(1/t)$ convergence rate of FW. Under additional regularity conditions, it achieves nonexponential finite convergence over the polytope and group norm ball and linear convergence over the spectrahedron and nuclear norm ball, as shown in Theorem 6, 7, and 10. These convergence results are beyond the reach of FW and many of its variants [GM86, LJJ15, GM16, FGM17].
- **Storage:** The storage required by $k$FW is $O(kn)$, needed to store the $k$ best directions computed in each step, while the pairwise step, away step, and fully corrective step based FW [LJJ15] require $O(\min(tn, n^2))$ storage to accumulate vectors in $n$-dimensional Euclidean space computed from LOO.

A comparison of $k$FW with FW, away-step FW [GM86], and fully corrective FW (FCFW) [Jag13, Algorithm 4] is shown in Table 1. A recent result [Gar20] shows that away-step FW can have better

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Figure 1: The Zigzag phenomenon and optimization over $\text{conv}(x_\star, v_1^\star, v_2^\star)$ (green). Here, the solution $x_\star$ is a convex combination of $v_1^\star$ and $v_2^\star$, and $r_\star = 2$. The grey arrows are the negative gradients $-\nabla f$. 

(a) Zig-Zag: black arrows show trajectory of the iterates.

(b) Optimization over $\text{conv}(x_\star, v_1^\star, v_2^\star)$ (green).
Table 1: Comparison of $kFW$, FW, FW with away step, and FCFW for Problem (1), smooth convex optimization over a constraint set $\Omega$ in a $n$-dimensional Euclidean space. We display the per iteration computation (per iter. comp.), storage, faster rate (compared to $O\left(\frac{1}{t}\right)$ rate) under the condition on $\Omega$, extra conditions on Problem (1) to achieve the faster rate (Ex. Cond.), and the reference providing the proof of the rate. A recent result [Gar20] shows that away-step FW can have better convergence and storage after a initial burn-in period under similar assumptions as ours. However, it is hard to quantify the burn-in period as it depends on the parameter of the face where the solution lies. Even without the extra conditions listed in the table, all algorithms admit a $O\left(\frac{1}{t}\right)$ convergence rate (see [Jag13] and Theorem 6). Here $t \wedge n = \min(t, n)$. Definitions of the sparsity measure $r_*$, strict complementarity (str. comp.), and quadratic growth (q.g.) can be found in Section 3.1.

| Algorithm | Per iter. comp. | Storage | Rate and $\Omega$ Shape | Ex. Cond. | Reference |
|-----------|-----------------|---------|-------------------------|-----------|-----------|
| FW        | LOO, 1DS        | $O(n)$  | finite polytope, group norm ball | str. comp., q.g., and $r_* = 1$ | Theorem 7 |
|           |                 |         | linear spectrahedron $B\|\cdot\|_{\text{nuc}}$ |           | [Theorem 10] |
| Away-step FW | LOO, 1DS, and $t \wedge n$ inner products | $O(n(t \wedge n))$ | linear polytope | q.g. | [LJJ15], [Gar20] |
| FCFW      | LOO, and $(t \wedge n)\text{DS}$ | $O(n(t \wedge n))$ | linear polytope | q.g | [LJJ15] |
| $kFW$     | $k$LOO, and $k$DS | $O(kn)$ | finite polytope, group norm ball | str. comp., q.g., and $k \geq r_*$ | Theorem 7 |
|           |                 |         | linear spectrahedron $B\|\cdot\|_{\text{nuc}}$ |           | [Theorem 10] |

Interestingly, in our experiments in Section 4, we did not observe much of the benefit.

Paper Organization. The rest of the paper is organized as follows. In Section 2, we explain how to solve the two subproblems over a polytope $\Omega$, and how to extend the idea to group norm ball, spectrahedron, and nuclear norm ball. In Section 3, we describe a few analytical conditions, and then present the faster convergence guarantees of $kFW$ under these conditions for the polytope, group norm ball, spectrahedron, and nuclear norm ball. We demonstrate the effectiveness of $kFW$ numerically in Section 4. In Section 5, we conclude the paper and present a discussion on related work and future direction is presented.

Notation. The Euclidean spaces of interest in this paper are the $n$-th dimensional real Euclidean space $\mathbb{R}^n$, the set of real matrices $\mathbb{R}^{n_1 \times n_2}$, and the set of symmetric matrices $\mathbb{S}^n$ in $\mathbb{R}^{n \times n}$. We equip the first one with the standard dot product and the latter two with the trace inner product. The induced norm is denoted as $\|\cdot\|$ if not specified. For a linear map $B : E_1 \to E_2$ between two Euclidean spaces, we define its operator norm as $\|B\|_{\text{op}} = \max_{\|x\| \leq 1} \|B(x)\|$. We denote the eigenvalues of a symmetric matrix $A \in \mathbb{S}^n$ as $\lambda_1(A) \geq \cdots \geq \lambda_n(A)$. The $i$-th largest singular value of a rectangular matrix $B \in \mathbb{R}^{n_1 \times n_2}$ is denoted as $\sigma_i(B)$. A matrix $A \in \mathbb{S}^n$ is positive semidefinite if all its eigenvalues are nonnegative and is denoted as $A \succeq 0$ or $A \in \mathbb{S}^n_+$. The column space of a matrix $A$ is written as $\text{range}(A)$. The $i$-th standard basis vector with appropriate dimension is denoted as $e_i$. 

4
2 Stronger subproblem oracles for polytopes and beyond

In Section 2.1, we explain when the subproblem oracles can be implemented efficiently for polytopes. We then show how to extend \( k \)-FW to more complex constraint sets by an appropriate definition of \( k \)LOO and \( k \)DS in Section 2.2.

2.1 Stronger subproblem oracles for polytopes

Let us first explain when the \( k \)LOO can be implemented efficiently for a polytope \( \Omega \subseteq \mathbb{R}^n \).

Solving \( k \)LOO. Computing a LOO can be NP-hard for some constraint sets \( \Omega \): for example, the 0-1 knapsack problem can be formulated as linear optimization over an appropriate polytope.

Hence we should not expect that we can compute a \( k \)LOO efficiently without further assumptions on the polytope \( \Omega \subseteq \mathbb{R}^n \). Since many polytopes come from problems in combinatorics, for these polytopes, computing a \( k \)LOO is equivalent to computing the \( k \)best solutions to a problem in the combinatorics literature, and polynomial time algorithms are available for many polytopes [Mur68, Law72, HQ85, Epp14]. We present the time complexity of computing \( k \)LOO for many interesting problems in Table 5 in the appendix.

Efficient \( k \)LOO. Unfortunately, for some polytopes, the time required to compute a \( k \)LOO grows superlinearly in \( k \) even if \( k \leq n \). Hence we restrict our attention to special structured polytopes for which the time complexity of \( k \)LOO is no more than \( k \) times the complexity of LOO.

Our primary example is the probability simplex \( \Delta^n = \text{conv}(\{e_i\}_{i=1}^n) \) in \( \mathbb{R}^n \). Since the vertices of \( \Delta^n \) are the coordinate vectors \( e_i \), \( i = 1, \ldots, n \), the inner product of vertex \( e_i \) with a vector \( y \in \mathbb{R}^n \) is \( \langle y, e_i \rangle = y_i \). Hence in this case, \( k \)LOO with input \( y \in \mathbb{R}^n \) simply outputs the coordinate vectors corresponding to the smallest \( k \) values of \( y \). Using a binary heap of \( k \) nodes, we can scan through the entries of \( y \) and update the heap to keep the \( k \) smallest entries seen so far and their indices.

Since each heap update takes time \( O(\log k) \), the time to compute \( k \)LOO is \( O(n \log k) \).

A more sophisticated procedure called quickselect improves the time to \( O(n + k) \) [MR01], [Epp14, Section 2.1]. Other examples of efficient \( k \)LOO includes, the \( \ell_1 \) norm ball, the spanning tree polytope [Epp90], the Birkhoff polytope, [Mur68], and the path polytope of a directed acyclic graph [Epp98]. More details of each example and its application can be found in Section A.2 in the appendix.

Next, we explain how to compute the \( k \) direction search.

\( k \) direction search. The \( k \) direction search problem optimizes the objective \( f(x) \) over \( x \in \text{conv}(w, v_1, \ldots, v_k) = \{ \sum_{i=1}^k \lambda_i v_i + \eta w \mid (\eta, \lambda) \in \Delta^{k+1} \} \). We parametrize this set by \( (\eta, \lambda) \in \Delta^{k+1} \) and employ the accelerated projected gradient method (APG) to solve

\[
\min_{(\eta, \lambda) \in \Delta^{k+1}} f \left( \sum_{i=1}^k \lambda_i v_i + \eta w \right). \tag{3}
\]

The constraint set here is a \( k + 1 \) dimensional probability simplex; projection onto this set requires time \( O(k \log k) \) [CY11]. Hence for small \( k \), we can solve (3) efficiently. We recover the output \( x_{k-\text{DS}} = \sum_{i=1}^k \lambda_i^* v_i + \eta^* w \) of \( k \)DS from the optimal solution \( (\eta^*, \lambda^*) \) of (3).

Remark 1. Optimizing over \( \text{conv}(w, v_1, \ldots, v_k) = \{ \sum_{i=1}^k \lambda_i v_i + \eta w \mid (\eta, \lambda) \in \Delta^{k+1} \} \) using the representation \( (\eta, \lambda) \) can be challenging due to the high dimension \( k \) of this parametrization. Here we discuss a few alternative parametrizations that facilitate optimization.
For example, consider the product of simplices \( \prod_{j=1}^{d} \Delta_{k_j} \subset \mathbb{R}^\sum_{j=1}^{d} k_j \), which appears in a variety of applications \cite{LJJSPT13}. Denote the \( j \)-th block of \( w \in \mathbb{R}^\sum_{j=1}^{d} k_j \) as \([w]^j \in \mathbb{R}^{k_j}\), and let \( e^j_i \in \mathbb{R}^\sum_{j=1}^{d} k_j \) be the indicator of the \( i \)-th position in \( j \)-th block (1 there, and 0 everywhere else). Write \( e_{i_1 \ldots i_d} = \sum_{j=1}^{d} e^j_i \). Define the set \( I = \prod_{j=1}^{d} I_j \) where \( I_j \subset \{1, \ldots, k_j\} \), which might be the generated when we apply |\( I_j \)LOO in each block within \( \mathcal{O}((\sum_{j=1}^{d} k_j) \log(\max_j |I_j|)) \) time. Suppose we want to optimize over \( \sum_{j=1}^{d} k_j \) variables and hence should be easier to optimize over. One strategy is to use bisection to choose \( \eta \) approach. However, note that optimizing over variables in \( \{A_\alpha \}_{\alpha \in \Omega} \) by optimizing over \( \sum_{j=1}^{n} \eta \) is not easily computable.

\( \langle \eta w, \{e_{i_1 \ldots i_d}\}_{(i_1, \ldots, i_d) \in I} \rangle \) is a \( \mathbb{R}^\sum_{j=1}^{d} k_j \) representation, the size of \( \eta, \lambda \) is \( \prod |I_j| + 1 \) which can be much larger than the number of nonzeros, \( \sum_{j=1}^{n} |I_j| \), of the solution \( x_* \) or even larger than the total dimension \( \sum_{j=1}^{n} k_j \), even if the support of \( x_* \) in \( j \)-th block is exactly \( I_j \).

An alternative parametrization introduces a slightly larger convex set. Indeed, \( B_{w,I} = \{ (\alpha_{ij}), \eta_{ij} \}_{1 \leq j \leq d, i \in I_j} \mid \alpha_{ij} \geq 0 \forall i, j, \eta_{ij} \geq 0 \forall j, \sum_{i \in I_j} \alpha_{ij} + \eta_{ij} = 1 \} \). Then

\[
\text{conv}(w, \{e_{i_1 \ldots i_d}\}_{(i_1, \ldots, i_d) \in I}) \subset \left\{ \sum_{j=1}^{d} \left( \sum_{i \in I_j} \eta_{ij} [w]^j_i e^j_i + \sum_{i \in I_j} \alpha_{ij} e^j_i \right) \left| (\alpha_{ij}, \eta_{ij}) \in B_{w,I} \right. \right\}.
]\]

Note the latter set has \( \sum_{j=1}^{d} |I_j| + d \) variables instead of \( \sum_{j=1}^{d} |I_j| + 1 \) variables as in the previous approach. However, note that optimizing over variables in \( B_{w,I} \) is actually easier as \( B_{w,I} \) is a product of scaled simplices which enables faster projection.

**Algorithm 1** Frank-Wolfe with line search

**Input:** initialization \( x_0 \in \mathcal{E} \)

for \( t = 1, 2, \ldots \) do

- Linear optimization oracle (LOO): Compute \( v_t \in \arg \min_{v \in \mathcal{E}} \langle v, \nabla f(x) \rangle \).

- Line search: solve \( \hat{\eta} = \arg \min_{\eta \in [0,1]} f(\eta x_t + (1 - \eta)v_t) \) and set \( x_{t+1} = \hat{\eta} x_t + (1 - \hat{\eta})v_t \).

end for

**Algorithm 2** \( k \)FW for polytope

**Input:** initialization \( x_0 \in \Omega \), and an integer \( k > 0 \)

for \( t = 1, 2, \ldots \) do

- \( k \) linear optimization oracle (kLOO): compute \( k \) extreme points, \( v_1, \ldots, v_k \) with smallest \( \langle v, \nabla f(x_t) \rangle \) among all extreme points of \( v \in \Omega \).

- \( k \) direction search (kDS): Solve \( \min_{x \in \text{conv}(v_1, \ldots, v_k, x_t)} f(x) \) to obtain \( x_{t+1} \).

end for

**Algorithm 3** \( k \)FW for other \( \Omega \)

Same as Algorithm 2 replacing the kLOO (with input \( \nabla f(x_t) \)) and kDS (with input consisting of \( x_t \) and the output of kLOO, and output \( x_{t+1} = x_{k\text{DS}} \), as described in Section 2.2.
2.2 Stronger subproblem oracle for nonpolytope $\Omega$

In this section, we explain how to extend $k$FW to operate on the unit group norm ball, spectrahedron, and nuclear norm ball. We shall redefine the $k$LOO and $k$DS accordingly.

2.2.1 Group norm ball

Let us first define the group norm ball. Given a partition $\mathcal{G} = \{g_1, \ldots, g_l\}$ of the set $[n] = \{1, \ldots, n\}$ ($\cup_{g \in \mathcal{G}} g = [n]$ and $g_i \cap g_j = \emptyset$ for $i \neq j$), the group norm and the unit group norm ball are

$$\|x\|_\mathcal{G} := \sum_{g \in \mathcal{G}} \|x_g\|, \forall x \in \mathbb{R}^n \quad \text{and} \quad B_{\|\cdot\|_\mathcal{G}} = \{x \in \mathbb{R}^n : \|x\|_\mathcal{G} \leq 1\}, \text{ respectively.} \quad (4)$$

Here the base norm $\|\cdot\|$ can be any $\ell_p$ norm, or even some matrix norms. We restrict our attention to the $\ell_2$ norm in the main text for ease of presentation. The vector $x_g$ is formed by the entries of $x$ with indices in $g$.

Let us now define $k$LOO and $k$DS for the group norm ball $B_{\|\cdot\|_\mathcal{G}}$.

**$k$LOO.** Given an input $y \in \mathbb{R}^n$, $k$LOO outputs the $k$ groups $v_1, \ldots, v_k \in \mathcal{G}$ with largest $\|y_{v_i}\|$ among all $v \in \mathcal{G}$. Here the $k$ best “directions” are not vectors, but groups. Notice the groups $g \in \mathcal{G}$ are disjoint, so $\sum_{i=1}^k \|y_{v_i}\| \leq \|y\|_\mathcal{G}$. In this sense, $k$LOO for the group norm ball generalizes $k$LOO for the simplex.

**$k$DS.** Given inputs $w \in B_{\|\cdot\|_\mathcal{G}}$ and $v_1, \ldots, v_k \in \mathcal{G}$, $k$DS for the group norm ball optimizes the objective $f(x)$ over convex combinations of $w$ and vectors supported on $\cup_{i=1}^k v_i$. To parametrize vectors supported on $\cup_{i=1}^k v_i$, we introduce a variable $\lambda^{v_1,\ldots,v_k} \in \mathbb{R}^n$ supported on $\cup_{i=1}^k v_i$. That is, $\lambda^{v_1,\ldots,v_k} = 0$ for all $i \not\in \cup_{i=1}^k v_i$. Our decision variable $x$ is written as

$$x = \eta w + \lambda^{v_1,\ldots,v_k}, \quad \text{where} \quad \eta + \|\lambda^{v_1,\ldots,v_k}\|_\mathcal{G} \leq 1, \eta \geq 0. \quad (5)$$

We solve the following problem to obtain $x_{kDS}$:

$$\text{minimize } f(\eta w + \lambda^{v_1,\ldots,v_k}) \quad \text{subject to } \eta + \|\lambda^{v_1,\ldots,v_k}\|_\mathcal{G} \leq 1, \eta \geq 0. \quad (6)$$

We can again employ APG to solve this problem, as the projection step only requires $O(k \log k + \sum_{i=1}^k |v_i|)$ time. (See more details in Section A.4.)

2.2.2 Nuclear norm ball

We now define $k$LOO and $k$DS for the unit nuclear norm ball $B_{\|\cdot\|_{\text{nuc}}} = \{X \in \mathbb{R}^{n_1 \times n_2} : \|X\|_{\text{nuc}} \leq 1\}$, where $\|X\|_{\text{nuc}} = \sum_{i=1}^{\min(n_1,n_2)} \sigma_i(X)$, the sum of singular values.

**$k$LOO.** Given an input matrix $Y \in \mathbb{R}^{n_1 \times n_2}$, define the $k$ best directions of the linearized objective $\min_{V \in \Omega(\alpha)} \langle V, Y \rangle$ to be the pairs $(u_1, v_1), \ldots, (u_k, v_k)$, the top $k$ left and right orthonormal singular vectors of $Y$. Collect the output as $U = [u_1, \ldots, u_k] \in \mathbb{R}^{n_1 \times k}$ and $V = [v_1, \ldots, v_k] \in \mathbb{R}^{n_2 \times k}$.

\[\text{See Section A.5 in the appendix for further discussion.}\]
Take as inputs $W \in B_{\|\cdot\|_{\text{nuc}}}^n$ and $(U,V) \in \mathbb{R}^{n_1 \times k} \times \mathbb{R}^{n_2 \times k}$ with orthonormal columns. Inspired by [HR00], we consider the spectral convex combinations of $W$ and $u_i v_i^\top$ instead of just convex combination:

$$X = \eta W + USV^\top$$

where $\eta \geq 0$, $\eta + \|S\|_{\text{nuc}} \leq 1$.

Next, we minimize the objective $f(X)$ parametrized by $(\eta, S) \in \mathbb{R}^{1+k^2}$ to obtain $X_{\text{kDS}}$:

$$\text{minimize } f(\eta W + USV^\top) \text{ subject to } \eta + \|S\|_{\text{nuc}} \leq 1, \eta \geq 0.$$  

Again, we use APG to solve this problem. Projection requires singular value decomposition of a $k^2$ matrix, which is tolerable for small $k$. (See Section A.6 for details.)

A summary of $k\text{LOO}$ and $k\text{DS}$ for these sets appears in Table 6 and 7 in the appendix respectively. The case of spectrahedron has been addressed very recently by [DFXY20]. We give a self-contained description of its $k\text{LOO}$ and $k\text{DS}$ in Section A.1. The kFW algorithm for unit group norm ball, spectrahedron, and unit nuclear norm ball is presented as Algorithm 3.

**Remark 2.** (Choice of $k$) Having discussed kFW for various constraint sets, here we discuss the choice of $k$. Determining the choice of $k$ is of great importance as our guarantees require $k$ to be larger or equal to the underlying sparsity measure to observe significant speedup, see Definition 2 and results in Section 3. Domain knowledge is then particular helpful in this regard. In our experiments, for synthetic datasets, we have set $k$ to be the ground truth of the sparsity measure. On real data, we determine $k$ according to the expected sparsity level of the data (e.g. the expected number of support vectors in SVM, see Section 4 for details.)

Here we provide a adaptive method to adjust $k$, which is shown in Algorithm 4. The main idea is to increase $k$ in every iteration until it cannot improve the relative decrease of the objective function. We found that setting the increasing factor $\zeta = 2$ works every well in practice. For example, Figure 2 shows the results of kFW with adaptive $k$ on the Lasso problem. We see that the algorithm is able to find a (possibly) optimal $k$ effectively with different initialization $k_0$. We also found similar performance (not shown here) in the experiments of other tasks discussed in Section 4.

**Algorithm 4** kFW with adaptive $k$

**Input:** initialization $x_0$ and $k_0$, parameter $\zeta > 1$, $inc = True$

for $t = 0, 1, \ldots,$ do

Compute $f(x_t)$

if $t = 2$ then

$k_t = \zeta k_{t-1}$

end if

if $t > 2$ and $inc = True$ then

if $(f(x_{t-1}) - f(x_t))/f(x_{t-1}) > (f(x_{t-2}) - f(x_{t-1}))/f(x_{t-2})$ then

$k_t = \zeta k_{t-1}$

else

$inc = False$

end if

end if

$k\text{LOO}$ step

$k\text{DS}$ step

end for
3 Theoretical guarantees

In this section, we first present a few definitions and conditions required to state our results. Then we present the theorems and provide intuitions. Proofs are deferred to Section B.4 and B.5.

3.1 Analytical conditions

Here we define the sparsity measure $r_*$ for each constraint set $\Omega$ and the complementarity measure $\delta$.

Definition 3 (Sparsity measure $r_*$). Suppose the solution $x_*$ of (1) is unique.

- Polytope: The sparsity measure $r_*$ is the number of extreme points of the smallest face $F(x_*)$ of $\Omega$ containing $x_*$. 
- Group norm ball: The sparsity measure $r_*$ is the number of groups $g \in \mathcal{G}$ such that $(x_*)_g \neq 0$, or equivalently, the cardinality of the set $F(x_*) := \{ g \mid (x_*)_g \neq 0 \}$.
- Spectrahedron and unit nuclear norm ball: The sparsity measure $r_*$ is rank$(X_*)$, or equivalently, the dimension of $F(X_*) = \text{range}(X_*)$.

In short, the sparsity is the cardinality or the dimension of the support set $F(x_*)$.

Definition 4 (Strict complementarity). Problem (1) admits strict complementarity if it has a unique solution $x_* \in \partial \Omega$ and $-\nabla f(x_*) \in \text{relint}(N_\Omega(x_*))$.

The complementarity measure $\delta$ is the gap between the inner products of $x_*$ and the elements of the complementary set $F^c(x_*)$ defined below:

$$\delta = \min \{ \langle u, \nabla f(x_*) \rangle - \langle x_*, \nabla f(x_*) \rangle \mid u \in F^c(x_*) \subseteq \Omega \}. \quad (7)$$

The complementary set $F^c(x_*)$. Morally, the complementary set $F^c(x_*)$ is the complement (in $\Omega$) of elements supported in $F(x_*)$. Our formal definition also respects the vector structure of these sets.

- Polytope: The complementary space $F^c(x_*)$ is the convex hull of all vertices not in $F(x_*)$.
- Group norm ball: The complementary space $F^c(x_*)$ is the set of all vectors in $\Omega$ not supported in $F(x_*) = \{ g \mid (x_*)_g \neq 0 \}$.
- Spectrahedron and nuclear norm ball: The complementary space $F^c(X_*)$ is the set of all matrices in $\Omega$ with column space orthogonal to $F(X_*) = \text{range}(X_*)$.

\footnote{Here $\partial \Omega$ is the topological boundary of $\Omega$ under the standard topology of $E$. The set $N_\Omega(x_*)$ is the normal cone of $\Omega$ at $x_*$, i.e. $N_\Omega(x_*) = \{ y \mid \langle y, x \rangle \leq \langle y, x_* \rangle, \forall x \in \Omega \}$, and relint(·) is the relative interior.}
Table 8 in the appendix catalogues $r^*, \mathcal{F}(x^*_*)$, $\mathcal{F}^c$, and $\delta$ for several sets $\Omega$. Note that the definition of the gap $\delta$ is always nonnegative due to optimality condition of (1). It is indeed positive when strict complementarity holds as shown in Lemma 11 in the appendix.

**Remarks on strict complementarity.** Two aspects of strict complementarity have important implications for $k$FW. (See further discussion in B.1) First, structurally, the strict complementarity condition ensures robustness of $r^*$ under perturbations of the problem. Indeed, consider the problem

$$\min_{x \in \Delta^n} \|x - \sigma e_1\|^2 + \langle c, x \rangle. \quad (8)$$

For $c = 0$ and any $\sigma \in [0, 1]$, the unique solution $x^* = \sigma e_1$, which is also sparse. However, it can be easily verified that strict complementarity fails in this case. As a result, almost any small perturbation $c \neq 0$ results in a solution with sparsity $r^* > 1$. We refer the reader to Example B.1 in the appendix and to [Gar20, Table 2], and to [Gar19a, Lemma 2 and 10] for more discussion on the relationship between complementarity and robustness of the solution sparsity.

Second, algorithmically, the proof of Theorem 7 and 10 reveal that $k$FW identifies the support set $\mathcal{F}(x^*)$ once the iterate is near $x^*$. The gap $\delta$ tells us how close it must be to identify the support.

We introduce the quadratic growth condition, a strictly weaker version of strong convexity. It is has been studied in [DL18, NNG19] to ensure linear convergence of some first order algorithms, and is also necessary as shown in [NNG19].

**Definition 5 (Quadratic growth).** Problem (1) admits quadratic growth with parameter $\gamma > 0$ if it has a unique solution $x^*$ and for all $x \in \Omega$, $f(x) - f(x^*) \geq \gamma \|x - x^*\|^2$.

**Remarks on quadratic growth.** For all constraint set $\Omega$ considered in this paper, quadratic growth holds under strict complementarity for strongly convex $g$ in (1), $\min_{x \in \Omega} g(Ax) + \langle c, x \rangle$. (See Theorem 12 in the appendix for a proof.) Quadratic growth also holds for almost all $c$ if $g$ and $\Omega$ are semi-algebraic [DIL16, Corollary 4.8].

### 3.2 Guarantees for $k$FW

Our first theorem states that $k$FW never requires more iterations than FW.

**Theorem 6.** Suppose $f$ is $L_f$-smooth and convex and $\Omega$ is convex compact with diameter $D$. Then for any $k \geq 1$ and for all $t \geq 1$, the iterate $x_t$ in $k$FW (Algorithm 2 and 3) satisfies

$$f(x_t) - f(x^*) \leq \frac{L_f D^2}{t}. \quad (9)$$

**Proof.** The inequality (9) follows from the proof of convergence of FW as in [Jag13] by noting that the vector $v_t = \arg \min_{v \in \Omega} \langle \nabla f(x_t), v \rangle$ is feasible for the $k$DS minimization problem.

The theorem shows that $k$FW converges faster when $k \geq r^*$ for the polytope and group norm ball.

**Theorem 7.** Suppose that $f$ is $L_f$-smooth and convex, $\Omega$ is convex compact with diameter $D$, Problem (1) satisfies strict complementarity and quadratic growth, and $k \geq r^*$. If the constraint set $\Omega$ is a polytope or a unit group norm ball, then the gap $\delta > 0$ and $k$FW finds $x^*$ in at most $T + 1$ iterations, where $T$ is

$$T = \frac{4L_f^3 D^4}{\gamma \delta^2}. \quad (10)$$

Proof. The proof follows from the intuition that once \( x_t \) is close to \( x_\ast \), the set \( \mathcal{F}(x_\ast) \) can be identified using \( \nabla f(x_t) \). The fact that \( \delta > 0 \) is shown in Lemma 11. Let us now consider Algorithm 2 whose constraint set \( \Omega \) is a polytope. Using quadratic growth in the following step (a), and Theorem 6 in the following second step (b), and the choice in the following step (c), the iterate \( x_t \) with \( t \geq T \) satisfies that
\[
\|x_t - x_\ast\| \leq \sqrt{\frac{1}{\gamma} (f(x_t) - f(x_\ast))} \leq \sqrt{\frac{L_f D^2}{\gamma T}} \leq \frac{\delta}{2L_f D}.
\] (11)

Next, for any \( t \geq T \), we have that for any vertex \( v \) in \( \mathcal{F}(x_\ast) \), and any vertices \( u \) in \( \mathcal{F}^c(x_\ast) \),
\[
\langle \nabla f(x_t), v \rangle - \langle \nabla f(x_t), u \rangle = \langle \nabla f(x_\ast), v - u \rangle + \langle \nabla f(x_t) - \nabla f(x_\ast), v - u \rangle \leq -\delta + \langle \nabla f(x_t) - \nabla f(x_\ast), v - u \rangle \leq \frac{\delta}{2}.
\] (12)

Here in step (a), we use the definition of \( \delta \) in (7) and \( \langle x_\ast, \nabla f(x_\ast) \rangle = \langle v, \nabla f(x_\ast) \rangle \) using the optimality condition for Problem (1) and \( \mathcal{F}(x_\ast) \) being the smallest face containing \( x_\ast \). In step (b), we use the bound in (11), Lipschitz continuity of \( \nabla f(x) \), and \( \|v - u\| \leq D \).

Thus, the \( kLOO \) step will produce all the vertices in \( \mathcal{F}(x_\ast) \) as \( k \geq r_\ast \) after \( t \geq T \), and so \( x_\ast \) is a feasible and optimal solution of the optimization problem in the \( k \) direction search step. Hence, Algorithm 2 finds the optimal solution \( x_\ast \) within \( T + 1 \) many steps. The case for unit group norm ball can be similarly analyzed and we defer the detail to Section B.4 in the appendix.

Remark 8 (The burn-in period \( T \)). The initial “burn-in” period scales as \( \mathcal{O}\left(\frac{4L_f^2 D^4}{\gamma \delta^2}\right) \), which is arguably too large for certain choice of \( L_f, D, \gamma \), and \( \delta \). It is possible to remedy the situation for many polytopes by incorporating the technique from [GM16] by simply adding the atom \( \gamma_t(v_t^+ - v_t^-) \) proposed in [GM16, Algorithm 3] into our \( kDS \). Utilizing their convergence rate result [GM16, Theorem 1], the time \( T \) an be improved to \( \text{card}(x_\ast) 2L_f D^2 \log \left(\frac{4L_f^2 D^2}{\delta^2} \right) \), where \( \text{card}(x_\ast) \) is the number of nonzeros in \( x_\ast \). However, we note that in our experiments, the number of iterations of \( kFW \) is extremely low and the estimate \( T \) is too pessimistic.

Remark 9 (Subproblem complexity). The finite complexity result for the polytope and group norm ball requires that each \( kDS \) solves the subproblem [3] exactly. A closer look reveals that the proof basically assumes that \( kFW \) achieves the worst case rate \( \mathcal{O}(1/t) \) rate in the beginning, and once the iterate is close to \( x_\ast \), \( kLOO \) finds the optimal face and \( kDS \) finds the solution \( x_\ast \). For a theoretical analysis purpose of lowering the complexity in terms of gradient computation, \( LOO \), and \( kLOO \), one can modify the algorithm (assuming knowing the constant \( L_f, D, \gamma \), and \( \delta \)) so it first perform \( T \) many iterations of \( FW \) with stepsize rule \( O(1/t) \); and then perform one \( kLOO \) and one \( kDS \). This algorithm will require \( T \) many gradient computation in the first stage and \( k \) many \( LOO \), and one \( kLOO \) and one \( kDS \) in the second stage. If \( APG \) is employed in solving the problem in \( kDS \), one requires \( \mathcal{O}\left(\frac{1}{\sqrt{\epsilon}}\right) \) gradient computation. In our experiments, we found the subproblem is not too hard to solve to high accuracy and employing \( kDS \) in the beginning significantly reduces the total time.

Convergence for the spectrahedron and nuclear norm ball differs because any neighborhood of \( X_\ast \), contains infinitely many matrices with rank \( \leq r_\ast \). The proof appears in Section B.5 in the appendix.
Theorem 10. Instate the assumption of Theorem 7. Then if the constraint set is the spectrahedron or the unit nuclear norm ball, the gap $\delta > 0$ and $kFW$ satisfies that for any $t \geq T := \frac{72L_f^3}{\gamma \delta^2}$,

$$f(X_{t+1}) - f(X_*) \leq \left(1 - \min \left\{ \frac{\gamma}{4L_f}, \frac{\delta}{12L_f} \right\} \right) (f(X_t) - f(X_*)).$$ (13)

3.3 A limitation of $kFW$ for polytopes and potential fixes

As stated in Theorem 7, $kFW$ needs the parameter $k$ to be greater than or equal to the sparsity level $r_*$, which is the number of vertices of the optimal face instead of $1 + \dim(\mathcal{F}(x_*))$, the face dimension plus one. The number $r_*$ can be arbitrarily larger than the dimension $1 + \dim(\mathcal{F}(x_*))$ for some sets $\Omega$. This in turn means that $k$ has to be very large, at least in theory.

Indeed, the following Example 3.1 shows that if $k$ is only larger than $1 + \dim(\mathcal{F}(x_*))$, but not larger than $r_*$, $kFW$ can behave as bad as standard Frank-Wolfe. The slowdown occurs for the same reason as the zigzagging slowdown in Frank Wolfe: if all the vertices selected are nearly linearly dependent, they do not necessarily span the whole face, so $x_*$ may lie far from their convex hull even though they lie on the same face as $x_*$.

Example 3.1 (A worst case example). Consider the following problem:

$$\begin{align*}
\text{minimize} & \quad f(x, y, z) := x^2 + y^2 + z \\
\text{subject to} & \quad x \in \Omega := \{(x, y, z) \mid \sqrt{x^2 + y^2} \leq 1 - z\}. \tag{14}
\end{align*}$$

The constraint set $\Omega$ is an ice-cream cone. It is easily verified that the origin $(0, 0, 0)$ is the solution and that strict complementarity holds for this problem. Now, if we start at $x^0 = (x_0, y_0, z_0) = (0, 0, 0.1)$ and use FW to solve the problem, it can be shown that FW will produce iterates $x^1, x^2, x^3, \ldots, x^t, \ldots$ that converge to the solution $(0, 0, 0)$ with rate $f(x^t) \geq \frac{c}{t}$ for some constant $c$. A numerical demonstration of the slow convergence is shown by the line “FWSOC” in Figure 5 for the objective value of the first 30 iterations.

Next consider the constraint set $\Omega_n = \text{conv}((0, 0, 1), \{\theta_i\}_{i=1}^n)$ where $\theta_i = (\cos(2\pi i/n), \sin(2\pi i/n), 0)$. In other words, $\Omega_n$ is the polytope being a convex hull of the vertex $(0, 0, 1)$ and a $n$-polygon on the $x$-$y$ plane. We now consider

$$\begin{align*}
\text{minimize} & \quad f(x, y, z) := x^2 + y^2 + z \\
\text{subject to} & \quad x \in \Omega_n. \tag{15}
\end{align*}$$

The $n$-polygon on the $x$-$y$ plane approximates the unit disk for large $n$, also see Figure 3 for an illustration of this approximation. Hence, the feasible region $\Omega_n$ approximates $\Omega$ for large $n$ (see 3 for a comparison), and we expect FW applied to Problem (14) and (15) behaves similarly. One can verify that the origin is still the solution and that strict complementarity continues to holds for $n \geq 3$. Moreover, the strict complementarity parameter $\delta_0$ for this problem is exactly the same for all $n \geq 3$. The quadratic growth parameter $\gamma$ also stabilizes for all large $n$. Now consider running $kFW$ starting from $x^0 = (x_0, y_0, z_0) = (0, 0, 0.1)$. Then for any $T$ and $k$, there is an $N$ such that for all $n > N$, the $kFW$ iterate $x^{t,kFW}$ does not stop after $T$ iterations and $f(x^{t,kFW}) \geq \frac{c}{t}$ for all $t \leq T$. This is because for each $T$ and $k$, we can increase $n$ so that $\Omega_n$ is close enough to $\Omega$. The closeness in the feasible region make the vertices found by $kFW$ tend to be quite close to each other (just like the vertices found by FW), and they fail to form a convex combination of the optimal solution. Hence $x^{t,kFW}$ will be very close to $x^t$ and by our result from previous paragraph, we should have $f(x^{t,kFW}) \geq \frac{c}{t}$ for all $t \leq T$. A numerical illustration of this fact for the first 30 iterations of FW and $kFW$ can be found in Figure 5. In this case, the dimension of the optimal face is always 2, but the number of vertices on the optimal face, $r_*$, grows with $n$ and can be arbitrarily larger than 2.
Figure 3: The left plot shows a second order cone in (14). The right plot shows a polyhedron in (15) that approximates the second order cone.

Figure 4: From left to right, we show the $n$-polygon, the bottom of the feasible region (15), that approximates the disk, the bottom of the second order cone.
Figure 5: The objective value of different algorithms for (14) and (15). FWSOC shows the behavior of FW applied to (14). The other lines are different algorithms applies to (15). LFW stands for limited memory Frank-Wolfe, which always keep the most recent 2 vertices found by LOO, and optimal over the convex hull of the current iterate and these two past vertices. PairFW stands for pairwise FW.

A quick fix  We could remedy the problem with a stronger oracle: for example, one that outputs vertices that are always linear independent, or (even better) an oracle that can output a set of vertices whose convex hull contains $x^\star$ whenever the iterate is close to $x^\star$. If the oracle can achieve this latter property, then $k = 1 + \dim(F(x^\star))$ suffices for fast convergence by Caratheodory's theorem. Hence we avoid the dependence on $r^\star$ defined here. These strong oracles exist for some sets, such as the simplex, the $\ell_1$ norm ball, and the spanning tree in a graph (in the sense of orthogonality), but in general they may be prohibitively expensive to compute.

The relation between $r^\star$ and $\dim(F(x^\star))$  For polytopes encountered in practice, the relation between $r^\star$ and the face dimension varies. For the probability simplex and the $\ell_1$ norm ball, $r^\star = 1 + \dim(F(x^\star))$. Frank Wolfe is often used to optimize over these sets, and our algorithm presents a substantial advantage here. For other types of polytope, the dependence of $r^\star$ on the face dimension can be polynomial or exponential, e.g., products of simplices and Birkhoff polytopes.

Our responses to the limitation  The limitation of $k \geq r^\star$ instead of $k \geq \dim(F(x^\star)) + 1$ of our theory need not spell disaster in practice: small $k$ can still work. First, if $x^\star$ is a vertex or $x^\star$ lies on a 1 dimensional line segment, then $r^\star = 2$ suffices. More generally, if $x^\star$ lies on a face with dimension independent of the ambient dimension $n$, then $r^\star$ is independent of $n$ even if it is exponential in $\dim(F(x^\star))$. Second, even if $r^\star$ is polynomial or exponential in the dimension of the face $F(x^\star)$, it is sometimes still easy to solve the $k$LOO and $k$DS subproblem: for example, these subproblem are still easy for the simplex, a product of simplices, the $\ell_1$ norm ball, or a product of $\ell_1$ norm balls. See Remark 1 for a detailed discussion. Finally, as shown by the following example,
Figure 6: Relative objective \( \frac{f(x) - f(x^\star)}{f(x^\star)} \) for the hypercube problem (16) of different algorithms.

we found that in numerics, a modified version of \( k \)FW which incorporates limited past information can limit the choice of \( k \) to \( \mathcal{O}(\dim(F(x^\star))) \) even though the vanilla version may fail.

Example 3.2. We consider the problem of projection to the hypercube \([0, 1]^n\):

\[
\begin{align*}
\text{minimize} & \quad f(x) := \|x - x_0\|_2^2 \\
\text{subject to} & \quad x \in [0, 1]^n.
\end{align*}
\]  

We perform experiments with \( n = 50 \) and set the first 10 coordinates of \( x_0 \) to be uniformly chosen from \([0, 1]\), and set the rest of the coordinates to be \( 2 \). This choice of \( x_0 \) ensures the strict complementarity condition is satisfied. We compute the optimal solution of (16) via Sedumi \cite{Stu99} and found it is has 40 ones and all the other entries are in \((0, 1)\). Note this face has \( 2^{40} \) many vertices though. Hence the optimal face is \( F(x^\star) \) is 10 dimensional. We set \( k = 10 \) and we try (1) FW, (2) \( k \)FW with \( k = 11 \), (3) \( k \)FW with limited memory (\( Lk \)FW), that is, we also keep the most recent \( k - 1 \) vertices found by LOO in the past \( k - 1 \) iterations, and then add them together with the output of \( k \)LOO into \( 2k - 1 \)-DS. (4) FW with limited past information (LFW), which call LOO once in every iteration, but keep the most recent \( k - 1 \) vertices found by LOO in the past \( k - 1 \) iterations. The results of the objective value against the iteration is shown in Figure 6. It can be seen that once past information is incorporated, \( Lk \)FW is able to find the optimal solution in very few iterations while the vanilla \( k \)FW behaves similarly to FW. It is also interesting LFW itself is as fast as \( Lk \)FW for this problem.

4 Numerics

In this section, we perform experiments to see the empirical behavior of \( k \)FW. We first start with synthetic datasets, where we set \( k \) to be the ground truth of the sparsity measure. Next, we
experiment on real data, we determine $k$ according to the expected sparsity level of the data (e.g. the expected number of support vectors in SVM).

### 4.1 Synthetic data

We compare our method $k$FW with FW, away-step FW (awayFW) [GM86], pairwise FW (pairFW) [LJJ15], DICG [GM16], and blockFW [AZHHL17] for the Lasso, support vector machine (SVM), group Lasso, and matrix completion problems on synthetic data. Details about experimental settings appear in the Appendix D. All algorithms terminate when the relative change of the objective is less than $10^{-6}$ or after 1000 iterations. As shown in Figure 7, $k$FW converges in many fewer iterations than other methods. Table 2 shows that $k$FW also converges faster in wall-clock time, with one exception (blockFW in matrix completion). Note that blockFW is sensitive to the step size while $k$FW has no step size to tune. More numerics can be found in Appendix D.

![Figure 7: $k$FW vs. FW and its variants](image)

Table 2: Computation time (seconds): the algorithms terminate when the relative change of the objective $< 10^{-6}$ or after 1000 iterations. The dash - means the algorithm is not suited to the problem.

|                  | FW | awayFW | pairFW | DICG | blockFW | $k$FW |
|------------------|----|--------|--------|------|---------|-------|
| Lasso            | >14| 7      | 6      | 10   | -       | 0.5   |
| SVM              | 6  | 4.5    | 2.9    | 2.5  | -       | 0.6   |
| Group Lasso      | 17 | 6      | 1.8    | -    | -       | 0.3   |
| Matrix completion| >180| -      | -      | -    | 1.8     | 4.8   |

**Time of $k$LOO and $k$DS** In the experiments, the time cost ratios $k$LOO:$k$DS are approximately: Lasso 0.6:1, SVM 0.03:1, Group Lasso 0.2:1, MC 0.1:1. The time of $k$FW spends on $k$DS occupies a major fraction of the total time. However, the spend is worthwhile as the number of iteration is extremely reduced indicated by our experiments.

### 4.2 Real data

First, we randomly choose 5000 samples of each digit of the MNIST [LBBH98] dataset to form a dictionary $A \in \mathbb{R}^{784 \times 50000}$. Given an image $b$ from the rest of the dataset, we add Gaussian noise (zero mean and 0.1 variance) to it (denoted by $\tilde{b}$) and use sparse coding to denoise, i.e. $\hat{x} = \arg\min_x \|Ax - \tilde{b}\|^2$ subject to $\|x\| \leq 2$. In $k$FW, we set $k = 50$. In every algorithm, the optimization is terminated if the relative change of the objective function is less than $10^{-4}$ or the iteration number reaches 500. The recovered image is $\hat{b} = A\hat{x}$. The recovery error is defined as $RE = \|\hat{b} - b\|/\|b\|$. Table 3 shows three examples. We see that $k$FW is significantly faster than
other methods in all cases and the recovery error of $k$FW is much lower than DICG. Figure 8 shows some examples intuitively.

| digit | metric | FW | awayFW | pairFW | DICG | $k$FW |
|-------|--------|-----|--------|--------|------|-------|
| 0     | TC     | 18.2| 19.1   | 18.9   | 4.0  | 1.6   |
|       | RE     | **0.2634** | 0.2641 | 0.2645 | 0.2665 | 0.2639 |
| 1     | TC     | 18.7| 18.1   | 18.2   | 5.7  | **3.2** |
|       | RE     | 0.3725 | 0.3764 | 0.3731 | 0.4010 | **0.3632** |
| 2     | TC     | 18.3| 18.4   | 18.1   | 6.1  | **2.3** |
|       | RE     | 0.3272 | 0.3281 | 0.3267 | 0.3383 | **0.3258** |
| 3     | TC     | 18.2| 18.3   | 18.1   | 6.1  | **2.4** |
|       | RE     | **0.2577** | 0.2607 | 0.2587 | 0.2653 | 0.2581 |
| 4     | TC     | 18.4| 18.2   | 18.1   | 6.1  | **4.0** |
|       | RE     | **0.3240** | 0.3273 | 0.3263 | 0.3256 | 0.3249 |
| 5     | TC     | 18.7| 18.3   | 18.3   | 6.5  | **2.8** |
|       | RE     | 0.3136 | 0.3132 | 0.3134 | 0.3264 | **0.3110** |
| 6     | TC     | 18.6| 18.4   | 18.6   | 6.1  | **3.9** |
|       | RE     | **0.2772** | 0.2792 | 0.2800 | 0.2890 | **0.2772** |
| 7     | TC     | 18.2| 18.2   | 18.4   | 6.6  | **3.0** |
|       | RE     | 0.3315 | 0.3297 | 0.3301 | 0.3296 | **0.3237** |
| 8     | TC     | 17.4| 17.6   | 18.4   | 2.8  | **2.3** |
|       | RE     | 0.3072 | **0.3066** | 0.3072 | 0.3555 | 0.3069 |
| 9     | TC     | 18.3| 18.0   | 18.0   | 7.6  | **2.2** |
|       | RE     | 0.3575 | 0.3598 | 0.3573 | 0.3618 | **0.3535** |

Second, we consider the SVM classification task on the MNIST dataset. We randomly choose 5000 samples of digit “0” and 5000 samples of digit “6”. The training-testing ratio is 8:2. In $k$FW, we set $k = 50$. The time cost and classification accuracy (average of 10 trials) in the condition of different number of iterations are reported in Table 4. With 50 iterations, the SVM solved by $k$FW achieved a classification accuracy of 0.9934 while the accuracies of SVM solved by other algorithms are lower than 0.9. In general, the results in Table 4 indicate that $k$FW is much more efficient than other algorithms in solving the optimization of SVM.

Table 4: SVM (with second-order polynomial kernel, $C = 10$, and $\lambda = 0.1$) classification for digits “0” and “6” of MNIST (TC: time cost (second); Acc: classification accuracy).

| iterations | metric | FW | awayFW | pairFW | DICG | $k$FW |
|------------|--------|-----|--------|--------|------|-------|
| 10         | TC     | 6.6 | 7.5    | 3.8    | 3.1  | **1.2** |
|            | Acc    | 0.5094 | 0.6514 | 0.5691 | 0.6650 | **0.8199** |
| 50         | TC     | 44.0| 48.6   | 19.6   | 14.9 | **5.6** |
|            | Acc    | 0.8331 | 0.8364 | 0.7997 | 0.8728 | **0.9934** |
| 200        | TC     | 239.0| 261.1  | 90.1   | 60.9 | **22.6** |
|            | Acc    | 0.9236 | 0.9852 | 0.9503 | 0.9915 | **0.9966** |
| 500        | TC     | 722.3| 743.5  | 265.1  | 155.4 | **55.7** |
|            | Acc    | 0.9834 | 0.9931 | 0.9916 | 0.9957 | **0.9962** |

Finally, we consider an inpainting problem for the gray-scale image shown in Figure 9. We
randomly remove 50% of the pixels. Since the image matrix $X_{\text{org}}$ is approximately low-rank, we use $\|X\|_{\text{nuc}} \leq 0.8\alpha$, where $\alpha$ is the value of the nuclear norm of $X_{\text{org}}$. In blockFW and $k$FW, we set $\eta = 5$. In Figure 9, we see that blockFW with $\eta = 0.1$ outperformed our $k$FW slightly in terms of PSNR. In addition, the time cost of $k$FW is 2.5 times of blockFW. However, blockFW requires a well determined step size $\eta$.
5 Conclusion and discussion

This paper presented a new variant of FW, \( k \text{FW} \), that takes advantage of sparse structure in problem solutions to offer much faster convergence than other variants of FW, both in theory and in practice. \( k \text{FW} \) avoids the Zigzag phenomenon by optimizing over a convex combination of the previous iterate and \( k \) extreme points of the constraint set, rather than one, at each iteration. The method relies on the ability to efficiently compute these \( k \) extreme points (\( k \text{LOO} \)) and to compute the update (\( k \text{DS} \)), which we demonstrate for a variety of interesting problems.

Apart from the algorithmic advance of the introduction of \( k \text{LOO} \) and \( k \text{DS} \) for various settings, theoretically, a more uniform, geometric definition of strict complementarity that unifies and extends previous work \[ \text{DFXY20} \] [Gar19a] [Gar20], and allows us to handle a wide range of problems in a coherent framework.

**Related work and comparison** A recent line of work \[ \text{DFXY20} \] [Gar19a] [Gar20] [DCP20] [CDLP21] utilizes the concept of strict complementarity or the local geometry of (1) near \( x^* \) to show faster convergence when the iterate is near the solution. [Gar19a] studies vanilla FW for spectrahedron with rank one solution and [DFXY20] shows how to deal with general rank by utilizing \( k \text{LOO} \) and \( k \text{DS} \) (specFW in their language). The work [Gar20] revisits away-FW and show the method achieves better local convergence rate. In [DCP20] [CDLP21], the authors tries to accelerate away-FW when the iterate is close to the solution for polytope constraint.

Comparably, these past works are rather specific, in particular, strict complementarity is defined specific to each setting rather than in a uniform way. Nevertheless, the present work is inspired from [DFXY20] and the contribution of the present work is to distill and generalize the ideas there to various settings such as polytope, group norm ball, and nuclear norm ball. In particular, the extension to the nuclear norm from the spectrahedron is important for several reasons: (i) The nuclear norm ball (NNB) formulation is the natural problem form for rectangular matrix recovery problems; (ii) To apply the spectrahedron formulation to NNB formulation would require dilation, which doubles the number of variables. Moreover, a quadratic growth objective does not have quadratic growth after dilation, so existing theory for the spectrahedral case does not apply; (iii) Technically, our analysis is similar to [DFXY20] but introduces several novel elements; note in particular that the SC defined in the present paper generalizes that in [DFXY20].

The idea of utilizing multiple directions instead of just one is rooted in fully-corrective FW and related variants. It is also explored in recent works such as [AZHHL17] [BRZ20]. [AZHHL17] deals with nuclear norm ball and computes multiple singular vectors in each iteration in order to make a gradient step. Note that even though [AZHHL17] considers computing \( k \) singular vectors, the \( k \text{LOO} \) is not based on the gradient but rather primal iterate - gradient, which may induces some computation difficulty due to the higher rank of iterates. More importantly, it may not converge for \( k < r^* \) as shown in [AZHHL17] Figure 1, while kFW converges always as shown in Theorem 6. The work [BRZ20] considers how to identify the vertices on the optimal face via away-FW, however, the result is limited to probability simplex.

**Future work** We expect the core ideas that undergird \( k \text{FW} \) can be generalized to a wide variety of atomic sets in addition to those considered in this paper. We also expect the idea of \( k \text{DS} \) and a limited memory Frank-Wolfe, which uses most recent \( k \) points found by LOO, can still succeed for polytopes with \( r^* \), much larger than the dimension of the optimal face.
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A Table and Procedures for Section 2

A.1 kLOO and kDS for Spectrahedron

We define kLOO and kDS for the spectrahedron $\mathcal{SP}^n = \{ X \in \S^n \mid X \succeq 0, \, \text{tr}(X) = 1 \}$ in this section.

**kLOO.** Given an input matrix $Y \in \S^n$, define the $k$ best directions of the linearized objective $\min_{V \in \mathcal{SP}^n} \langle V, Y \rangle$ as the bottom $k$ eigenvectors of $Y$, the eigenvectors corresponding to the $k$ smallest eigenvalues. Call these vectors $v_1, \ldots, v_k$ and collect the output as $V = [v_1, \ldots, v_k] \in \R^{n \times k}$.

**kDS.** Take as inputs $W \in \mathcal{SP}^n$ and $V = [v_1, \ldots, v_k] \in \R^{n \times r}$ with orthonormal columns. Instead of convex combinations of $W$ and $v_i v_i^\top$, we consider a spectral variant inspired by [HR00]:

$$X = \eta W + VS V^\top \quad \text{where} \quad \eta \geq 0, \, S \in \S^k_+, \, \eta + \text{tr}(S) = 1.$$  

We minimize the objective $f(X)$ over this constraint set to obtain the solution $X_{kDS}$ to kDS:

$$\minimize \ f(\eta W + VS V^\top) \quad \text{subject to} \quad \eta \geq 0, \, S \in \S^k_+, \, \text{and} \, \eta + \text{tr}(S) = 1.$$  

Again, we use APG to solve this problem. Projection onto the constraint set requires eigenvalue decomposition (EVD) of a $k^2$ matrix, which is tolerable for small $k$. (See more detail in Section A.6)
A.2 \(k\text{LOO} \) of combinatorial optimization

In this section, we present Table 5 of the computational complexity of finding the \(k\) best solution for combinatorial optimizations. In our setting, the \(k\) best solution corresponds to the \(k\) best directions of \(k\text{LOO}\). We then point out those \(k\text{LOO}\) that can be efficiently computed.

Let us first look at Table 5 for the complexity of \(\text{LOO}\) and \(k\text{LOO}\).

Table 5: The time complexity of \(\text{LOO}\) for different combinatorial problems. The matroid \(M = (E, \mathcal{I})\) consists of the ground set \(E\) with \(n\) elements and the set of bases \(\mathcal{I}\). The polytope is the convex hull of all bases in \([0, 1]^m\). The quantity \(\alpha\) is the complexity of checking independence of a set. Here \(r(M)\) is the rank of the matroid \(M\). The \(s - t\) cut is for a directed graph with \(n\) nodes, \(m\) edges, a source node \(s\), and a sink node \(t\). For each \(s - t\) cut, a partition \(S, S^c\) of the vertex set with \(s \in S\) and \(t \in S^c\), we define its cut point as a vector in \([-1, 1]^m\) that has entry 1 for an edge from \(S\) to \(S^c\), and an entry \(-1\) for an edge from \(S^c\) to \(S\). The \(s - t\) cut polytope is the convex hull of all cut points in \([-1, 1]^m\). The path polytope considers all simple path from \(s\) to \(t\) for a directed acyclic graph with \(n\) nodes and \(m\) edges. The polytope is then the convex hull of all simple path point in \([0, 1]^m\).

For an undirected graph with \(n\) nodes and \(m\) edges, the spanning tree polytope is the convex hull of all spanning tree in \([0, 1]^m\).

| Polytope name                        | LOO complexity    | \(k\text{LOO}\) complexity |
|--------------------------------------|-------------------|------------------------------|
| Probability simplex                  | \(O(n)\)          | \(O(n + k)\) [MR01]         |
| Polytope of bases of a matroid \(M\) | \(O(n \log n, n\alpha)\) | \(O(n \log n + knr(M)\alpha)\) [HQ85] |
| The Birkhoff polytope                | \(O(n^3)\)        | \(O(kn^3)\) [Mur68]         |
| \(s - t\) Cut Polytope (Directed Graph) | \(O(nm \log n)\)   | \(O(nm \log n)\) [Epp98]    |
| \(s - t\) path Polytope (DAG)       | \(O(m + n \log n)\) | \(O(m + n \log n + k\min(n, k)^{1/2})\) [Epp90] |
| Spanning tree Polytope               | \(O(m + n \log n)\) | \(O(m \log n + k\min(n, k)^{1/2})\) [Epp90] |

Let us now list other polytopes with efficient \(k\text{LOO}\) with the assumption that \(k \leq n\):

- The \(\ell_1\) norm ball \(\{x \in \mathbb{R}^n \mid \sum_{i=1}^n |x_i| \leq \alpha\}\) admits a \(k\text{LOO}\) with time complexity \(O(n + k)\) by simply considering finding the \(k\) largest elements among \(2n\) elements.
- The spanning tree polytope of an undirected graph \(G(V, E)\) in \(\mathbb{R}^{|E|}\) admits a \(k\text{LOO}\) with time complexity \(O(m \log n + k^2)\), where \(m = |E|\) and \(n = |V|\) [Epp90].
- The Birkhoff polytope, the convex hull of permutation matrices in \(\mathbb{R}^{n \times n}\), admits a \(k\text{LOO}\) with time complexity \(O(kn^3)\) [Mur68].
- The path polytope of a directed acyclic graph \(G(V, E)\) in \(\mathbb{R}^{|E|}\) admits a \(k\text{LOO}\) with time complexity \(O(m + n \log n + k \min(n, k)^{1/2})\), where \(m = |E|\) and \(n = |V|\) [Epp98].

Optimization over the probability simplex is useful for fitting support vector machines [Cla10, Problem (24)]. The \(\ell_1\) norm ball plays a key role in sparse signal recovery [CDS01]. The path polytope appears in applications in video-image co-localization [JTFF14].

A.3 Examples of \(k\text{LOO}\) and \(k\text{DS}\)

This section presents Table 6 which presents examples of efficiently-computable \(k\text{LOO}\), and which presents examples of efficiently-computable \(k\text{DS}\).
Table 6: kLOO examples: The input is a vector $y$ for the polytope and unit group norm ball (with base norm $\ell_2$ norm), and a matrix $Y$ for the spectrahedron and unit nuclear norm ball.

| Name               | $k$ best direction and output                                      | kLOO cost                      |
|--------------------|-------------------------------------------------------------------|--------------------------------|
| Polytope           | $k$ extreme points $v_i$'s with $k$ smallest $\langle v, y \rangle$ among all extreme points $v$ | See Table 5                   |
| Unit group norm ball| $k$ groups $v_1, \ldots, v_k \in G$ of the largest $\ell_2$ norm of $y$ | $O(\sum_{i=1}^k |v_i|) + k \log k)$ |
| Spectral simplex   | bottom $k$ eigenvector $v_i$'s of $Y$, output $V = [v_1, \ldots, v_k]$ | Computing bottom $k$ eigenvectors |
| Unit nuclear norm Ball | top $k$ left, right singular vectors $(u_i, v_i)$ of $Y$, output $U = [u_1, \ldots, u_k], V = [v_1, \ldots, v_k]$. | Computing top $k$ singular vectors |

Table 7: $k$ direction search examples. We present the parametrization of the vector $x$ or matrix $X$ in the second column. The $k$DS optimization problem is to minimize $f(x)$ or $f(X)$ over the parametrization. The input is a vector $w$ or a matrix $W$ in $\Omega$ and another of the form output by kLOO.

| Name               | Parametrization of $x$ or $X$ | Parameter variable | Parameter constraint (p.r.) | Main cost of proj to p.r. |
|--------------------|--------------------------------|--------------------|----------------------------|---------------------------|
| Polytope           | $\eta w + \sum_{i=1}^k \lambda_i v_i$ | $(\eta, \lambda) \in \mathbb{R}^{k+1}$ | $(\eta, \lambda) \in \Delta^{k+1}$ | $O(k \log(k))$            |
| Unit Group norm ball | $\eta w + \lambda_1 v_1, \ldots, \lambda_k v_k$ | $(\eta, \lambda v_1, \ldots, \lambda_k v_k)$ | $\eta + \|\lambda v_1, \ldots, \lambda_k v_k\|_G \leq 1$ | $O(k \log(k)) + O\left(\sum_{i=1}^k |v_i|\right)$ |
| Spectrahedron      | $\eta W + VSV^T$               | $(\eta, S) \in \mathbb{R} \times S^k$ | $\eta \geq 0, S \succeq 0, \eta + \text{tr}(S) = 1$ | $\text{a full EVD}$       |
| Unit nuclear norm Ball | $\eta W + USV^T$               | $(\eta, S) \in \mathbb{R}^{1+k^2}$ | $\eta \geq 0, \eta + \|S\|_{\text{nuc}} \leq 1$ | $\text{a full SVD of a } k^2 \text{ matrix}$ |

A.4 Projection Step in APG for $k$DS of group norm ball

Here we described the projection procedure in $k$DS for group norm ball when the base norm is $\ell_2$ norm. Suppose we want to solve the projection problem given $(\eta_0, \lambda_0 v_1, \ldots, \lambda_k v_k) \in \mathbb{R}^{1+n}$ with decision variable $\eta$ and $\lambda v_1, \ldots, v_k$:

$$\text{minimize } \|\eta_0, \lambda_0 v_1, \ldots, \lambda_k v_k\|_2 \text{ subject to } \eta + \|\lambda v_1, \ldots, v_k\|_G \leq 1, \eta \geq 0. \quad (17)$$

Here we further require that $\lambda_0 v_1, \ldots, v_k$ and $\lambda v_1, \ldots, v_k$ are supported on $\cup_{i=1}^k v_i$. We denote the optimal solution as $(\eta^*, (\lambda v_1, \ldots, v_k)^*)$.

Since $\lambda v_1, \ldots, v_k$ is only supported on $\cup_{i=1}^k v_i$, we can consider it as a vector in $\mathbb{R}^{v_1 + \cdots + v_k}$ and $\|\lambda v_1, \ldots, v_k\|_G = \sum_{i=1}^k \|\lambda v_i \|_G$. The procedure for projection is as follows:

1. First compute the $(\eta^*, a^*)$ that solves

$$\text{minimize}_{\eta, a} \|\eta_0, \lambda_0 v_1, \ldots, \lambda_k v_k\|_2 \text{ subject to } \eta + \|\lambda v_1, \ldots, v_k\|_G \leq 1, \eta \geq 0, \sum_{i=1}^k a_i \leq 1. \quad (18)$$

Here $\mathbb{R}^{k+1}_+$ is the nonnegative orthant in $\mathbb{R}^{k+1}$. 

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2. Next, for each $v_i$, we compute $(\lambda v_1^{v_i}, \ldots, v_k)_{v_i}$ by solving
\[
(\lambda v_1^{v_i}, \ldots, v_k)_{v_i} = \arg \min_{\|\lambda v_1^{v_i}, \ldots, v_k\| \leq a_i^*} \|v_i - \lambda v_1^{v_i}, \ldots, v_k v_i\|_2.
\]

The first step requires a projection to the convex hull of simplex and 0 and can be done in time $O(k \log k)$. The second step requires projection to $\ell_2$ norm ball which is a simple scaling. The correctness can be verified by decomposing each $\lambda v_1^{v_i}, \ldots, v_k v_i = \alpha_i w_i$ where $\alpha_i \geq 0$ and $w_i$ has $\ell_2$ norm 1. For general $\ell_p$ norm, one has to find a root of a monotone function. This problem can be solved by bisection \[Sra11\].

A.5 Discussion on the norm of group norm ball

For the main Theorems 6, 7, and 10, the results holds for any arbitrary norm. The positive gap in Lemma 11 also holds for an arbitrary norm. However, the authors have not been able to verify whether strict complementarity implies quadratic growth for norms other than the $\ell_2$ norm.

A.6 Projection Step in APG for $k$DS of spectrahedron, and nuclear norm ball

We consider how to compute the projection step of $k$DS for the spectrahedron and nuclear norm ball.

**Spectrahedron** We want to find $(\eta^*, S^*)$ that solves
\[
\begin{align*}
\text{minimize} \quad & \| (\eta, S) - (\eta_0, S_0) \|_2, \\
\text{subject to} \quad & S \in \mathbb{S}_k^+, \eta \geq 0, \text{tr}(S) + \eta = 1.
\end{align*}
\]

Here $\| (\eta, S) \|_2 = \sqrt{\eta^2 + \|S\|_F^2}$. The procedures are as follows:

1. Compute the eigenvalue decomposition of $S_0 = V \Lambda_0 V^T$, where $\Lambda_0 \in \mathbb{S}_k^+$ is a diagonal matrix with diagonal $\vec{\lambda}_0 = (\lambda_1, \ldots, \lambda_k)$.

2. Compute $(\eta^*, \vec{\lambda}^*) = \arg \min_{(\eta, \vec{\lambda})\in\Delta_{k+1}} \| (\eta_0, \vec{\lambda}_0) - (\eta, \vec{\lambda}) \|_2$.

3. Form $S^* = V \text{diag}(\vec{\lambda}^*) V^T$. Here $\text{diag}(\lambda)$ forms a diagonal matrix with the vector $\lambda$ on the diagonal.

The main computational step is the eigenvalue decomposition which requires $O(k^3)$ time. The correctness of the procedure can be verified as in [AZHHL17, Lemma 3.1] and [Gar19b, Lemma 6].

**Unit nuclear ball** We want to find $(\eta^*, S^*)$ that solves
\[
\begin{align*}
\text{minimize} \quad & \| (\eta, S) - (\eta_0, S_0) \|_2, \\
\text{subject to} \quad & \eta + \|S\|_{nuc} \leq 1, \eta \geq 0.
\end{align*}
\]

The procedures are as follows:

1. Compute the singular value decomposition of $S_0 = U \Lambda_0 V^T$, where $\Lambda_0 \in \mathbb{S}_k^+$ is a diagonal matrix with diagonal $\vec{\lambda}_0 = (\lambda_1, \ldots, \lambda_k)$.

2. Compute $(\eta^*, \vec{\lambda}^*) = \arg \min_{(\eta, \vec{\lambda})\in\Delta_{k+1}} \| (\eta_0, \vec{\lambda}_0) - (\eta, \vec{\lambda}) \|_2$.

3. Form $S^* = U \text{diag}(\vec{\lambda}^*) V^T$. Here $\text{diag}(\lambda)$ forms a diagonal matrix with the vector $\vec{\lambda}^*$ on the diagonal.

The main computational step is the singular value decomposition which requires $O(k^3)$ time. The correctness of the procedure can be verified as in [AZHHL17, Lemma 3.1] and [Gar19b, Lemma 6].
B  Examples, lemmas, tables, and Proofs for Section 3

B.1  Further discussion on strict complementarity

We give two additional remarks on the strict complementarity.

1. Traditionally, the boundary location condition \( x \in \partial \Omega \) is not included in the definition of strict complementarity. We include this condition for two reasons: first, the extra location condition excludes the trivial case that the dual solution of (1) is 0, and \( x_* \) in the interior of \( \Omega \), in which case FW can be proved to converges linearly [GH15]; second, as we shall see in Example B.1, such assumption ensures the robustness of the sparsity of \( x_* \).

2. Strict complementarity (without the boundary location condition) holds generically: more precisely, it holds for almost all \( c \) in our optimization problem (1), \( \min_{x \in \Omega} g(Ax) + \langle c, x \rangle \), [DL11] Corollary 3.5.

Example B.1. Consider the problem

\[
\min_{x \in [\alpha \Delta^\alpha]} \frac{1}{2} \|x - e_1 - \frac{1}{n} 1\|^2.
\]

Here \( 1 \) is the all one vector and \( \alpha > 0 \). If we set \( \alpha = 1 \), then \( x_* = e_1 \) and the gradient \( \nabla f(x_*) = -\frac{1}{n} 1 \). Hence we see that strict complementarity does not hold, using Lemma 11. In this case, even though \( x_* = e_1 \) is sparse for \( \alpha = 1 \), the solution is no longer sparse when \( \alpha \) is slightly larger than 1. Hence, we see a perturbation to the constraint can cause instability of the sparsity when strict complementarity fails.

B.2  Lemmas and tables for strict complementarity

In this section, we show that the gap quantity defined in Definition 2 is indeed positive when strict complementarity holds. We then present a table of summarizing the notations \( F(x_*), F^c(x_*), \) and the gap \( \delta \).

Here, for the group norm ball, we consider a general norm denoted as \( \| \cdot \| \) which is not necessarily the Euclidean \( \ell_2 \) norm. The dual norm of \( \| \cdot \| \) is defined as \( \|x\|_* = \max_{\|y\| \leq 1} \langle y, x \rangle \). We note here the group norm ball is assumed to have radius one.

Lemma 11. When \( \Omega \) is a polytope, group norm ball, spectrahedron, and nuclear norm ball, if strict complementarity holds for Problem (1), then the gap \( \delta \) is positive. Moreover, we can characterize the gradient at the solution and the size of the gap in each case:

- Polytope: order the vertices \( v \in \Omega \) according to the inner products \( \langle \nabla f(x_*), v \rangle \) in ascending order as \( v_1, \ldots, v_{r_*}, \ldots, v_l \) where \( l \) is the total number of vertices. Then \( \langle \nabla f(x_*), v_i \rangle, i = 1, \ldots, r_* \) are all equal and the gap \( \delta \) is \( \delta = \langle \nabla f(x_*), v_{r_*+1} \rangle - \langle \nabla f(x_*), v_{r_*} \rangle \).

- Group norm ball for arbitrary base norm: order vectors \( \|\nabla f(x_*)\|_g, g \in G \) according to their dual norm in descending order as \( \|\nabla f(x_*)\|_{g_1}, \ldots, \|\nabla f(x_*)\|_{g_{|G|}} \). Then \( \|\nabla f\|_{g_i} \), \( i = 1, \ldots, r_* \) are all equal, and the gap \( \delta \) is \( \delta = \|\nabla f(x_*)\|_{g_{r_*+1}} - \|\nabla f(x_*)\|_{g_{r_*}} \).

- Spectrahedron: The smallest \( r_* \) eigenvalues of \( \nabla f(X_*) \) are all equal and \( \delta = \lambda_{n-r_*}(\nabla f(X_*)) - \lambda_{n-r_*+1}(\nabla f(X_*)) \).

- Nuclear norm ball: The largest \( r_* \) singular values of \( \nabla f(X_*) \) are all equal and \( \delta = \sigma_{r_*}(\nabla f(X_*)) - \sigma_{r_*+1}(\nabla f(X_*)) \).

Proof. Let us first consider the polytope case.
**Polytope.** Since the constraint set is a polytope and \( x_* \in \partial \Omega \), we know the smallest face \( F(x_*) \) containing \( x \) is proper and admits a face-defining inequality \( \langle a, x \rangle \leq b \) for some \( a \in \mathbb{R}^n \) and \( b \in \mathbb{R} \). That is, \( F(x_*) = \{ x \mid \langle a, x \rangle = b \} \cap \Omega \) and for every \( x \in \Omega \), \( \langle a, x \rangle \leq b \). In particular, this implies that (1) for any vertex \( v \) that is not in \( F(x_*) \), \( \langle a, v \rangle < b \), and (2) \( \langle a, x_* \rangle = b \).

Let us now characterize the normal cone \( N_\Omega(x_*) \). Let \( \mathcal{V} \) be the set of vertices in \( \Omega \). Since \( \Omega \) is bounded, we know that every point in \( \Omega \) is a convex combination of the vertices. Hence \( N_\Omega(x_*) \) is the set of solutions \( g \) to the following linear system:

\[
\langle g, v \rangle \leq \langle g, x_* \rangle, \quad \text{for all} \quad v \in \mathcal{V}. \tag{19}
\]

Since \( F(x_*) \) is the smallest face containing \( x_* \), we know that \( x_* \in \text{relint}(F(x_*)) \), and so the description of normal cone \( N_\Omega(x_*) \) in (19) reduces to

\[
\langle g, v_1 \rangle = \langle g, x_* \rangle, \quad \text{for all} \quad v_1 \in F(x_*), \tag{20}
\]

\[
\langle g, v_2 \rangle \leq \langle g, x_* \rangle, \quad \text{for all} \quad v_2 \text{ being vertices of } \mathcal{F}^c(x_*). \tag{21}
\]

Note that the vector \( a \) in the face-defining inequality satisfies (20) and satisfies (21) with strict inequality. Hence, the relative interior of \( N_\Omega(x_*) \) consists of those vectors \( g \) that satisfy (20) and satisfy (21) with a strict inequality. As \( -\nabla f(x_*) \in \text{relint}(N_\Omega(x_*)) \), we know by the previous argument that \( -\nabla f(x_*) \) satisfies (21) with strict inequality, which is exactly the condition \( \delta > 0 \). We arrive at the formula for \( \delta \) by noting that \( \langle \nabla f(x_*), v \rangle = \langle \nabla f(x_*), x_* \rangle \) for every \( v \in \mathcal{F}(x_*) \) due to (20).

**Group norm ball.** Again, recall we here define the group norm ball using any general norm \( \| \cdot \| \). The normal cone at \( x_* \) for unit group norm ball is defined as

\[
N_\Omega(x_*) = \{ y \mid \langle y, x \rangle \leq \langle y, x_* \rangle, \quad \text{for all} \quad \sum_{g \in \mathcal{G}} \| x_g \| \leq 1 \}.
\]

Standard convex calculus reveals the following properties:

1. The normal cone is a linear multiple of the subdifferential for \( x_* \in \partial \Omega \): \( N_\Omega(x_*) = \{ y \mid y \in \lambda \partial \| x_* \|_{\mathcal{G}} , \lambda \geq 0 \} \).
2. The product rule applies to \( \partial \| x_* \|_{\mathcal{G}} \) as \( \mathcal{G} \) forms a partition: \( \partial \| x_* \|_{\mathcal{G}} = \prod_{g \in \mathcal{G}} \partial \| (x_*)_g \| \).
3. Any vector in the subdifferential of a group \( g \) in the support of the solution has norm 1: for every \( g \in \mathcal{F}(x_*) \) and every \( y_g \in \partial \| (x_*)_g \| , \| y_g \| \leq 1 \) and \( \langle y_g, (x_*)_g \rangle = \| (x_*)_g \| \).
4. The subdifferential for groups \( g \) not in the support is a unit dual norm ball: for every \( g \notin \mathcal{F}(x_*) \),

\[
\partial \| (x_*)_g \| = B_{\| \cdot \|}, \quad \{ y_g \in \mathbb{R}^{|g|} \mid \| y_g \| \leq 1 \}.
\]

The above properties reveal that the normal cone is the set

\[
N_\Omega(x_*) = \{ y \mid y \in \lambda \left( \prod_{g \in \mathcal{F}(x_*)} \partial \| (x_*)_g \| \times \prod_{g \notin \mathcal{G} \setminus \mathcal{F}(x_*)} B_{\| \cdot \|} \right) , \lambda \geq 0 \}, \tag{22}
\]

where for every \( g \in \mathcal{F}(x_*) \) and every \( y_g \in \partial \| (x_*)_g \| , \| y_g \| = 1 \). Hence, we know that the relative interior of \( N_\Omega(x_*) \) is simply

\[
\text{relint} (N_\Omega(x_*)) \]

\[
= \{ y \mid y \in \lambda \left( \prod_{g \in \mathcal{F}(x_*)} \text{relint} (\partial \| (x_*)_g \|) \times \prod_{g \notin \mathcal{G} \setminus \mathcal{F}(x_*)} \text{relint} (B_{\| \cdot \|}) \right) , \lambda > 0 \}, \tag{23}
\]

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where for every \( g \in \mathcal{F}(x_\ast) \), and every \( y_g \in \text{relint}(\partial \|x_\ast\|_g) \), \( \|y_g\|_\ast = 1 \), and for every \( g \in \mathcal{G} - \mathcal{F}(x_\ast) \), and every \( y_g \in \text{relint}(B_{\|\cdot\|_\ast}) \), \( \|y_g\|_\ast < 1 \). Because of the strict inequality of \( \lambda \) in (23), and strict inequality for \( \|y_g\|_\ast < 1 \) for \( y_g \in \text{relint}(B_{\|\cdot\|_\ast}) \), we see that
\[
\|\nabla f(x_\ast)\|_{g_\ast} = \cdots = \|\nabla f(x_\ast)\|_{g_{\ast+r}} \ast, \quad \text{and}
\|\nabla f(x_\ast)\|_{g_{\ast+r}} - \|\nabla f(x_\ast)\|_{g_{\ast+r+1}} > 0
\]
(24) as \( -\nabla f(x_\ast) \in \text{relint}(N_{\Omega}(x_\ast)) \). Using the condition that for every \( g \in \mathcal{F}(x_\ast) \) and every \( y_g \in \partial \|x_\ast\|_g \), \( \|y_g\|_\ast = 1 \), and \( \langle y_g, (x_\ast)_g \rangle = \|\|x_\ast\|_g \rangle \), we know \( \langle -\nabla f(x_\ast), x_\ast \rangle = \|\nabla f(x_\ast)\|_{g_{\ast+r}} \ast. \) Furthermore, using generalized Cauchy-Schwarz, it can be proved that \( \min_{x \in \mathcal{F}(x_\ast)} \langle \nabla f(x_\ast), x \rangle = -\|\nabla f(x_\ast)\|_{g_{\ast+r+1}} > 0 \). Hence, combining the two equalities with (24), we see that \( \delta > 0 \) and arrive at the stated formula for \( \delta \).

**Spectrahedron.** We first note that \( X_\ast \in \partial \Omega \) and \( \text{tr}(X) = 1 \) imply that \( 1 \leq r_\ast < n \). To compute the normal cone, we can apply the sum rule of subdifferentials to
\[
\chi(\{X \in \mathbb{S}^n \mid \text{tr}(X) = 1\}) + \chi(X \geq 0),
\]
where \( \chi \) is the characteristic function, which takes value 0 for elements belonging to the set and \(+\infty \) otherwise) of \( \{X \in \mathbb{S}^n \mid \text{tr}(X) = 1\} \) and \( \mathbb{S}^n \) and reach
\[
N_{\Omega}(x_\ast) = \{sI \mid s \in \mathbb{R}\} + \{-Z \mid Z \geq 0, \text{range}(Z) \subseteq \text{nullspace}(X_\ast)\}.
\]
(25)
We note that the sum rule for the relative interior is valid here because \( \frac{1}{n} I \) belongs to the interior of both sets. Applying the sum rule to (25), we find that
\[
\text{relint}(N_{\Omega}(x_\ast)) = \{sI \mid s \in \mathbb{R}\} + \{-Z \mid Z \geq 0, \text{range}(Z) = \text{nullspace}(X_\ast)\}.
\]
Or equivalently,
\[
\text{relint}(N_{\Omega}(x_\ast)) = \{sI \mid s \in \mathbb{R}\} + \{-Z \mid Z \geq 0, \text{nullspace}(Z) = \text{range}(X_\ast)\}.
\]
Using the above equality and \( -\nabla f(X_\ast) \in \text{relint}(N_{\Omega}(x_\ast)) \), we know there are \( Z_\ast \geq 0 \) and \( s_\ast \in \mathbb{R} \)
\[
\nabla f(X_\ast) = -s_\ast I + Z_\ast, \quad \text{and} \quad \text{nullspace}(Z_\ast) = \text{range}(X_\ast).
\]
(26)
Denote the eigenspace corresponding to the smallest \( r_\ast \) values of \( \nabla f(X_\ast) \) as \( \text{EV}_{r_\ast}(\nabla f(X_\ast)) \). From (26), it is immediate that
\[
\text{EV}_{r_\ast}(\nabla f(X_\ast)) = \text{range}(X_\ast).
\]
Moreover, from (26), we also have
\[
\lambda_{n-r_\ast+1}(\nabla f(X_\ast)) - \lambda_{n-r_\ast}(\nabla f(X_\ast)) > 0, \quad \text{and} \quad \langle \nabla f(X_\ast), X_\ast \rangle = -s_\ast = \lambda_{n-i+1}(\nabla f(X_\ast)), \quad i = 1, \ldots, r_\ast.
\]
(27)
Combining (27) and the well-known fact that
\[
\min_{X \in \Omega, \text{range}(X) \perp \text{EV}_{r_\ast}(\nabla f(X_\ast))} \langle \nabla f(X_\ast), X \rangle = \lambda_{n-r_\ast+1}(\nabla f(X_\ast)),
\]
we see that \( \delta \) is indeed positive, and the formula for \( \delta \) holds.
Nuclear norm ball. We first note that \( X_* \in \partial \Omega \) imply that \( 1 < r_* < \min(n_1, n_2) \), and \( \| X_* \|_{\text{nuc}} = 1 \). Let the singular value decomposition of \( X_* \) as \( X_* = U \Sigma V \) with \( U \in \mathbb{R}^{n_1 \times r_*} \) and \( V \in \mathbb{R}^{n_2 \times r_*} \). The normal cone of the unit nuclear norm ball is

\[
N_{\Omega}(X_*) = \{ Y \mid Y = \lambda Z, \ Z = UV^T + W, \ W^T U = 0, \ WV = 0, \| W \|_{\text{op}} \leq 1 \text{ and } \lambda \geq 0 \}. \quad (28)
\]

Hence, the relative interior is

\[
N_{\Omega}(X_*) = \{ Y \mid Y = \lambda Z, \ Z = UV^T + W, \ W^T U = 0, WV = 0, \| W \|_{\text{op}} < 1 \text{ and } \lambda > 0 \}, \quad (29)
\]

Since \( -\nabla f(X_*) \in \text{relint}(N_{\Omega}(X_*)) \), we know immediately that

\[
\sigma_{r_*}(\nabla f(X_*)) - \sigma_{r_*+1}(\nabla f(X_*)) > 0, \quad (30)
\]

and the top \( r_* \) left and right singular vectors of \( \nabla f(X_*) \) are just the columns of \( -U \) and \( V \), and \( \langle \nabla f(X_*), X_* \rangle = -\sigma_i(\nabla f(X_*)) \) for \( i = 1, \ldots, r_* \). Combining pieces and the standard fact that

\[
\min_{\text{range}(U) \subseteq \partial \text{range}(U), \| X \|_{\text{nuc}} \leq 1} \langle \nabla f(X_*), X \rangle = -\sigma_{r_*+1}(\nabla f(X_*)),
\]

we see the gap \( \delta \) is indeed positive and the formula is correct.

A table of the notions \( \mathcal{F}(x_*), \mathcal{F}^c(x_*), \) and the formula of gap \( \delta \) is shown as Table 8.

| Constraint \( \Omega \)         | \( \mathcal{F}(x_*) \)                | \( \mathcal{F}^c \)                | \( \delta \) formula                                      |
|---------------------------------|----------------------------------------|------------------------------------|-----------------------------------------------------------|
| polytope                        | smallest face containing \( x_* \)    | convex hull of all the vertices not in \( \mathcal{F}(x_*) \) | \( \langle \nabla f(x_*), v_{r_*+1} \rangle \)  \(-\langle \nabla f(x_*), v_{r_*} \rangle \) |
| group norm ball                 | \( \{ g \in \mathcal{G} \mid (x_*)_g \neq 0 \} \) | \( \{ x \mid x_g = 0, \forall g \in \mathcal{F}(x_*) \} \) | \( \frac{\| \nabla f(x_*) \|_{\text{gr}, r_*} }{2} \)  \(-\frac{\| \nabla f(x_*) \|_{\text{gr}, r_*+1} }{2} \) |
| spectrahedron                   | range(\( X_* \))                      | \( \{ X \in \text{range}(X_*) \} \cap \mathcal{S}P^n \) | \( \lambda_{n-r_*}(\nabla f(x_*)) \)  \(-\lambda_{n-r_*+1}(\nabla f(x_*)) \) |
| nuclear norm ball               | range(\( X_* \))                      | \( \{ X \in \text{range}(X_*) \} \) \cap \mathcal{B}_{\| \text{nuc} \|} | \( \sigma_{r_*}(\nabla f(x_*)) \)  \(-\sigma_{r_*+1}(\nabla f(x_*)) \) |

B.3 Quadratic growth under strict complementarity

This section develops that quadratic growth does hold under strict complementarity and the condition \( g \) in (1) is strongly convex.

Theorem 12. Suppose Problem (1), \( \min_{x \in \Omega} g(Ax) + \langle c, x \rangle \), satisfies that \( g \) is strongly convex and the constraint set \( \Omega \) is one of the four sets (i) polytope, (ii) unit group norm ball, (iii) spectrahedron, and (iv) unit nuclear norm ball. Further suppose that strict complementarity holds. Then quadratic growth holds for Problem (1) as well.
We will use the machinery developed in [ZS17] for the case of the group norm. We define a few notions and notations for later convenience. We define the projection to $\Omega$ as $\mathcal{P}_\Omega(x) := \arg\min_{v \in \Omega} \|x - v\|_2$. The difference of iterates for projected gradient with step size $t$ is defined as $\mathcal{G}_t(x) := \frac{1}{t}(x - \mathcal{P}_\Omega(x - \nabla f(x)))$. Note that $\mathcal{G}_t(x) = 0$ implies $x = x_*$. Finally, for an arbitrary set $\mathcal{S}$, we define the distance of $x \in \mathbb{R}^n$ to it as $\text{dist}(x, \mathcal{S}) := \inf_{v \in \mathcal{S}} \|x - v\|_2$.

Proof. The proof for the polytope appears in [BS17, Lemma 2.5]. The proof of the Spectrahedron appears in [DFXY20, Theorem 6]. Here, we address the case of the group norm ball and Nuclear norm ball. Let us first consider the case of the group norm ball with the $\ell_2$ norm.

**Unit group norm ball.** Using [DL18] Corollary 3.6, we know that if the error bound condition holds for some $t, \gamma > 0$ then the quadratic growth condition holds with some parameter $\gamma'$. The error bound condition with parameter $t, \gamma, \epsilon > 0$ means that for all $x \in \Omega$ and $\|x - x_*\|_2 \leq \epsilon$, the following the inequality holds:

$$\|x - x_*\|_2 \leq \gamma \|\mathcal{G}_t(x)\|_2. \quad (31)$$

Define $\tilde{y} = \mathcal{A}(x_*)$ and $\tilde{h} = \nabla f(x_*)$. Now using [ZS17] Corollary 1 and Theorem 2, we need only verify the following two conditions to establish (31):

1. **Bounded linear regularity:** The two sets $\Gamma_f(\tilde{y}) := \{x \in \mathbb{E} \mid \tilde{y} = \mathcal{A}(x)\}$ and $\Gamma_\Omega(\tilde{h}) := \{x \in \mathbb{E} \mid -\tilde{h} \in \mathcal{N}_\Omega(x)\}$ satisfy that for every bounded set $B$, there exists a constant $\kappa$ such that

$$\text{dist}(x, \Gamma_f(\tilde{y}) \cap \Gamma_\Omega(\tilde{h})) \leq \kappa \max\{\text{dist}(x, \Gamma_f(\tilde{y})), \text{dist}(x, \Gamma_\Omega(\tilde{h}))\}, \text{ for all } x \in \Omega.$$  

2. **Metric subregularity:** there exists $\kappa, \epsilon > 0$ such that for all $x$ with $\|x - x_*\|_2 \leq \epsilon$,

$$\text{dist}(x, \Gamma_\Omega(\tilde{h})) \leq \kappa \text{dist}(-\tilde{h}, \mathcal{N}_\Omega(x)). \quad (32)$$

Let us first verify bounded linear regularity. First, the subdifferential of the Euclidean norm $\|\cdot\|_2$ is

$$\partial\|x\|_2 = \begin{cases} \frac{x}{\|x\|_2} & x \neq 0, \\ \mathcal{B}_{\|\cdot\|_2} & x = 0. \end{cases}$$

Here $\mathcal{B}_{\|\cdot\|_2} := \{x \mid \|x\|_2 \leq 1\}$ is unit $\ell_2$ norm ball.

From the characterization (23) of the interior of the normal cone, we know that $\tilde{h} = \nabla f(x_*)$ is nonzero due to strict complementarity, and hence any $x \in \Gamma(\tilde{h})$ must satisfy $x \in \partial \Omega$. Following the derivation of the normal cone in (22), we have for any $x \in \partial \Omega$,

$$\mathcal{N}_\Omega(x) = \{y \mid y \in \lambda \left( \prod_{g \in \mathcal{F}(x)} \partial\|x_g\|_2 \times \prod_{g \in \mathcal{G} - \mathcal{F}(x)} \mathcal{B}_{\|\cdot\|_2} \right), \lambda \geq 0\}. \quad (33)$$

Here the support set $\mathcal{F}(x)$ is the set of groups in the support of $x$. Let us pick a $i^* \in \mathcal{F}(x_*)$. For each $i \in \mathcal{G}$, define the vector $\tilde{h}_i = \frac{-\tilde{h}_i}{\|\tilde{h}_i\|_2} \in \mathbb{R}^{|v_i|}$. Recall from (24), we have $\|\tilde{h}_i\|_2$ all equal for

---

*The error bound condition considered in [DL18] Corollary 3.6 actually require the bound (31) to hold for all $x$ in the intersection of $\Omega$ and a sublevel set of $f$. Note there is a difference between a sublevel set and a neighborhood of $x_*$. However, as $f$ is continuous and $\Omega$ is compact, when restricted to $\Omega$ any neighborhood of $x_*$ is contained in a sublevel set and vice versa. Moreover, the quadratic growth condition of [DL18] Corollary 3.6 is only required to hold for $x$ in $\Omega$ and a sublevel set of $f$. Again, this condition is equivalent to ours as to $\Omega$ is compact and $f$ is continuous.*
For each $i \in \mathcal{F}(x_*)$, define $\tilde{h}^i \in \mathbb{R}^n$ so that it is only supported on group $i$ with vector value $\tilde{h}_i$ and is 0 elsewhere. Again, from [24] and Lemma [11], we have $\|\tilde{h}^i\|_2$ all equal for $i \in \mathcal{F}(x_*)$, and is larger than those $i$ not in $\mathcal{F}(x_*)$. To remember the notation, we use $\tilde{h}^i$, upper index $i$, to mean a vector in $\mathbb{R}^n$. We use the notation $\tilde{h}_i$, lower index $i$, to mean the shorter vector in $\mathbb{R}^{n_i}$.

Combining the facts about $\tilde{h}_i$, the formula (33), the formula of $\partial \| \cdot \|_2$, and $x \in \partial \Omega$, we find that actually
\[
\Gamma_\Omega(\tilde{h}) = \{ x | \sum_{i \in \mathcal{F}(x_*)} \alpha_i \tilde{h}^i, \alpha_i \in \Delta^{\mathcal{F}(x_*)} \},
\]
which is a convex polyhedral. Because $\Gamma_f(\bar{y})$ and $\Gamma_\Omega(\tilde{h})$ are both convex polyhedral, we know from [BBL99] Corollary 3 that bounded linear regularity holds.

We verify metrical subregularity now. Note that from previous calculation of $\Gamma_\Omega(\tilde{h})$, we know
\[
\text{dist}(x, \Gamma_\Omega(\tilde{h}))^2 = \min_{\alpha_i \in \Delta^{\mathcal{F}(x_*)}} \sum_{i \in \mathcal{F}(x_*)} \| x_i - \alpha_i \tilde{h}_i \|_2^2 + \sum_{i \notin \mathcal{F}(x_*)} \| x_i \|_2^2.
\]
By choosing $\epsilon$ sufficiently small, say $\epsilon < \epsilon_0$, we have $\mathcal{F}(x) \supseteq \mathcal{F}(x_*)$. The quantity, $\text{dist}(\tilde{h}, N_\Omega(x))$, on the RHS of (32) for all $x$ within an $\epsilon$ neighborhood of the solution $x_*$ satisfies that
\[
\text{dist}^2(\tilde{h}, N_\Omega(x)) = \begin{cases} +\infty, & x \notin \Omega, \\ \| \tilde{h} \|_2^2, & x \in \text{int}(\Omega), \end{cases}
\]
where $\text{int}(\Omega)$ is the interior of $\Omega$. For $x \in \partial \Omega$, $\text{dist}^2(\tilde{h}, N_\Omega(x))$ satisfies that
\[
\text{dist}^2(\tilde{h}, N_\Omega(x)) = \| h_i * \|_2^2 \min_{\lambda \geq 0, v_i \in B} \sum_{i \in \mathcal{F}(x)} \| \tilde{h}_i - \lambda \tilde{x}_i \|_2^2 + \sum_{i \notin \mathcal{F}(x)} \| \tilde{h}_i - \lambda v_i \|_2^2,
\]
where $\tilde{x} = \frac{x}{\|x\|_2}$, and $\tilde{x}_i$ is the vector with components in group $i$. The case of $x \notin \Omega$ is trivial. The case of $x \in \text{int}(\Omega)$ can be proved by choosing a large enough $\kappa$, say $\kappa > K_0$, as $\text{dist}(x, \Gamma_\Omega(\tilde{h}))^2$ is upper bounded for any $x \in \text{int}(\Omega)$, and $\text{dist}^2(\tilde{h}, N_\Omega(x))$ in this case is fixed. We are left with the most challenging case $x \in \partial \Omega$, where the normal cone is non-trivial. First, we upper bound $\text{dist}(x, \Gamma_\Omega(\tilde{h}))^2$ by choosing $\alpha_i = \| x_i \|_2$. The numbers $\alpha_i$ sum to one because $x \in \partial \Omega$. In this case, $\text{dist}(x, \Gamma_\Omega(\tilde{h}))^2$ satisfies the bound
\[
\text{dist}(x, \Gamma_\Omega(\tilde{h}))^2 \leq \sum_{i \in \mathcal{F}(x_*)} \| x_i - \tilde{h}_i \|_2 + \sum_{i \notin \mathcal{F}(x_*)} \| x_i \|_2,
\]
where step (a) is due to $\mathcal{F}(x) \supseteq \mathcal{F}(x_*)$ by our choice of small enough $\epsilon$. We next lower bound $\text{dist}^2(\tilde{h}, N_\Omega(x))$ by ignoring the term not in $\mathcal{F}(x)$:
\[
\text{dist}^2(\tilde{h}, N_\Omega(x)) \geq \| g_* * \|_2^2 \min_{\lambda \geq 0} \sum_{i \in \mathcal{F}(x)} \| \tilde{h}_i - \lambda \tilde{x}_i \|_2^2
\]
Now if $\mathcal{F}(x) = \mathcal{F}(x_*)$, then it is tempting to set $\lambda = 1$ above and compare the inequality with (34) to claim victory. This does not work directly due to the minimization over $\lambda$ and the fact $\mathcal{F}(x) \supseteq \mathcal{F}(x_*)$.
Let $\lambda_* = \arg \min_{\lambda \geq 0} \sum_{i \in \mathcal{F}(x)} \| \hat{h}_i - \frac{\lambda x_i}{\|x_i\|_2} \|^2_2$. In this case, we have an explicit formula of $\lambda_*:

\lambda_* = \max \left\{ 0, \frac{\sum_{i \in \mathcal{F}(x)} \langle \hat{h}_i, \tilde{x}_i \rangle |\mathcal{F}(x)|}{\| \mathcal{F}(x) \|} \right\}.

If $\lambda_* = 0$, then we can simply pick some $\kappa > K_0$ as done in the case of $x \in \text{int}(\Omega)$. So we assume $\lambda_* > 0$ in the following. Next let $\lambda_i = \arg \min_{\lambda \geq 0} \| \hat{h}_i - \frac{\lambda x_i}{\|x_i\|_2} \|^2_2$ for each $i \in \mathcal{F}(x_*)$. With such choice of $\lambda_i$ and $\lambda^*$, we can further lower bound $\text{dist}^2(\tilde{h}, N_\Omega(x))$ by splitting the terms in $\mathcal{F}(x)$ and those are not:

$$
\text{dist}^2(\tilde{h}, N_\Omega(x)) \geq \| g_i^* \|^2_2 \left( \sum_{i \in \mathcal{F}(x_*)} \| \tilde{h}_i - \frac{\lambda_i x_i}{\|x_i\|_2} \|^2_2 + \sum_{i \in \mathcal{F}(x) \setminus \mathcal{F}(x_*)} \| \tilde{h}_i - \frac{\lambda_* x_i}{\|x_i\|_2} \|^2_2 \right). 
$$

(35)

We bound the two terms separately. Let us first deal with $R_1$. From the expression of normal cone $\mathcal{N}_\Omega(x_*)$ and $-\tilde{h} \in N_\Omega(x_*)$ by our assumption, we know $\hat{h}_i = \frac{(x_i)}{\|x_i\|_2}$ for every $i \in \mathcal{F}(x_*)$. Hence by choosing a (possibly smaller) $\epsilon$, say $\epsilon < \epsilon_1$, we can ensure that for any $x$ within an $\epsilon_1$ neighborhood of the solution $x_*, \langle \tilde{x}_i, \hat{h}_i \rangle \geq 0$ for every $i \in \mathcal{F}(x_*)$. Moreover, for a small enough $\epsilon_1$, we know each $\lambda_i = \langle \tilde{x}_i, \hat{h}_i \rangle$ and is very close to 1. Thus the condition of Lemma 13 is fulfilled, and we have

$$
R_1 \geq \frac{1}{2} \sum_{i \in \mathcal{F}(x_*)} \| x_i \|_2 \| \tilde{h}_i - \tilde{x}_i \|^2_2.
$$

(36)

Next, to deal with $R_2$, let us examine the expression of $\lambda_* = \frac{\sum_{i \in \mathcal{F}(x)} \langle \hat{h}_i, \tilde{x}_i \rangle |\mathcal{F}(x)|}{\| \mathcal{F}(x) \|}$. Recall $\langle \hat{h}_i, \tilde{x}_i \rangle$ is close to 1 for small enough $\epsilon$. Due to strict complementarity, for each $i \in \mathcal{F}(x) \setminus \mathcal{F}(x_*)$, we know $\| \hat{h}_i \|_2 < 1 - \delta_0$ for some $\delta_0 > 0$ that depends only on $\hat{h}$. Combining these two facts, we know that $i' = \arg \min_{i \in \mathcal{F}(x)} \langle \hat{h}_i, \tilde{x}_i \rangle$ must belong to $\mathcal{F}(x) \setminus \mathcal{F}(x_*)$. Moreover, by choosing an even smaller $\epsilon$, say $\epsilon < \epsilon_2$, we have $\lambda_* \geq \delta_1 + \min_i \langle \hat{h}_i, \tilde{x}_i \rangle$ for some $\delta_1 > 0$ that only depends on $\hat{h}$, $\delta$, and $\epsilon_2$. We can now lower bound $R_2$ as follows:

$$
R_2 \geq \| \tilde{h}_i - (\delta_1 + \langle \hat{h}_i, \tilde{x}_i \rangle) \tilde{x}_i \|^2_2
= \| \tilde{h}_i - \langle \hat{h}_i, \tilde{x}_i \rangle \tilde{x}_i \|^2_2 + \delta_1^2
+ 2 \delta \langle \tilde{h}_i - (\langle \hat{h}_i, \tilde{x}_i \rangle) \tilde{x}_i, \tilde{x}_i \rangle
\geq \delta_1^2.
$$

(37)

Combining the bounds (36) and (37) on $R_1$ and $R_2$, we find that

$$
\text{dist}^2(\tilde{h}, N_\Omega(x)) \geq \frac{\| g_i^* \|^2_2}{2} \sum_{i \in \mathcal{F}(x_*)} \| \tilde{h}_i - \tilde{x}_i \|^2_2 + \| g_i^* \|^2_2 \delta_1^2
\geq \frac{\| g_i^* \|^2_2}{2} \sum_{i \in \mathcal{F}(x_*)} \| x_i \|_2 \| \tilde{h}_i - \tilde{x}_i \|^2_2 + \| g_i^* \|^2_2 \delta_1^2 \sum_{i \in \mathcal{F}(x) \setminus \mathcal{F}(x_*)} \| x_i \|_2^2.
$$

(38)

Here, for the step (a), we use $\| x_i \|_2 \leq 1$ as $x \in \partial \Omega$. Hence, by taking $\epsilon = \min(\epsilon_1, \epsilon_2)$ and $\kappa = \max\{K_0, \| g_i \|^2_2 \delta_1, \| g_i \|^2_2 \delta_1 \}$, and comparing (38) with (34), a bound on $\text{dist}(x, \Gamma_\Omega(\tilde{h}))$, we see that metric subregularity is satisfied and our proof for unit group norm ball is complete.

Finally, we consider the unit nuclear norm ball.
We claim that it satisfies strict complementarity and its solution $\tilde{X}$. To see this proves quadratic growth.

Let $\tilde{n} = n_1 + n_2$. For any $\tilde{X} \in S^\tilde{n}$, denote its eigenvalues as $\lambda_1(\tilde{X}) \geq \cdots \geq \lambda_{\tilde{n}}(\tilde{X})$. Also, for any $X \in B_{\|\cdot\|_{\text{nuc}}}^n$, denote its singular value decomposition as $X = U_X \Sigma_X V_X^\top$ where $U_X \in \mathbb{R}^{n_1 \times r_X}$, $V_X \in \mathbb{R}^{n_2 \times r_X}$, and $r_X = \text{rank}(X)$. Define the dilation $X^\sharp \in S^\tilde{n}$ of a $X \in \mathbb{R}^{n_1 \times n_2}$ as

$$X^\sharp = \frac{1}{2} \begin{bmatrix} X_1 & X \end{bmatrix},$$

where the $X_1 = U_X (\Sigma_X + \xi_X I) U_X^\top$, and $X_2 = V_X (\Sigma_X + \xi_X I) V_X^\top$. The number $\xi_X \geq 0$ is chosen so that $X^\sharp$ has trace 1. Note that $X^\sharp$ is positive semidefinite as $X^\sharp = \frac{1}{2} \begin{bmatrix} U_X^\top & \Sigma_X [U_X^\top V_X^\top] + \xi_X X \end{bmatrix}$. For any $\tilde{Y} = \frac{1}{2} \begin{bmatrix} Y_1 & Y \end{bmatrix}$ with $Y_1 \in S^{n_1}$, and $Y_2 \in S^{n_2}$, we denote its off diagonal component as $\tilde{Y}^\flat = Y$.

Note here that $X^\sharp$ denotes the dilation of a matrix $X \in \mathbb{R}^{n_1 \times n_2}$, while $\tilde{X}$ means a generic matrix in $S^\tilde{n}$ which is not necessarily related to $X$. We also have the relation that $(X^\sharp)_{\tilde{b}} = X$ for any $X \in \mathbb{R}^{n_1 \times n_2}$.

Consider the problem

$$\begin{align*}
\text{minimize} & \quad \tilde{f}(\tilde{X}) := f(\tilde{X}_b) = g(A(\tilde{X}_b)) + \langle C, (\tilde{X})_{\tilde{b}} \rangle \\
\text{subject to} & \quad \tilde{X} = 1 \quad \tilde{X} \succeq 0.
\end{align*}$$

We claim that it satisfies strict complementarity and its solution $\tilde{X}_*$ is unique and is equal to $X^\sharp$. Suppose the claim is proved for the moment. Note that $X_* \in \partial \Omega$ implies that $\text{rank}(X^\sharp) = \text{rank}(X_*) < \tilde{n}$. Hence, the condition of [DFXY20, Theorem 6] is fulfilled, and we know there is some $\tilde{\gamma} > 0$, such that for all $\tilde{X} \in SP^\tilde{n}$, we have

$$\tilde{f}(\tilde{X}) - \tilde{f}(X^\sharp) \geq \tilde{\gamma} \|\tilde{X} - X^\sharp\|_F.$$

Hence, for any $X \in \Omega$, by construction of $\tilde{f}$, we have

$$f(X) - f(X_*) = \tilde{f}(X^\sharp) - \tilde{f}(X^\sharp) \geq \tilde{\gamma} \|X^\sharp - X^\sharp\|_F^2 \geq \frac{\tilde{\gamma}}{2} \|X - X_*\|_F^2.$$

This proves quadratic growth.

We now verify our claim that $X^\sharp$ is the unique solution to (40) and $X^\sharp \in \partial SP^\tilde{n}$ with $\nabla \tilde{f}(X^\sharp) \in \partial N_{SP^\tilde{n}}(X^\sharp)$. First, consider feasibility and whether $X^\sharp \in \partial SP^\tilde{n}$. The condition $X_* \in \partial \Omega$ implies that $1 \leq r_* < \min(n_1, n_2)$ and $\|X_*\|_{\text{nuc}} = 1$. Hence we do have $\text{tr}(X^\sharp) = 1$ and $X^\sharp \in \partial SP^\tilde{n}$ as $\text{rank}(X^\sharp) = \text{rank}(X_*) = r_* < n_1 + n_2$. Next, consider optimality. Given any $\tilde{X} \in SP^\tilde{n}$, we may write it as $\tilde{X} = \frac{1}{2} \begin{bmatrix} X_1 & X \end{bmatrix}$. By [JS10, Lemma 1], we have

$$\|X\|_{\text{nuc}} \leq 1.$$  (41)

To see $X^\sharp$ is optimal for (40), note that

$$f((\tilde{X})_{\tilde{b}}) = f(X) \geq f(X_*) = f((X^\sharp)_{\tilde{b}}),$$

where $f$ is the objective function of (40).
where step (a) is due to optimality of $X_*$ in (1) and $X$ is feasible as just argued. Thirdly, we argue that $X^*_2$ is a unique solution to (40). For any optimal solution $\tilde{X}_* = \frac{1}{2} \begin{bmatrix} X^*_1 & X_0 & X^*_2 \end{bmatrix}$ of (40), we have $X_0$ is optimal to (1) as

$$f(X_0) = f((\tilde{X}_*)_0) = f((X^*_2)_0) = f(X_*),$$

where step (a) is because $X^*_2$ is optimal to (40). Hence due to uniqueness of $X_*$, we know $X_0 = X_*$. Because $\|X_*\|_{\text{nuc}} = 1$, using [DU20, Lemma 3], we know in fact $X^*_2 = \tilde{X}_*$ and uniqueness of solution to (40) is proved. Finally, we verify strict complementarity that $\nabla \tilde{f}(X^*_2) \in \text{relint} \left( N_{\mathcal{SP}^n}(X^*_2) \right)$. Recall from (26), that we need to show

$$-\nabla \tilde{f}(X^*_2) \in \text{relint} \left( N_{\mathcal{SP}^n}(\tilde{X}_*) \right) = \{ sI | s \in \mathbb{R} \} + \{-\tilde{Z} | \tilde{Z} \succeq 0, \text{range}(\tilde{Z}) = \text{nullspace}(X^*_2) \}.$$  

Using the definition of $X^*_2$, we know

$$\nabla \tilde{f}(X^*_2) = \begin{bmatrix} 0 & \nabla f(X_*) \end{bmatrix}.$$  

Recall from Lemma 11 we have $\sigma_1(\nabla f(X_*)) = \cdots = \sigma_r(\nabla f(X_*)) = \delta + \sigma_{r_1+1}(\nabla f(X_*))$ for some gap $\delta > 0$. Hence we see that $\nabla \tilde{f}(X^*_2)$ has all its smallest $r_*$ eigenvalues equal as $-\sigma_{r_1}(\nabla f(X_*))$ and the gap between its $r_*$-th smallest eigenvalue and the $r_* + 1$-th eigenvalue is simply $\delta > 0$. Moreover, let the singular value decomposition of $X_*$ as $X_* = U_* \Sigma V_*^T$ with $U_* \in \mathbb{R}^{n \times r_*}$ and $V_* \in \mathbb{R}^{n \times r_*}$. From the description of normal cone of nuclear norm ball in (29), we know $U_*, -V_*$ are the matrices formed by the top $r_*$ left and right vectors of $\nabla f(X_*)$. Hence, the bottom $r_*$ eigenvector of $\nabla f(X_*)$ is simply $\frac{1}{\sqrt{2}} \begin{bmatrix} U_* \\ -V_* \end{bmatrix}$. Since $\text{range}(X^*_2) = \text{range}(\begin{bmatrix} U_* \\ V_* \end{bmatrix})$, we may take $s = \sigma_1(\nabla f(X_*))$ and $\tilde{Z} = \sigma_1(\nabla f(X_*))I + \nabla \tilde{f}(X^*_2)$. Using the eigengap condition on $\nabla \tilde{f}(X^*_2)$, we see $\text{range}(\tilde{Z}) = \text{nullspace}(X^*_2)$ and our claim is proved. 

\hfill \Box

### B.3.1 Additional Lemma for quadratic growth

We establish the following lemma for the proof of unit group norm ball.

**Lemma 13.** For any two $x, y \in \mathbb{R}^d$ with $\ell_2$ norm one, and $a := \langle x, y \rangle \geq 0$, we have

$$2 \min_{\lambda \geq 0} \|x - \lambda y\|_2^2 \geq \|x - y\|_2^2.$$  

**Proof.** Simple calculus reveals that the optimal solution $\lambda^*$ of the LHS of the inequality is $\lambda^* = a \geq 0$. We know $a \in [0, 1]$ due to Cauchy-Schwarz and our assumption on $a$. Direct calculation of the difference yields

$$2 \min_{\lambda \geq 0} \|x - \lambda y\|_2^2 - \|x - y\|_2^2 = 2 + 2a^2 - 4a^2 - 2 + 2a = -2a^2 + 2a \geq 0,$$

where the last line is due to $a \in [0, 1]$. 

\hfill \Box
B.4 Proofs of Theorem 7 for group norm ball

Proof. Let us now consider Algorithm 2 whose constraint set $\Omega$ is a unit group norm ball with arbitrary base norm $\| \cdot \|$. Using quadratic growth (a), Theorem 6 in the second step (b), and the choice of $T$ in the following step (c), the iterate $x_t$ with $t \geq T$ satisfies that

$$
\| x_t - x_* \| \leq \frac{1}{\gamma} h_1 \leq \sqrt{\frac{L_f D^2}{\gamma T}} \leq \frac{\delta}{2L_f D}.
$$

(43)

Next recall the definition of $F(x_*)$ implies $(x_*)_g \neq 0$ for any $g \in F(x_*)$. The optimality conditions and $\| x_* \|_g = 1$ (due to $x_* \in \partial \Omega$) implies that for every $g \in F(x_*)$,

$$
\langle \nabla f(x_*), [x_*)_g \rangle = ||\nabla f(x_*)||_g ||x_*||_g, \quad \text{and} \quad \langle \nabla f(x_*), x_* \rangle = ||\nabla f(x_*)||_g ||x_*||_g.
$$

For any $g \in F(x_*)$, define a vector $x_\delta^g \in \Omega$ as $x_\delta^g := \begin{cases} \left( \frac{[x_*)_g}{\|x_*\|_g} \right)_i, & i \in g \setminus g_* \\ 0, & i \notin g \setminus g_* \end{cases}$. So $x_\delta^g \in \Omega$ is an extended vector of the normalized vector $\frac{[x_*)_g}{\|x_*\|_g}$. Combining this definition with previous two equalities, we see

$$
\langle \nabla f(x_*), x_\delta^g \rangle = \langle \nabla f(x_*), x_* \rangle.
$$

(44)

Now, for any $t \geq T$, we have for any group $g \in F(x_*)$, and any vector $v \in \Omega$ that is in $F^c(x_*)$,

$$
\langle \nabla f(x_t), x_\delta^g \rangle - \langle \nabla f(x_t), v \rangle = \langle \nabla f(x_*), x_\delta^g - v \rangle + \langle \nabla f(x_t) - \nabla f(x_*), v - u \rangle \leq -\delta + \langle \nabla f(x_t) - \nabla f(x_*), v - u \rangle \leq -\frac{\delta}{2}.
$$

(45)

Here in step (a), we use the definition of $\delta$ in (7) and (44). In step (b), we use the bound in (11), Lipschitz continuity of $\nabla f(x)$, and $\|v-u\| \leq D$.

Thus, the kLOO step will produce all the groups in $F(x_*)$ as $k \geq r_*$ after $t \geq T$, and so $x_*$ is a feasible and optimal solution of the optimization problem in the $k$ direction search step. Hence Algorithm 2 finds the optimal solution $x_*$ within $T + 1$ steps.

B.5 Proofs of Theorem 10

We state one lemma that is critical to our proof of linear convergence. It is proved in Section B.5.1.

Lemma 14. Given $Y \in \mathbb{R}^{n_1 \times n_2}$ with $\sigma_r(Y) - \sigma_{r+1}(Y) = \delta > 0$. Denote the matrices formed by the top $r$ left and right singular vectors of $Y$ as $U \in \mathbb{R}^{n_1 \times r}$, $V \in \mathbb{R}^{n_2 \times r}$ respectively. Then for any $X \in \mathbb{R}^{n_1 \times n_2}$ with $\|X\|_{\text{nuc}} = 1$, there is an $S \in \mathbb{R}^{r \times r}$ with $\|S\|_{\text{nuc}} = 1$ such that

$$
\langle X - USV^T, Y \rangle \geq \frac{\delta}{2} \|X - USV^T\|_F^2.
$$

Equipped with this lemma, let us now prove Theorem 10.

Proof of Theorem 10. The case of the spectrahedron is proved in [DFXY20, Theorem 3] by using the eigengap formula in Lemma 11 and [DFXY20, Section 2.2 “relation with the eigengap assumption”]. Here, we need only to address the case of the unit nuclear norm. The proof that we present here for the case of the nuclear norm ball is quite similar. For notation convenience, for each $t$, let $U_t, V_t$ be matrices formed by top $r_*$ left and right singular vectors of $\nabla f(X_t)$. Define the set $N_{r_*,t} = \{U_tSV_t^T \mid \|S\|_{\text{nuc}} \leq 1\}$.
The term $R$, where we use the triangle inequality and the basic inequality (b) in step (a), that is, the quadratic growth condition in step (a), we have for any $t \geq 1$, $\eta \in [0, 1]$, and any $W \in \mathcal{N}_{\mathcal{r}, t}$:

$$
f(X_{t+1}) \leq f(X_t) + (1 - \eta)\langle W - X_t, \nabla f(X_t) \rangle + \frac{(1 - \eta)^2 L_f}{2} \|W - X_t\|_F^2. \tag{46}
$$

For $t \geq T$, we find that $\|X_t - X_\ast\|_F \leq \frac{\delta}{6\sqrt{2L_f}}$, and

$$
\sigma_{r_\ast}(\nabla f(X_t)) - \sigma_{r_\ast+1}(\nabla f(X_t)) = \sigma_{r_\ast}(\nabla f(X_\ast)) - \sigma_{r_\ast+1}(\nabla f(X_\ast)) + (\sigma_{r_\ast}(\nabla f(X_t)) - \sigma_{r_\ast+1}(\nabla f(X_\ast)))
\leq -\frac{\delta}{3}.
\tag{47}
$$

Here in step (a), we use the singular value gap formula of $\delta$ in Lemma 11; step (b) is due to Weyl’s inequality, the Lipschitz continuity of $\nabla f$, and the inequality $\|X_t - X_\ast\|_F \leq \frac{\delta}{6\sqrt{2L_f}}$.

Now we subtract the inequality (46) both sides by $f(X_\ast)$, and denote $h_t = f(X_t) - f(X_\ast)$ for each $t$ to arrive at

$$
h_{t+1} \leq h_t + (1 - \eta)\langle W - X_t, \nabla f(X_t) \rangle + \frac{(1 - \eta)^2 L_f}{2} \|W - X_t\|_F^2. \tag{47}
$$

Using Lemma 14, the inequality (47), and the assumption $X_\ast \in \partial \Omega$, we can choose $W \in \mathcal{N}_{\mathcal{r}, t}$ such that

$$
\langle W - X_\ast, \nabla f(X_t) \rangle \leq -\frac{\delta}{6} \|X_\ast - W\|_F^2. \tag{48}
$$

Let us now analyze the term $R_1 = \langle W - X_t, \nabla f(X_t) \rangle$ using (48) and convexity of $f$:

$$
R_1 = \langle W - X_t, \nabla f(X_t) \rangle = \langle W - X_\ast, \nabla f(X_t) \rangle + \langle X_\ast - X_t, \nabla f(X_t) \rangle \\ \leq -\frac{\delta}{6} \|X_\ast - W\|_F^2 + h_t.
$$

The term $R_2 = \|X_t - W\|_F^2$ can be bounded by

$$
R_2 = \|X_t - W\|_F^2 \leq 2(\|X_t - X_\ast\|_F^2 + \|X_\ast - W\|_F^2) \leq \gamma h_t + \frac{2\|X_\ast - W\|_F^2},
$$

where we use the triangle inequality and the basic inequality $(a + b)^2 \leq 2a^2 + 2b^2$ in step (a), and the quadratic growth condition in step (b).
Writing the equation in block form reveals that
\[ h_{t+1} \leq h_t + \xi \left( -\frac{\delta}{6} \| X_* - W \|_F^2 - h_t \right) + \frac{\xi^2 L_f}{2} \left( \frac{2}{\gamma} h_t + 2 \| X_* - W \|_F^2 \right) \]
\[ = \left( 1 - \xi + \frac{\xi^2 L_f}{\gamma} \right) h_t + \left( \xi^2 L_f - \frac{\xi \delta}{6} \right) \| X_* - W \|_F^2. \]

A detailed calculation below and a careful choice of \( \xi \) below yields the factor \( 1 - \min\{ \frac{\gamma}{4 L_f}, \frac{\delta}{2 L_f} \} \) in the theorem.

We show here how to choose \( \xi \in [0,1] \) so that \( 1 - \xi + \frac{\xi^2 L_f}{\gamma} \) is minimized while keeping \( \xi^2 L_f - \frac{\xi \delta}{6} \leq 0 \).

For \( \xi^2 L_f - \frac{\xi \delta}{6} \leq 0 \), we need \( \xi \leq \frac{\delta}{6 L_f} \). The function \( q(\xi) = 1 - \xi + \frac{\xi^2 L_f}{\gamma} \) is decreasing for \( \xi \leq \frac{\gamma}{4 L_f} \) and increasing for \( \xi \geq \frac{\gamma}{4 L_f} \). If \( \frac{\gamma}{2 L_f} \leq \frac{\delta}{6 L_f} \), then we can pick \( \xi = \frac{\gamma}{2 L_f} \), and \( q(\xi) = 1 - \frac{\gamma}{4 L_f} \). If \( \frac{\gamma}{2 L_f} \geq \frac{\delta}{6 L_f} \Rightarrow \frac{\gamma}{\delta} \leq 3 \), then we can pick \( \xi = \frac{\delta}{6 L_f} \), and \( q(\xi) = 1 - \frac{\delta}{6 L_f} + \frac{\delta^2}{36 L_f} = 1 + \frac{\delta}{6 L_f} \left( \frac{\delta}{\delta} - 1 \right) \leq 1 - \frac{\gamma}{12 L_f} \).

**B.5.1 Additional lemmas for the proof of Theorem 10**

Here we give a proof of Lemma 14.

**Proof of Lemma 14.** We utilize the result in [DFXY20, Lemma 5]: given any \( \bar{Y} \in S^n \) with eigenvalues \( \lambda_0(\bar{Y}) \leq \cdots \leq \lambda_{n-r+1}(\bar{Y}) \leq \lambda_{n-r}(\bar{Y}) - \delta' \leq \cdots \leq \lambda_1(\bar{Y}) - \delta' \) for some \( \delta' > 0 \). Denote the matrices by the bottom \( r \) eigenvectors of \( \bar{Y} \) as \( \bar{V} \in \mathbb{R}^{n \times r} \) respectively. Then for any \( \bar{X} \in S^n \) with \( \text{tr}(\bar{X}) = 1 \), there is an \( S \in \mathbb{R}^{r \times r} \) with \( \text{tr}(S) = 1 \) such that
\[
\langle \bar{X} - \bar{V} S \bar{V}^T, \bar{Y} \rangle \geq \frac{\delta'}{2} \| \bar{X} - \bar{V} S \bar{V}^T \|_F^2. \tag{49}
\]

To utilize this result, we consider the dilation of the matrices \( X \) and \( Y \):
\[
\bar{X} := \frac{1}{2} \begin{bmatrix} X_1 & X_2 \\ X_1^T & X_2 \end{bmatrix}, \quad \text{and} \quad \bar{Y} := \begin{bmatrix} 0 & Y \\ Y^T & 0 \end{bmatrix}. \tag{50}
\]

Here the matrices \( X_1 = U_X \Sigma_X U_X^T, \quad X_2 = V_X \Sigma_X V_X^T \) where \( U_X \Sigma_X V_X \) is the SVD of \( X \) and the number \( r_X = \text{rank}(X) \). Since \( \bar{X} = \begin{bmatrix} U_X^T \\ V_X \end{bmatrix} \begin{bmatrix} U_X & V_X \end{bmatrix}^T \), the matrix \( \bar{X} \in S^{n_1+n_2} \). The trace of \( \bar{X} \) is \( \text{tr}(\bar{X}) = 1 \) as \( \| X \|_{\text{nuc}} = 1 \). Note that the bottom \( r + 1 \) eigenvalues of \( \bar{Y} \) is simply \( -\sigma_1(Y), \ldots, -\sigma_r(Y), -\sigma_{r+1}(Y) \), and the matrix \( \bar{V} \in \mathbb{R}^{(n_1+n_2)r} \) defined below is formed by the matrix eigenvectors corresponds the smallest \( r \) eigenvalues:
\[
\bar{V} := \frac{1}{\sqrt{2}} \begin{bmatrix} U \\ -V \end{bmatrix}. \tag{51}
\]

Using [DFXY20, Lemma 5], we can find a matrix \( S \in S^r \) with \( \text{tr}(S) = 1 \) such that (49) holds. Writing the equation in block form reveals that
\[
\langle X - U(-S)V^T, Y \rangle = \langle \bar{X} - \bar{V} S \bar{V}^T, \bar{Y} \rangle \geq \frac{\delta}{2} \| \bar{X} - \bar{V} S \bar{V}^T \|_F^2 \overset{(a)}{\geq} \frac{\delta}{2} \| X - U(-S)V^T \|_F^2, \tag{52}
\]
where the last step is due to Lemma 15. Note that the matrix \( U(-S)V^T \) is the matrix we seek as \( \| -S \|_{\text{nuc}} = \text{tr}(S) = 1 \). Hence the proof is completed. \( \square \)
Lemma 15. Suppose two matrices $X, Y \in \mathbb{R}^{n_1 \times n_2}$, and $X = U_1 S_1 V_1^T$ and $Y = U_2 S_2 V_2^T$ for some unitary $U_i, V_i$ that for some integers $r_1, r_2$, they satisfy $U_i \in \mathbb{R}^{n_1 \times r_i}, i = 1, 2$ and $V_i \in \mathbb{R}^{n_2 \times r_i}, i = 1, 2$. The matrices $S_i \in S_+^{r_i}$ are positive semidefinite. Then

$$
\|U_1 S_1 U_1^T - U_2 S_2 U_2^T\|_F^2 + \|V_1 S_1 V_1^T - V_2 S_2 V_2^T\|_F^2 \geq 2\|U_1 S_1 V_1^T - U_2 S_2 V_2^T\|_F^2.
$$

Proof. This result follows by direct computation. Consider the difference $\|U_1 S_1 U_1^T - U_2 S_2 U_2^T\|_F^2 + \|V_1 S_1 V_1^T - V_2 S_2 V_2^T\|_F^2 - 2\|U_1 S_1 V_1^T - U_2 S_2 V_2^T\|_F^2$. Expanding the square and using the orthogonal invariance of the Frobenius norm, we find that

$$
\|U_1 S_1 U_1^T - U_2 S_2 U_2^T\|_F^2 + \|V_1 S_1 V_1^T - V_2 S_2 V_2^T\|_F^2 - 2\|U_1 S_1 V_1^T - U_2 S_2 V_2^T\|_F^2
= 2\text{tr}(S_1 U_1^T U_2 S_2 (U_2^T U_1 - V_2^T V_1)) + 2\text{tr}(S_1 (V_1^T V_2 - U_1^T U_2) S_2 V_2^T V_1)
= 2\text{tr}(S_1 (U_1^T U_2 - V_1^T V_2) S_2 (U_2^T U_1 - V_2^T V_1)),
$$

where step (a) is due to the fact that $\text{tr}(A) = \text{tr}(A^T)$ and step (b) is due to the cyclic property of trace. By factorizing $S_i = S_i^{1/2}$ for $i = 1, 2$ and the cyclic property of trace again, we find that

$$
\|U_1 S_1 U_1^T - U_2 S_2 U_2^T\|_F^2 + \|V_1 S_1 V_1^T - V_2 S_2 V_2^T\|_F^2 - 2\|U_1 S_1 V_1^T - U_2 S_2 V_2^T\|_F^2
= \text{tr}(S_1^{1/2} (U_1^T U_2 - V_1^T V_2) S_2^{1/2} S_1^{1/2} (U_2^T U_1 - V_2^T V_1) S_1^{1/2})
= \|S_2^{1/2} (U_2^T U_1 - V_2^T V_1) S_1^{1/2}\|_F^2 \geq 0.
$$

Hence the lemma is proved. $\square$

C Extension for multiple solutions

When the problem has more than one solution, let $\mathcal{X}$ be the solution set. This set is convex and closed. We change the term $\|x - x_*\|$ in the quadratic growth condition to $\text{dist}(x, \mathcal{X}) = \min_{x_* \in \mathcal{X}} \|x - x_*\|$.

For strict complementarity, we remove the condition that $x_*$ is unique and demand instead that some $x_* \in \mathcal{X}$ satisfies the conditions listed in strict complementarity. The support set $\mathcal{F}(x_*)$ and complementary set $\mathcal{F}^c(x_*)$ are defined via the $x_*$ that satisfies strict complementarity. Note that the dual vector $\nabla f(x_*)$ is the same for every $x_* \in \mathcal{X}$ [ZS17 Proposition 1]. The algorithmic results, Theorem 6, 7 and 10 hold almost without any change of the proof using the new definition of $r_*$ and $\delta$. The argument to establish quadratic growth via strict complementarity is more tedious and we defer it to future work.

D Numerical Experiment setting for Section 4

We detail the experiment settings of Lasso, support vector machine (SVM), group Lasso, and matrix completion problems. The compared methods include FW, away-step FW (awayFW) [GMS6], pairwise FW (pairFW) [LL15], DICO [GM16], and blockFW [AZHI17]. All codes are written by MATLAB and performed on a MacBook Pro with Processor 2.3 GHz Intel Core i5 and Memory 8 GB 2133 MHz LPDDR3. In our k-FW, we solve the kDS by the FASTA toolbox [GSB14, GSB15]: https://github.com/tomgoldstein/fasta-matlab. In DICO (as well as FW, awayFW, pairFW in Group Lasso and SVM), the step size is determined by backtracking line search. The ball sizes of $\ell_1$ norm, group norm, and nuclear norm are set to be the ground truth respectively.
D.1 Lasso

The experiment is the same as that in [LJJ15] except that the data size in our setting is ten times of that in [LJJ15]: $A \in \mathbb{R}^{2000 \times 5000}$ and $b \in \mathbb{R}^{2000}$. The large size is more reasonable for comparing the computational costs of FW, awayFW, pairFW, DICG and our k-FW. For FW, awayFW and pairFW, we use the MATLAB codes provide by [LJJ15]: https://github.com/Simon-Lacoste-Julien/linearFW. In DICG (as well as FW, awayFW, pairFW in Group Lasso and SVM), the step size is determined by backtracking line search.

D.2 SVM

We generate the synthetic data for two-class classification by the following model

$$X = [X_1, X_2] = [U_1V_1 + 1, U_2V_2 - 1], \quad X \leftarrow X + E,$$

where the elements of $U_1 \in \mathbb{R}^{20 \times 5}$, $V_1 \in \mathbb{R}^{5 \times 500}$, $U_2 \in \mathbb{R}^{20 \times 5}$, and $V_2 \in \mathbb{R}^{5 \times 500}$ are drawn from $\mathcal{N}(0, 1)$. $E$ consists of noise drawn from $\mathcal{N}(0, 0.1\sigma_X)$, where $\sigma_X$ denotes the standard deviation of the entries of $X$. Thus, in $X$, the number of samples is 1000 and the number of features is 20. We use 80% of the data as training data to classify the remaining data. In SVM, we use a polynomial kernel $k(x, y) = (x^\top y + 1)^2$.

D.3 Group Lasso

We generate a $100 \times 1000$ matrix $X$ whose entries are drawn from $\mathcal{N}(0, 1)$ and a $10 \times 100$ matrix $W$ with 10 nonzero columns drawn from $\mathcal{N}(0, 1)$. Then let $Y = WX$ and set $Y \leftarrow Y + E$, where the entries of noise matrix $E$ are drawn from $\mathcal{N}(0, 0.01\sigma_Y)$. Then we estimate $W$ from $Y$ and $X$ by solving a Group Lasso problem with kFW.

D.4 Matrix Completion

We generate a low-rank matrix as $X = UV^\top$, where the entries of $U \in \mathbb{R}^{500 \times 5}$ and $V \in \mathbb{R}^{5 \times 500}$ are drawn from $\mathcal{N}(0, 1)$. We sample 50% of the entries uniformly at random and recover the unknown entries by low-rank matrix completion.

D.5 Objective function vs running time

See Figure 10. kFW uses considerably less time compared to other FW variants for Lasso, SVM, and Group Lasso problems. It takes longer time than blockFW for the matrix completion problem.

Figure 10: Objective against time cost