Fusion over the Grassmann Manifold for Incomplete-Data Clustering

Abstract

This paper presents a new paradigm to cluster incomplete vectors using subspaces as proxies to exploit the geometry of the Grassmannian. We leverage this new perspective to develop an algorithm to cluster and complete data in a union of subspaces via a fusion penalty formulation. Our approach does not require prior knowledge of the number of subspaces, is naturally suited to handle noise, and only requires an upper bound on the subspaces' dimensions. In developing our model, we present local convergence guarantees. We describe clustering, completion, model selection, and sketching techniques that can be used in practice, and complement our analysis with synthetic and real-data experiments.

1 Introduction

Suppose we observe a subset of entries in a data matrix $\mathbf{X}$ whose columns lie near a union of subspaces. Our goals are (i) to learn the underlying subspaces, (ii) to fill the unobserved entries, and (iii) to cluster the columns according to the subspaces. This problem is often known as *high-rank matrix completion* (HRMC) [22, 19], and it has a wide range of applications, including tracking moving objects in computer vision [12, 13, 26, 27, 29, 30, 35], predicting target interactions for drug discovery [24, 36, 37, 40], and identifying groups in recommender systems [32, 54, 65].

Prior work. Due to its broad applicability, HRMC has attracted considerable attention in recent years. Existing approaches can be divided in four major groups: (1) *naive* methods that fill missing entries (with zeros, means, or low-rank matrix completion) prior to clustering with a full-data method, like sparse subspace clustering [20, 34, 63], (2) *neighborhood* methods that cluster points according to their overlapping coordinates [22], (3) *alternating* methods, like EM [41], k-subspaces [6], and group-lasso [43, 45], and (4) *liftings*, which exploit the second-order algebraic structure of unions of subspaces [56, 58]. Unfortunately, each of these methods present shortcomings. For instance, naive methods may work if data is missing at a rate inversely proportional to the dimension of the subspace [53], but fail with moderate volumes of missing data, as data filled naively no longer lies in a union of subspaces [19]. Neighborhood methods require either abundant observations or a super-polynomial number of samples (to produce enough overlaps). Liftings require squaring the dimension of an already high-dimensional problem, which severely limits their applicability.

The fundamental difficulty that all approaches face lies in assessing distances (e.g., euclidean, or in the form of inner products) between partially observed vectors, for the simple reason that this requires overlapping observations which become increasingly unlikely in low-sampling regimes [22]. **To circumvent this problem,** we introduce a new paradigm to cluster incomplete vectors, using subspaces as proxies, thus avoiding the need to calculate distances or inner products or other notions of similarity between incomplete vectors, as other methods require. To this end we assign each (incomplete-data) point its own (full-data) subspace, and simultaneously minimize over the Grassmann manifold: (a) the chordal distance between each point and its assigned subspace, to guarantee that the subspace stays *near* the observed entries, and (b) the geodesics between subspaces of all data, to encourage the subspaces from points that belong together to *fuse* (i.e, represent the same space). At the end of this minimization, clustering the proxy subspaces using standard procedures

like k-means or spectral clustering [8, 21, 47, 50, 55, 59, 61] can be done as a proxy for clustering the incomplete-data (goal iii). The ability to cluster the subspace rather than the incomplete-data is the key strength we gain by moving to the Grassmannian. After clustering, the missing entries can be inferred (goal ii) using low-rank matrix completion. Once the data is clustered and completed, the underlying subspaces can be trivially inferred (goal i) with a singular value decomposition. Local convergence guarantees follow easily from known manifold optimization results. We complement this with experiments on both synthetic and real data that show the potential of the foundational fusion-over-the-Grassmann formulation.

HRMC vs LRMC. Low-rank matrix completion (LRMC) seeks to exactly recover the missing entries of a data matrix $\mathbf{X}$ whose columns lie in a single low-dimensional subspace [10]. One can view HRMC as a generalization of LRMC, where the columns of $\mathbf{X}$ are known to lie in a union of subspaces, each of low dimension, but it is not known to which subspace each column belongs. While much research has been devoted to HRMC (see [33] for a recent survey), current algorithms have shortcomings, as mentioned in the prior work section, and even less is known regarding theoretical guarantees. In contrast, research in LRMC over the last decades have resulted in theory and algorithms that guarantee perfect recovery under reasonable assumptions (e.g., random sampling and bounded-coherence of the data) [9, 10, 14, 15, 25, 44]. Hence, given a HRMC problem, if the number of underlying subspaces, say K, and the maximum of their dimension, say r, are low, one could be tempted to cast it as a LRMC problem. In such case, the single subspace containing all the columns of $\mathbf{X}$ would have dimension no larger than $r' := r \cdot K$. This would, however, completely ignore the union structure present in the data, and therefore require more observed entries in order to complete $\mathbf{X}$. We can see this by noting that each column must have more observed entries than the subspace containing it [42]. This means that even in the fortunate case where r' is low enough, using LRMC would require K times more observations than HRMC. This is especially prohibitive when considering applications such as Metagenomics or Drug Discovery, where data is extremely sparse and costly to acquire. In general, r' may be too large to even allow the use of LRMC.

Our work in context. This paper is tightly related to [39], which uses a similar Grassmannian optimization model to study the single-subspace problem of LRMC. This paper generalizes these ideas to the much harder multiple-subspace problem of HRMC, while maintaining the local convergence guarantees of Proposition 5.1 in [39]. The main difference between [39] and our formulation is that the former only considers a predefined subset of geodesic distances (see equations (17)-(19) in [39]), which determine the Grassmannian points that must be matched. In [39], these subsets of geodesics can be chosen somewhat arbitrarily, because in LRMC all points belong to the same subspace. A so-called *gossip* protocol is therefore suitable in the easier problem of LRMC. In contrast, HRMC requires that only certain subsets of the Grassmannian be matched (the points corresponding to the unknown clustering to be learnt). Without knowing a priori the correct clusters, one cannot utilize the *gossip* method and must therefore use *all* pairwise geodesics so as to not introduce bias.

2 MODEL AND MAIN RESULTS

Let $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^m$ lie near a union of subspaces with dimension upper bounded by r. Let $\mathbf{x}_i^\Omega \in \mathbb{R}^{|\Omega_i|}$ denote the observed entries of $\mathbf{x}_i$, indexed by $\Omega_i \subset \{1, \ldots, m\}$. We propose assigning to each observed vector $\mathbf{x}_i^\Omega$ a proxy subspace $\mathcal{U}_i := \mathrm{span}(\mathbf{U}_i)$. Our goal is to estimate the true subspace $\mathcal{U}_i^\star$ to which $\mathbf{x}_i$ belongs by (a) enforcing that the proxy space $\mathcal{U}_i$ contains a possible completion of $\mathbf{x}_i^\Omega$ and (b) minimizing the distance between individual proxy spaces $\mathcal{U}_i$ and $\mathcal{U}_j$ to build consensus. This is done via the following optimization problem, where the first term achieves goal (a) and the second term achieves goal (b):

$$\min_{\mathbf{U}_1,\ldots,\mathbf{U}_n \in \mathbb{S}(m,r)} \quad \sum_{i=1}^n d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) \;+\; \frac{\lambda}{2} \sum_{i,j=1}^n d_g^2(\mathbf{U}_i, \mathbf{U}_j), \tag{1}$$

where

$$d_c(\mathbf{x}_i^\Omega, \mathbf{U}_i) := \sqrt{1 - \sigma_1^2(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i)} \qquad \text{and} \qquad d_g(\mathbf{U}_i, \mathbf{U}_j) := \sqrt{\sum_{\ell=1}^r \arccos^2 \sigma_\ell(\mathbf{U}_i^\mathsf{T}\mathbf{U}_j)}.$$

Here $\mathbb{S}(m, r)$ denotes the Stiefel manifold of $m \times r$ orthonormal matrices, $\lambda \geq 0$ is a regularization parameter, $\sigma_\ell(\cdot)$ denotes the ℓth largest singular value, and $\mathbf{X}_i^0$ is the orthonormal matrix spanning all the possible completions of a non-zero $\mathbf{x}_i^\Omega$. The space of all possible completions of $\mathbf{x}_i^\Omega$ is therefore $\mathcal{X}_i^0 := \text{span}(\mathbf{X}_i^0)$, which clearly contains the true data $\mathbf{x}_i$. The matrix $\mathbf{X}_i^0$ can be easily constructed as follows. If $\mathbf{x}_i^\Omega = \mathbf{0}$, then $\mathbf{X}_i^0 = \mathbf{I}$, the identity matrix. Otherwise, $\mathbf{X}_i^0$ is the $m \times (m - |\Omega_i| + 1)$ matrix formed with $\mathbf{x}_i^\Omega$ normalized and filled with zeros in the unobserved rows, concatenated with the $(m - |\Omega_i|)$ canonical vectors indicating the unobserved rows of $\mathbf{x}_i^\Omega$. For example, if $\mathbf{x}_i^\Omega \neq \mathbf{0}$ is observed in the first $|\Omega_i|$ rows, then

$$\mathbf{X}_i^0 \;=\; \left[\begin{array}{c|c} \frac{\mathbf{x}_i^\Omega}{\|\mathbf{x}_i^\Omega\|} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{I} \end{array} \right] \begin{array}{l} \left.\rule{0pt}{12pt}\right\} |\Omega_i| \\ \left.\rule{0pt}{12pt}\right\} m - |\Omega_i|. \end{array}$$
$$\underbrace{}_{m - |\Omega_i| + 1}$$

When $\mathbf{x}_i^\Omega$ is fully observed, $\mathbf{X}_i^0$ simplifies to $\mathbf{x}_i$ normalized. Recall that Grassmannians $\mathbb{G}(m, r)$ are quotient spaces of Stiefel manifolds $\mathbb{S}(m, r)$ by action of the orthogonal group of $r \times r$ orthonormal matrices. Since both terms $d_c(\mathbf{x}_i^\Omega, \mathbf{U}_i)$ and $d_g(\mathbf{U}_i, \mathbf{U}_j)$ are invariant under this quotient, the objective function in (1) does not depend on the choice of basis, and descends to a function on the Grassmannian.

Why should this work? The *chordal distance* $d_c(\mathbf{x}_i^\Omega, \mathbf{U}_i)$, as defined in [60], is not a formal distance on the Grassmannian, but rather measures how far $\mathcal{U}_i$ is from containing a possible completion of $\mathbf{x}_i^\Omega$. More precisely, $d_c(\mathbf{x}_i^\Omega, \mathbf{U}_i)$ is the cosine of the angle between the nearest completion of $\mathbf{x}_i^\Omega$ and the r-plane $\mathcal{U}_i$. If the top singular value $\sigma_1(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i)$ is 1, then $\mathcal{X}_i^0$ and $\mathcal{U}_i$ intersect on at least a line, meaning that the proxy space $\mathcal{U}_i$ contains a possible completion of $\mathbf{x}_i^\Omega$. While merely forcing $\mathcal{U}_i$ to contain a possible completion offers no way to distinguish one possible completion to another, consensus among data is built as different proxies $\mathcal{U}_i$ and $\mathcal{U}_j$ are forced towards one another by the geodesic term. In other words, $\mathcal{U}_i$ and $\mathcal{U}_j$ are allowed to be near each other, and hence form clusters, only if they both contain possible completions of both $\mathbf{x}_i^\Omega$ and $\mathbf{x}_j^\Omega$. The term *chordal distance* used in this way is adopted from [60] and should not be confused with the more common chordal distance between points on the Grassmannian [17]. See Figure 1 to build some intuition.

Solving (1) The gradients of (1) with respect to $\mathbf{U}_i$ over the Grassmannian are given by:

$$\boldsymbol{\nabla} d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) \;=\; -2\sigma_1(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i)(\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T})\mathbf{v}_i\mathbf{w}_i^\mathsf{T}, \tag{2}$$

$$\boldsymbol{\nabla} d_g^2(\mathbf{U}_i, \mathbf{U}_j) \;=\; -\sum_{\ell=1}^r \frac{2\arccos \sigma_\ell(\mathbf{U}_i^\mathsf{T}\mathbf{U}_j)}{\sqrt{1 - \sigma_\ell^2(\mathbf{U}_i^\mathsf{T}\mathbf{U}_j)}} \cdot (\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T})\mathbf{v}_{ij}^\ell\mathbf{w}_{ij}^{\ell\mathsf{T}}, \tag{3}$$

where $\mathbf{v}_i$ and $\mathbf{w}_i$ are the leading left and right singular vectors of $\mathbf{X}_i^0\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i$, and $\mathbf{v}_{ij}^\ell$, $\mathbf{w}_{ij}^\ell$ are the ℓth left and right singular vectors of $\mathbf{U}_j\mathbf{U}_j^\mathsf{T}\mathbf{U}_i$. The key behind these expressions is that tangent vectors on the Grassmannian can be computed as projections of gradient vectors in Euclidean space [1, 18]. In fact, that is exactly what the gradient expressions in (2) and (3) are: $-2\sigma_1(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i)\mathbf{v}_i\mathbf{w}_i^\mathsf{T}$ in (2) is the gradient of $d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i)$ with respect to the entries of $\mathbf{U}_i$

Figure 1: The semi-spheres represent the Grassmannian $\mathbb{G}(m, r)$, where each point $\mathcal{U}_i$ represents a subspace (in the particular case of $\mathbb{G}(3, 1)$, the line going from the origin to $\mathcal{U}_i$). **Left:** Intuitively, the *chordal* distance $d_c(\mathbf{x}_i^\Omega, \mathbf{U}_i)$ is an informal measure of distance between the subspace $\mathcal{U}_i$ and an incomplete point $\mathbf{x}_i^\Omega$. The left image should only be taken as intuition since $\mathcal{X}_i^0$ may not live on the same Grassmannian and the chordal distance should not be thought of as a geodesic distance. **Center:** The *geodesic* distance $d_g(\mathbf{U}_i, \mathbf{U}_j)$ measures the distance over the Grassmannian between $\mathcal{U}_i$ and $\mathcal{U}_j$. **Right:** The Euclidean gradient vector $\boldsymbol{\nabla}_i$ *falls* out of the Grassmann manifold; to account for the Grassmannian curvature, each geodesic step needs to be adjusted according to (4).

in Euclidean space. The multiplication by $\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T}$ takes the horizontal direction of the tangent vector with respect to the quotient, thus mapping the gradient from Euclidean space to the Grassmannian. The same is true for the term $\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T}$ in (3). To summarize, (2) and (3) are gradient directions in the manifold of subspaces, rather than matrices: (2) is the steepest direction along which the subspace $\mathcal{U}_i$ can be descended to a potential subspace that contains $\mathbf{x}_i^\Omega$, and (3) is the steepest direction along which the subspace $\mathcal{U}_i$ can be descended to the subspace $\mathcal{U}_j$. The derivations of these gradients are in Section 4. Putting together the chordal and geodesic gradients, our overall descent direction for $\mathbf{U}_i$ is given by

$$\boldsymbol{\nabla}_i \; := \; \boldsymbol{\nabla} d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) + \frac{\lambda}{2} \sum_{j=1}^n \boldsymbol{\nabla} d_g^2(\mathbf{U}_i, \mathbf{U}_j).$$

Observe that $\mathbf{U}_i - \eta \boldsymbol{\nabla}_i$ *falls* out of the Grassmannian for every step size $\eta \neq 0$ (see Figure 1). To adjust for the curvature of the manifold, the update after taking a geodesic step of size η over the Grassmannian in the direction of $\boldsymbol{\nabla}_i$ is given by

$$\mathbf{U}_i \; \leftarrow \; \begin{bmatrix} \mathbf{U}_i\mathbf{E}_i & \boldsymbol{\Gamma}_i \end{bmatrix} \begin{bmatrix} \operatorname{diag}\cos(\eta\boldsymbol{\Upsilon}_i) \\ \operatorname{diag}\sin(\eta\boldsymbol{\Upsilon}_i) \end{bmatrix} \mathbf{E}_i^\mathsf{T}, \tag{4}$$

where $\boldsymbol{\Gamma}_i\boldsymbol{\Upsilon}_i\mathbf{E}_i^\mathsf{T}$ is the compact singular value decomposition of $\boldsymbol{\nabla}_i$. In our implementation, we use Armijo step sizes, given by $\eta = \beta^\nu \eta_0$, where $\eta_0 > 0$, and $\beta, \gamma \in (0, 1)$ are the Armijo tuning parameters related to the initial step size and step search granularity [1], and ν is the smallest non-negative integer such that

$$\sum_{i=1}^n f_i(\mathbf{U}_i) - f_i(R_{\mathbf{U}_i}(\beta^\nu\eta_0\boldsymbol{\nabla}_i)) \; \geq \; -\gamma \sum_{i=1}^n \langle \boldsymbol{\nabla}_i, \beta^\nu\eta_0(-\boldsymbol{\nabla}_i) \rangle,$$

where $f_i(\mathbf{U}_i)$ is the component of the objective function (1) holding i fixed and ranging over j, and $R_{\mathbf{U}_i}(\boldsymbol{\Delta})$ performs the geodesic step described by (4) in the direction of $\boldsymbol{\Delta}$.

Convergence guarantees. One advantage of our approach is that we can use standard techniques as in [39] to obtain local convergence guarantees like the following:

Proposition 1. Let $\{(\mathbf{U}_1, \mathbf{U}_2, \ldots, \mathbf{U}_n)\}$ be a sequence of iterates generated by Grassmannian Fusion. Then the sequence will converge to a critical point of (1).

Proof. We will demonstrate that the gradient steps in (4) are an instance of Accelerated Line Search (ALS), outlined in Algorithm 1, where the product manifold $\mathbb{G}^n$ will serve as the Riemannian manifold $\mathcal{M}$, the tangent space of which is the cartesian product of tangent spaces of each constituent $\mathbb{G}$. To see this, let $T\mathcal{M}$ denote the *tangent bundle* of (set of all

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Algorithm 1: Accelerated Line Search (ALS)

Require: Riemannian manifold $\mathcal{M}$; continuously differentiable scalar field f on $\mathcal{M}$; retraction R from $T\mathcal{M}$ to $\mathcal{M}$; scalars $\eta_0 > 0$, $c, \beta, \gamma \in (0, 1)$.
Input: Initial iterate $\mathcal{U} \in \mathcal{M}$
Output: Sequence of iterates $\{\mathcal{U}_t\}$.
for t = 0, 1, 2, . . . **do**

    Pick $\boldsymbol{\Delta}_t \in T_{\mathcal{U}_t}\mathcal{M}$ such that the sequence of tangent vectors $\{\boldsymbol{\Delta}_t\}$ is gradient related. Select $\mathcal{U}_{t+1}$ such that

$$f(\mathcal{U}_t) - f(\mathcal{U}_{t+1}) \geq c(f(\mathcal{U}_t) - f(R_{\mathcal{U}_t}(\eta_t \boldsymbol{\Delta}_t))), \tag{5}$$

    where η_t is the Armijo step size for the given $\eta_0, \beta, \gamma, \boldsymbol{\Delta}_t$.
end

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tangent vectors to) $\mathcal{M}$, and let $T_{\mathcal{U}}\mathcal{M}$ denote the tangent space of $\mathcal{M}$ at $\mathcal{U} \in \mathcal{M}$. In our case, $\mathcal{U}$ is the tuple $(\mathbf{U}_1, \ldots, \mathbf{U}_n)$, and equation (4) serves as the *retraction*[1] $R_{\mathbf{U}_i}$ on each component, so that $R_{\mathcal{U}} = (R_{\mathbf{U}_1}, \ldots, R_{\mathbf{U}_n})$. One can verify that this is indeed a retraction by recognizing (4) as the exponential map $\mathrm{Exp} : T_{\mathbf{U}}\mathbb{G} \to \mathbb{G}$ and noting that, on a Riemannian manifold, the exponential map is a retraction, and that the product of exponential maps is again an exponential map [1]. For our sequence of *gradient-related*[2] tangent vectors, we use the negative gradient, which is clearly always gradient-related. The gradient on the product manifold is the cartesian product of the gradients on each constituent manifold, i.e., $\boldsymbol{\nabla}(f) = (\boldsymbol{\nabla}(f_1), \ldots, \boldsymbol{\nabla}(f_n))$. Moreover, the inner product on the tangent space is the sum of the inner products on the constituent tangent spaces. Therefore, if $\{\boldsymbol{\Delta}_{i,t}\}$, $\boldsymbol{\Delta}_{i,t} \in T_{\mathcal{U}_t}\mathcal{M}_i$ is gradient-related for each $\mathcal{M}_i$, then $\{(\boldsymbol{\Delta}_{1,t}, \ldots, \boldsymbol{\Delta}_{n,t})\}$ is gradient-related on the product manifold. Furthermore, setting $\mathcal{U}_{t+1} = R_{\mathcal{U}_t}(\eta_t \boldsymbol{\Delta}_t)$ satisfies the bound in (5) with $c = 1$. Thus Proposition 1 follows as consequence of Theorem 4.3.1 and Corollary 4.3.2 in [1]. $\qquad\square$

3   Fusion in Practice

Clustering, completion, and subspace inference. Recall that the solution to (1) provides an estimator $\mathcal{U}_i$ of $\mathcal{U}_i^\star$, the true subspace from which $\mathbf{x}_i$ is drawn. After solving (1), one may form the matrix $\mathbf{D}$ whose $(i, j)^{\text{th}}$ entry is given by $d_g(\mathbf{U}_i, \mathbf{U}_j)$ and use it as input to any distance-based clustering method, such as k-means [8, 21, 47], spectral clustering [50, 55, 59, 61], or DBSCAN [23, 28, 46]. While prior knowledge of the number of subspaces K may be required for some clustering methods (e.g., k-means, or spectral clustering), it is not required at all to solve (1). Hence, by choosing a clustering method that doesn't require knowing K (e.g., DBSCAN), our approach can be applied to situations where K is unknown. After clustering, one can agglomerate all the data points corresponding to the kth cluster in the same matrix $\hat{\mathbf{X}}_k^\Omega$, and run any Low-Rank Matrix Completion (LRMC) algorithm (e.g., [5, 7, 9, 10, 11, 31, 44, 57]) to estimate its completion $\hat{\mathbf{X}}_k$. Finally, one can run Principal Component Analysis (PCA) [38, 62] on $\hat{\mathbf{X}}_k$ to recover an estimate basis $\hat{\mathbf{U}}_k$ of the kth underlying subspace $\mathcal{U}_k^\star$.

Penalty parameter and model selection. Intuitively, the chordal term in (1) forces each subspace to be close to its assigned data point, and the geodesic term forces subspaces from different data points to be close to one another. The tradeoff between these two quantities is determined by the penalty parameter $\lambda \geq 0$. If $\lambda = 0$, then the geodesic term is ignored and there is a trivial solution where each subspace exactly contains its assigned data point (thus attaining the minimum, zero, for the chordal distance). If $\lambda > 0$, the geodesic term forces

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[1]A mapping R from $T\mathcal{M}$ to $\mathcal{M}$ such that its restriction to $T_{\mathcal{U}}\mathcal{M}$, denoted $R_{\mathcal{U}}$, satisfies a local rigidity condition which preserves gradients at $\mathcal{U}$; see the rightmost illustration in Figure 1 to build some intuition, or Chapters 3 and 4 of [1] for a more careful treatment of these definitions.

[2]Given a cost function f on a Riemannian manifold $\mathcal{M}$, a sequence of tangent vectors $\{\boldsymbol{\Delta}_t\}$, $\boldsymbol{\Delta}_t \in T_{\mathcal{U}_t}\mathcal{M}$, is gradient-related if, for any sequence $\{\mathcal{U}_t\}_{t\in\mathcal{K}}$ that converges to a non-critical point of f, the corresponding subsequence $\{\boldsymbol{\Delta}_t\}_{t\in\mathcal{K}}$ is bounded and satisfies $\limsup_{t\to\infty, \ t\in\mathcal{K}} \langle \nabla f(\mathcal{U}_t), \boldsymbol{\Delta}_t \rangle < 0$.

Figure 2: $\lambda \geq 0$ in (1) regulates how clusters fuse together. If $\lambda = 0$, each point is assigned to a subspace that exactly contains it (overfitting). The larger λ, the more we penalize subspaces being apart, which results in subspaces getting closer to form fewer clusters. The extreme case $\lambda = \infty$ is the special case of PCA and LRMC, where only one subspace is allowed to explain all data.

subspaces from different data points to get closer, even if they no longer contain exactly their assigned data points. As λ grows, subspaces get closer and closer (see Figure 2). The extreme case ($\lambda = \infty$) forces all subspaces to fuse into one (to attain zero in the second term), allowing only one subspace to explain all data, which is the equivalent of PCA in the complete-data case, and LRMC if data is missing. In other words, PCA and LRMC are the special cases of our formulation with $\lambda = \infty$.

Ultimately, the effect of λ will be reflected in the distance matrix $\mathbf{D}$, which in turn determines the number of clusters. The smaller λ, the more clusters, up to the extreme where each data point is in its own cluster. Conversely, the larger λ, the fewer clusters, up to the extreme point where all points are clustered together. The more subspaces, the more accuracy, but the more degrees of freedom (overfitting). To determine the best λ, one can compute a goodness of fit test, like the minimum effective dimension [29, 56], that quantifies the tradeoff between accuracy and degrees of freedom. Similarly, we can iteratively increase r in (1) to find all the data points that lie in 1-dimensional subspaces, then all the data points that lie in 2-dimensional subspaces, and so on (pruning the data at each iteration). This will result in an estimate of the number of subspaces K, and their dimensions.

Initialization. In our implementation we initialize (1) with a solution to the problem when $\lambda = 0$, i.e., when each subspace perfectly contains the observed entries of its assigned data point. To this end, for each i we first construct an m × r matrix whose first column is equal to $\mathbf{x}_i^\Omega$ in its observed entries, and whose remaining entries are filled with standard normal entries, known to produce incoherent and uniformly distributed subspaces [22]. This matrix is then orthonormalized to produce the initial estimate $\mathbf{U}_i$, which, by construction, contains $\mathbf{x}_i^\Omega$, thus producing $d(\mathbf{x}_i^\Omega, \mathbf{U}_i) = 0$.

Computational complexity. We point out that the main caveat of our approach is its quadratic complexity in the number of samples. Fortunately, subspace clustering allows a simple approach to sketching both samples and features [51]. That is, one may solve (1) with a subset of $n' \leq n$ columns, and a subset of $m' \leq m$ rows (e.g., those with most observations), resulting in an improved complexity, quadratic in n' as opposed to n. With the solution of (1), one can use a clustering method, a LRMC algorithm, and PCA, as described above, to produce subspace estimates $\hat{\mathbf{U}}_1, \ldots, \hat{\mathbf{U}}_{K'}$, with $K' \leq K$. Each of the remaining $n - n'$ incomplete data points $\mathbf{x}_i^\Omega$ that were not used to solve (1) and that have more than r observations (a fundamental requirement of subspace clustering [42]) can be trivially assigned to the subspace estimate producing the largest projection coefficient $\boldsymbol{\theta}_i^k = (\hat{\mathbf{U}}_k^{\Omega\mathsf{T}}\hat{\mathbf{U}}_k^\Omega)^{-1}\mathbf{x}_i^\Omega$, where $\hat{\mathbf{U}}_k^\Omega \in \mathbb{R}^{|\Omega_i| \times r}$ denotes the restriction of $\hat{\mathbf{U}}_k$ to the observed rows of $\mathbf{x}_i^\Omega$ (notice that $\hat{\mathbf{U}}_k^{\Omega\mathsf{T}}\hat{\mathbf{U}}_k^\Omega$ is invertible for almost every rank-r $\hat{\mathbf{U}}_k$ whenever $|\Omega_i| > r$ [42]). If $\mathbf{x}_i^\Omega$ is assigned to $\hat{\mathbf{U}}_k$, its completion can be trivially estimated as $\hat{\mathbf{x}}_i = \hat{\mathbf{U}}_k\boldsymbol{\theta}_i^k$. All the data points $\mathbf{x}_i^\Omega$ that are too far from all of the subspace estimates (equivalently, the data points whose coefficients are smaller than a pre-determined parameter) can be used to solve (1) again for a refined clustering.

4 FUSION GRADIENTS

In this section, we derive the expressions in (2) and (3) that govern the fusion steps of our formulation.

Chordal gradient. To obtain the gradient of the chordal distance $d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i)$ presented in (2), consider the partial derivative with respect to the $(a, b)^{\text{th}}$ element of $\mathbf{U}_i$ [18]:

$$\left[\frac{\partial d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i)}{\partial \mathbf{U}_i} \right]_{ab} = \frac{\partial}{\partial [\mathbf{U}_i]_{ab}} d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) = -2\sigma_1(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i) \frac{\partial \sigma_1(\mathbf{X}_i^{0\mathsf{T}}\mathbf{U}_i)}{\partial [\mathbf{U}_i]_{ab}}.$$

To obtain the partial derivative of the leading singular value σ_1, observe that $\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i$ and $\mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i$ share singular values: if $\mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i = \mathbf{V}\boldsymbol{\Sigma}\mathbf{W}^\mathsf{T}$, then $\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i = (\mathbf{X}_i^0\mathbf{V})\boldsymbol{\Sigma}\mathbf{W}^\mathsf{T}$ with $\mathbf{X}_i^0\mathbf{V} \in \mathbb{S}(m, r)$, so the result is a compact singular value decomposition. Recall that $\mathbf{v}_i$ and $\mathbf{w}_i$ denote the leading left and right singular vectors of $\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i$. Since $\mathbf{v}_i^\mathsf{T} \mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i \mathbf{w}_i = \sigma_1$, we have that

$$\frac{\partial \sigma_1}{\partial [\mathbf{U}_i]_{ab}} = \frac{\partial \mathbf{v}_i^\mathsf{T}}{\partial [\mathbf{U}_i]_{ab}} \mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i \mathbf{w}_i + \mathbf{v}_i^\mathsf{T} \mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \frac{\partial \mathbf{U}_i}{\partial [\mathbf{U}_i]_{ab}} \mathbf{w}_i + v_i^\mathsf{T} \mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i \frac{\partial \mathbf{w}_i}{\partial [\mathbf{U}_i]_{ab}}.$$

The first and third terms are zero, because $\mathbf{w}_i$ is the leading right singular vector of $\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i$, so $(\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i)\mathbf{w}_i = \sigma_1 \mathbf{v}_i$, which implies

$$\frac{\partial \mathbf{v}_i^\mathsf{T}}{\partial [\mathbf{U}_i]_{ab}} (\mathbf{X}_i^0 \mathbf{X}_i^{0\mathsf{T}} \mathbf{U}_i)\mathbf{w}_i = \sigma_1 \frac{\partial \mathbf{v}_i^\mathsf{T}}{\partial [\mathbf{U}_i]_{ab}} \mathbf{v}_i,$$

and because $\frac{\partial \mathbf{v}_i^\mathsf{T}}{\partial [\mathbf{U}_i]_{ab}} \mathbf{v}_i = 0$, as seen by differentiating both sides of $\mathbf{v}_i^\mathsf{T}\mathbf{v}_i = 1$ (and similarly for the third term). To compute the second term, note that $\mathbf{v}_i \in \text{span}(\mathbf{X}_i^0)$ since it is a column of $\mathbf{X}_i^0\mathbf{V}$, and the space spanned by $\mathbf{X}_i^0$ is invariant under multiplication by $\mathbf{V}$. Now, $(\mathbf{v}_i^\mathsf{T}\mathbf{X}_i^0\mathbf{X}_i^{0\mathsf{T}})^\mathsf{T} = \mathbf{X}_i^0\mathbf{X}_i^{0\mathsf{T}}\mathbf{v}_i = \mathbf{v}_i$, since $\mathbf{X}_i^0\mathbf{X}_i^{0\mathsf{T}}$ acts on vectors as the projection onto $\text{span}(\mathbf{X}_i^0)$. Hence $\mathbf{v}_i^\mathsf{T}\mathbf{X}_i^0\mathbf{X}_i^{0\mathsf{T}} = \mathbf{v}_i^\mathsf{T}$. The second term then becomes $\mathbf{v}_i^\mathsf{T} \frac{\partial \mathbf{U}_i}{\partial [\mathbf{U}_i]_{ab}} \mathbf{w}_i = [\mathbf{v}_i]_a [\mathbf{w}_i]_b$. It follows that

$$\frac{\partial \sigma_1}{\partial [\mathbf{U}_i]_{ab}} = [\mathbf{v}_i]_a [\mathbf{w}_i]_b. \tag{6}$$

From this, we have $\boldsymbol{\nabla} d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) = -2(\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T})\sigma_1 \mathbf{v}_i \mathbf{w}_i^\mathsf{T}$, where multiplication by $\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T}$ projects onto the tangent space of the Grassmannian at $\mathbf{U}_i$, as described before [1, 18].

Geodesic gradient. For the gradient of the geodesic distance $d_g(\mathbf{U}_i, \mathbf{U}_j)$ in (3) let us use σ_ℓ as shorthand for $\sigma_\ell(\mathbf{U}_i^\mathsf{T}\mathbf{U}_j)$, and recall that $\mathbf{v}_{ij}^\ell$ and $\mathbf{w}_{ij}^\ell$ denote the ℓth left and right singular vectors of $\mathbf{U}_j\mathbf{U}_j^\mathsf{T}\mathbf{U}_i$. Then the partial derivative with respect to the $(a, b)^{th}$ element of $\mathbf{U}_i$ is

$$\left[\frac{\partial d_g^2(\mathbf{U}_i, \mathbf{U}_j)}{\partial \mathbf{U}_i} \right]_{ab} = \sum_{\ell=1}^{r} \frac{-2 \arccos \sigma_\ell}{\sqrt{1 - \sigma_\ell^2}} \frac{\partial \sigma_\ell}{\partial [\mathbf{U}_i]_{ab}} = \sum_{\ell=1}^{r} \frac{-2 \arccos \sigma_\ell}{\sqrt{1 - \sigma_\ell^2}} \mathbf{v}_{ij}^\ell \mathbf{w}_{ij}^{\ell\mathsf{T}},$$

where the first equality follows because $\sigma_\ell(\mathbf{U}_i^\mathsf{T}\mathbf{U}_j) = \sigma_\ell(\mathbf{U}_j^\mathsf{T}\mathbf{U}_i) = \sigma_\ell(\mathbf{U}_j\mathbf{U}_j^\mathsf{T}\mathbf{U}_i)$, and the second equality follows by parallel arguments as the derivation of (6) for the leading singular value. The last equation is the Euclidean gradient. Projecting onto the tangent space at $\mathbf{U}_i$, as described before [1, 18], we obtain the following gradient on the Grassmannian

$$\boldsymbol{\nabla} d_g^2(\mathbf{U}_i, \mathbf{U}_j) = \sum_{\ell=1}^{r} \frac{-2 \arccos \sigma_\ell}{\sqrt{1 - \sigma_\ell^2}} (\mathbf{I} - \mathbf{U}_i\mathbf{U}_i^\mathsf{T})\mathbf{v}_{ij}^\ell \mathbf{w}_{ij}^{\ell\mathsf{T}}.$$

5 EXPERIMENTS

In this section we present a series of experiments on real and synthetic data, in particular the Hopkins155 dataset [52], and the Smartphone dataset for Human Activity Recognition in Ambient Assisted Living (AAL) [3]. Rather than establishing a new state-of-the-art, these experiments have the intention to serve as proof of concept, showing the potential of our approach, which in this first introduction and basic formulation performs comparable to prominent methods [63]. In our experiments we initialize (1) as described in Section 3, with

Figure 3: Clustering error (average over 10 trials) as a function of sampling rate for different synthetic settings.

r fixed, as is known a priori in both, the simulations, and the real datasets. We do not specify K, and we make no special adjustments to handle noise, as is not required by our approach. The attained solution to (1) is used as input to spectral clustering [50, 55, 59, 61] (though, as described in Section 3, other clustering algorithms, such as k-means [8, 21, 47] or DBSCAN [23, 28, 46] could be used). We measure accuracy in terms of clustering error, given by $\min_M \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{M(\hat{\mathbf{y}}) \neq \mathbf{y}\}}$, where $\mathbb{1}$ denotes the indicator function, and M is a function that maps the estimated cluster labels $\hat{\mathbf{y}} \in \{1, \ldots, \hat{K}\}^n$ assigned to $\mathbf{x}_1^\Omega, \ldots, \mathbf{x}_n^\Omega$, to the true labels $\mathbf{y} \in \{1, \ldots, K\}^n$.

Synthetic data. In all our simulations we first generate K matrices $\mathbf{U}_k^\star \in \mathbb{R}^{m \times r}$ with i.i.d. $N(0,1)$ entries, to use as bases of the *true* subspaces. For each k we generate a matrix $\mathbf{\Theta}_k^\star \in \mathbb{R}^{r \times n_k}$, also with i.i.d. $N(0,1)$ entries, to use as coefficients of the columns in the kth subspace. We then form $\mathbf{X}$ as the concatenation $[\mathbf{U}_1^\star \mathbf{\Theta}_1^\star, \mathbf{U}_2^\star \mathbf{\Theta}_2^\star, \ldots, \mathbf{U}_K^\star \mathbf{\Theta}_K^\star]$. To induce missing data we sample each entry independently with probability p. Figure 3 shows the clustering results as a function of the sampling rate for a variety of settings, tuning the parameter λ manually. Notice that, even with this first formulation, we perform comparable to existing methods, and even better in some cases, especially in low-sampling regimes.

Object tracking in Hopkins 155. This dataset contains 155 videos of K = 2 or K = 3 moving objects, such as checkerboards, vehicles, and pedestrians. In each video, a collection of n mark points are tracked through all frames. The locations over time of the ith point are stacked to produce $\mathbf{x}_i \in \mathbb{R}^m$, so that the points corresponding to the same object lie near a low-dimensional subspace [49, 30] (r varies from video to video, from 1 to 3). In all cases we fixed the penalty parameter λ to 1. To induce missing data (e.g., produced by occlusions) we sample each entry independently with probability p. Figure 4 shows the clustering results.

Human activity recognition in Smartphone AAL Dataset. This dataset contains n = 5744 instances, each with m = 561 features related to pre-processed accelerometer and gyroscope time series and summary statistics [2], related to K = 2 activities: walking, and other movements, each approximated by a subspace of dimension r = 4. Recall that the complexity of (1) is quadratic in n, so if solved directly, this dataset that would produce an unmanageable computational complexity. However, using the sketching techniques described in Section 3, it can be solved quite efficiently. In particular, we only used $m' = 158$ features (related to the accelerometer's and gyroscope's minimum, maximum, standard deviation, and mean parameters over time), and $n' = 100$ samples selected at random, evenly distributed among classes. In all cases we fixed the penalty parameter λ to 10^{-5}. The results are summarized in Figure 4. Notice that our approach outperforms existing methods in the low-sampling regime.

Baseline comparisons and full-data sub-optimality. A recent survey [33] shows that most state-of-the-art algorithms for HRMC (including MC+SSC [63], EM [41], GSSC [43], k-subspaces [6], and more) have similar performance, with varying winners on specific scenarios depending on subspace vs ambient dimension gap, fraction of missing data, and number of subspaces. Based on this recent survey [33], and others [43], we chose a subset of representative algorithms as baseline (including EWZF-SSC, which as seen in [33] has a nearly identical performance as MC+SSC, EM, GSSC, and k-subspaces in the scenarios

Figure 4: Clustering error as a function of sampling rate for real datasets. **Left:** average over 120 videos with K = 2 objects, and 35 videos with K = 3 objects. **Right:** average over 20 trials.

discussed in our paper). Finally, HRMC counterparts of LRMC algorithms such as Grouse and Grasta (see, for example, k-GROUSE [6]) have comparable performance to our baselines.

Lastly, we note the disparity in performance between our model and existing algorithms when the missing data rate is low. The main motivation for our approach is incomplete data. While our formulation can certainly be used with full data, we acknowledge that it would be an over-kill, and consequently suboptimal in that scenario, which has been extensively studied. Hence, it is not surprising that methods tailored for full-data outperform ours in such setting. However, no full-data method outperforms ours when data is missing.

6 Future Directions and Challenges

The main formulation presented in this paper is a non-convex optimization that relies on the simultaneous interactions of many terms. A proper analysis of the model is therefore challenging. One difficulty confronted is the complex geometry of the zero-set of the chordal distance term, or more precisely, the intersections of many of these zero-sets, one for each column of data. While intuition suggests that the model is encouraged by the geodesic term to find regions of "dense" intersection, and therefore build consensus, a more precise formulation of this intuition has evaded us. This is further highlighted in Figures 3 and 4 by the fact that the performance of our model decreases as K grows, indicating that it is not currently understood how the combination of the chordal and geodesic terms encourage consensus amongst so many cross-cluster terms. It is our belief that a well-designed weighted version of (1), such as

$$\min_{\mathbf{U}_1,\ldots,\mathbf{U}_n \in \mathbb{S}^{m \times r}} \quad \sum_{i=1}^{n} d_c^2(\mathbf{x}_i^\Omega, \mathbf{U}_i) \; + \; \frac{\lambda}{2} \sum_{i,j=1}^{n} w_{ij} d_g^2(\mathbf{U}_i, \mathbf{U}_j), \tag{7}$$

where the weights $w_{ij} \geq 0$ quantify how much attention is given to each penalty, is key to unlocking better performance and understanding of the model. Our immediate future work will focus on investigating options for these weights, such as inverse distance functions, or k-nearest neighbors, known to dramatically improve the performance, computational complexity, and tolerance to K of fusion formulations in Euclidean space [4, 16, 48, 64].

7 Conclusions

This paper presents a new paradigm for clustering incomplete datapoints using subspaces as proxies to leverage the geometry of the Grassmannian. This new perspective enables clustering and completion of data in a union of subspaces. This work should be understood as the first introduction to the idea of fusion penalties in the Grassmann manifold, for the problem of *high-rank matrix completion*. Rather than establishing our approach as the state-of-the-art, our experiments have the intention to serve as proof of concept, showing that there is potential in our approach, in the hopes to ignite future work on several directions, such as the study of weighted versions described in (7), the choice of penalty parameters, and variants robust to outliers.

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