

Generalized Principal Component Analysis (GPCA)

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Abstract—This paper presents an algebro-geometric solution to the problem of segmenting an unknown number of subspaces of unknown and varying dimensions from sample data points. We represent the subspaces with a set of homogeneous polynomials whose degree is the number of subspaces and whose derivatives at a data point give normal vectors to the subspace passing through the point. When the number of subspaces is known, we show that these polynomials can be estimated linearly from data, hence subspace segmentation is reduced to classifying one point per subspace. We select these points optimally from the data set by minimizing certain distance function, thus dealing automatically with moderate noise in the data. A basis for the complement of each subspace is then recovered by applying standard PCA to the collection of derivatives (normal vectors). Extensions of GPCA that deal with data in a high-dimensional space and with an unknown number of subspaces are also presented. Our experiments on low-dimensional data show that GPCA out-performs existing algebraic algorithms based on polynomial factorization and provides a good initialization to iterative techniques such as K-subspace and Expectation Maximization. We also present applications of GPCA to computer vision problems such as face clustering, temporal video segmentation, and 3-D motion segmentation from point correspondences in multiple affine views.

Index Terms—Principal component analysis (PCA), subspace segmentation, Veronese map, dimensionality reduction, temporal video segmentation, dynamic scenes and motion segmentation.

I. INTRODUCTION

PRINCIPAL Component Analysis (PCA) [12] refers to the problem of fitting a linear subspace $S \subset \mathbb{R}^D$ of unknown dimension $d < D$ to N sample points $\{\mathbf{x}_j\}_{j=1}^N$ in S . This problem shows up in a variety of applications in many fields, e.g., pattern recognition, data compression, regression, image processing, etc., and can be solved in a remarkably simple way from the singular value decomposition (SVD) of the (mean-subtracted) data matrix $[\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N] \in \mathbb{R}^{D \times N}$.¹ With noisy data, this linear algebraic solution has the geometric interpretation of minimizing the sum of the squared distances from the (noisy) data points \mathbf{x}_j to their projections $\tilde{\mathbf{x}}^j$ in S .

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¹In the context of stochastic signal processing, PCA is also known as the Karhunen-Loeve transform [18]; in the applied statistics literature, SVD is also known as the Eckart and Young decomposition [4].

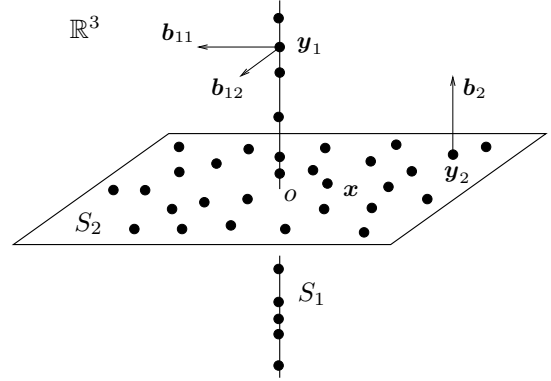


Fig. 1. Data points drawn from the union of one plane and one line (through the origin o) in \mathbb{R}^3 . The objective of subspace segmentation is to identify the normal vectors \mathbf{b}_{11} , \mathbf{b}_{12} and \mathbf{b}_2 to each one of the subspaces from the data.

In addition to these algebraic and geometric interpretations, PCA can also be understood in a probabilistic manner. In Probabilistic PCA [20] (PPCA), the noise is assumed to be drawn from an unknown distribution, and the problem becomes one of identifying the subspace and distribution parameters in a maximum likelihood sense. When the noise distribution is Gaussian, the algebro-geometric and probabilistic interpretations coincide [2]. However, when the noise distribution is non-Gaussian the solution to PPCA is no longer linear, as shown in [2], where PCA is generalized to arbitrary distributions in the exponential family.

Another extension of PCA is nonlinear principal components (NLPCA) or Kernel PCA (KPCA), which is the problem of identifying a *nonlinear* manifold from sample points. The standard solution to NLPCA [16] is based on first embedding the data into a higher-dimensional *feature* space F and then applying standard PCA to the embedded data. Since the dimension of F can be large, a more practical solution is obtained from the eigenvalue decomposition of the so-called *kernel* matrix, hence the name KPCA. One of the disadvantages of KPCA is that in practice, it is difficult to determine which kernel function to use, because the choice of the kernel naturally depends on the nonlinear structure of the manifold to be identified. In fact, learning kernels is an active topic of research in machine learning. To the best of our knowledge, our work is the first one to prove analytically that the Veronese map (a polynomial embedding) is the natural embedding for data lying in a union of multiple subspaces.

In this paper, we consider the following alternative extension of PCA to the case of data lying in a union of subspaces, as illustrated in Figure 1 for two subspaces of \mathbb{R}^3 .

Problem 1 (Subspace Segmentation)

Given a set of points $\mathbf{X} = \{\mathbf{x}_j \in \mathbb{R}^D\}_{j=1}^N$ drawn from $n \geq 1$ different linear subspaces $\{S_i \subseteq \mathbb{R}^D\}_{i=1}^n$ of dimension $d_i = \dim(S_i)$, $0 < d_i < D$, without knowing which points belong to which subspace:

- 1) Find the number of subspaces n and their dimensions $\{d_i\}_{i=1}^n$;
 - 2) Find a basis for each subspace S_i (or for S_i^\perp);
 - 3) Group the N sample points into the n subspaces.
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A. Previous work on subspace segmentation

Subspace segmentation is a fundamental problem in many applications in computer vision (e.g., image/motion/video segmentation), image processing (e.g., image representation and compression), and systems theory (e.g., hybrid system identification), which is usually regarded as “chicken-and-egg.” If the segmentation of the data was known, one could easily fit a single subspace to each group of points using standard PCA. Conversely, if the subspace bases were known, one could easily find the data points that best fit each subspace. Since in practice neither the subspace bases nor the segmentation of the data are known, most existing methods randomly choose a basis for each subspace, and then iterate between data segmentation and subspace estimation. This can be done using, e.g., K-subspace [10], an extension of K-means to the case of subspaces, subspace growing and subspace selection [15], or Expectation Maximization (EM) for mixtures of PCA’s [19]. Unfortunately, most iterative methods are in general very sensitive to initialization, hence they may not converge to the global optimum [21].

The need for initialization methods has motivated the recent development of algebro-geometric approaches to subspace segmentation that do *not* require initialization. In [13] (see also [3]) it is shown that when the subspaces are orthogonal, of equal dimension d , and intersect only at the origin, which implies that $D \geq nd$, one can use the SVD of the data to define a similarity matrix from which the segmentation of the data can be obtained using spectral clustering techniques. Unfortunately, this method is sensitive to noise in the data, as shown in [13], [26] where various improvements are proposed, and fails when the subspaces intersect arbitrarily [14], [22], [27]. The latter case has been addressed in an *ad-hoc* fashion by using clustering algorithms such as K-means, spectral clustering or EM [14], [27] to segment the data and PCA to obtain a basis for each group. The only algebraic approaches that deal with arbitrary intersections are [17], which studies the case of two planes in \mathbb{R}^3 , and [24] which studies the case of subspaces of co-dimension one, i.e. *hyperplanes*, and shows that hyperplane segmentation is equivalent to homogeneous polynomial factorization. Our previous work [23] extended this framework to subspaces of unknown and possibly different dimensions under the additional assumption that the number of subspaces is known. This paper unifies the results of [24] and [23] and extends to the case in which both the number and dimensions of the subspaces are unknown.

B. Paper organization and contributions

In this paper, we propose an algebro-geometric approach to subspace segmentation called *Generalized Principal Component Analysis* (GPCA), which is based on fitting, differentiating and dividing polynomials. Unlike prior work, we do not restrict the subspaces to be orthogonal, trivially intersecting, or with known and equal dimensions. Instead, we address the most general case of an *arbitrary number of subspaces of unknown* and possibly *different* dimensions (e.g., Figure 1) and with *arbitrary intersections* among the subspaces.

In Section II we motivate and highlight the key ideas of our approach by solving the simple example shown in Figure 1.

In Section III we generalize this example to the case of data lying in a known number of subspaces with unknown and possibly different dimensions. We show that one can represent the union of all subspaces as the zero set of a collection of homogeneous polynomials whose degree is the number of subspaces and whose factors encode normal vectors to the subspaces. The coefficients of these polynomials can be linearly estimated from sample data points on the subspaces and the set of normal vectors to each subspace can be obtained by evaluating the derivatives of these polynomials at any point lying on the subspace. Therefore, subspace segmentation is reduced to the problem of classifying one point per subspace. When those points are given (e.g., in semi-supervised learning), this means that in order to learn the mixture of subspaces, it is sufficient to have *one positive example per class*. When all the data points are unlabeled (e.g., in unsupervised learning), we use polynomial division to recursively select points in the data set that minimize their distance to the algebraic set, hence dealing automatically with moderate noise in the data. A basis for the complement of each subspace is then recovered by applying standard PCA to the derivatives of the polynomials (normal vectors) at those points. The final result is a global, non-iterative subspace segmentation algorithm based on simple linear and polynomial algebra.

In Section IV we discuss some extensions of our approach. We show how to deal with low-dimensional subspaces of a high-dimensional space via a linear projection onto a low-dimensional subspace that preserves the number and dimensions of the subspaces. We also show how to generalize the basic GPCA algorithm to the case in which the number of subspaces is unknown via a recursive partitioning algorithm.

In Section V, we present experiments on low-dimensional data showing that GPCA gives about half the error of existing algebraic algorithms based on polynomial factorization, and improves the performance of iterative techniques, such as K-subspace and EM, by about 50% with respect to random initialization. We also present applications of GPCA to computer vision problems such as face clustering, temporal video segmentation, and 3-D motion segmentation from point correspondences in multiple views.

II. AN INTRODUCTORY EXAMPLE

Imagine that we are given data in \mathbb{R}^3 drawn from a line $S_1 = \{\mathbf{x} : x_1 = x_2 = 0\}$ and a plane $S_2 = \{\mathbf{x} : x_3 = 0\}$, as

shown in Figure 1. We can describe the two subspaces as

$$\begin{aligned} S_1 \cup S_2 &= \{\mathbf{x} : (x_1 = x_2 = 0) \vee (x_3 = 0)\} \\ &= \{\mathbf{x} : (x_1 x_3 = 0) \wedge (x_2 x_3 = 0)\}. \end{aligned}$$

Therefore, even though each individual subspace is described with polynomials of degree one (linear equations), the mixture of two subspaces is described with two polynomials of degree two, namely $p_{21}(\mathbf{x}) = x_1 x_3$ and $p_{22}(\mathbf{x}) = x_2 x_3$. More generally, any two linear subspaces in \mathbb{R}^3 can be represented as the set of points satisfying some polynomials of the form

$$c_1 x_1^2 + c_2 x_1 x_2 + c_3 x_1 x_3 + c_4 x_2^2 + c_5 x_2 x_3 + c_6 x_3^2 = 0.$$

Although these polynomials are nonlinear in each data point $[x_1, x_2, x_3]^T$, they are actually linear in the vector of coefficients $\mathbf{c} = [c_1, \dots, c_6]^T$. Therefore, given enough data points, one can linearly fit these polynomials to the data.

Given the collection of polynomials that vanish on the data points, we would like to compute a basis for each subspace. In our example, let $P_2(\mathbf{x}) = [p_{21}(\mathbf{x}), p_{22}(\mathbf{x})]$ and consider the derivatives of $P_2(\mathbf{x})$ at two points in each of the subspaces $\mathbf{y}_1 = [0, 0, 1]^T \in S_1$ and $\mathbf{y}_2 = [1, 1, 0]^T \in S_2$:

$$DP_2(\mathbf{x}) = \begin{bmatrix} x_3 & 0 \\ 0 & x_3 \\ x_1 & x_2 \end{bmatrix} \Rightarrow DP_2(\mathbf{y}_1) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, DP_2(\mathbf{y}_2) = \begin{bmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 1 \end{bmatrix}.$$

Note that the columns of $DP_2(\mathbf{y}_1)$ span S_1^\perp and the columns of $DP_2(\mathbf{y}_2)$ span S_2^\perp (see Figure 1). Also, the dimension of the line is $d_1 = 3 - \text{rank}(DP_2(\mathbf{y}_1)) = 1$ and the dimension of the plane is $d_2 = 3 - \text{rank}(DP_2(\mathbf{y}_2)) = 2$. Thus, if we are given one point in each subspace, we can obtain the subspace bases and their dimensions from the derivatives of the polynomials at these points.

The final question is to find one point per subspace, so that we can obtain the normal vectors from the derivatives of P_2 at those points. With perfect data, we may choose a first point as any of the points in the data set. With noisy data, we may first define a distance from any point in \mathbb{R}^3 to one of the subspaces, e.g., the algebraic distance $d_2(\mathbf{x})^2 = p_{21}(\mathbf{x})^2 + p_{22}(\mathbf{x})^2 = (x_1^2 + x_2^2)x_3^2$, and then choose a point in the data set that minimizes this distance. Say we pick $\mathbf{y}_2 \in S_2$ as such point. We can then compute the normal vector $\mathbf{b}_2 = [0, 0, 1]^T$ to S_2 from $DP(\mathbf{y}_2)$. As it turns out, we can pick a second point in S_1 but not in S_2 by polynomial division. We can just divide the original polynomials of degree $n = 2$ by $(\mathbf{b}_2^T \mathbf{x})$ to obtain polynomials of degree $n - 1 = 1$:

$$p_{11}(\mathbf{x}) = \frac{p_{21}(\mathbf{x})}{\mathbf{b}_2^T \mathbf{x}} = x_1 \quad \text{and} \quad p_{12}(\mathbf{x}) = \frac{p_{22}(\mathbf{x})}{\mathbf{b}_2^T \mathbf{x}} = x_2.$$

Since these new polynomials vanish on S_1 but not on S_2 , we can find a point \mathbf{y}_1 in S_1 but not in S_2 , as a point in the data set that minimizes $d_1(\mathbf{x})^2 = p_{11}(\mathbf{x})^2 + p_{12}(\mathbf{x})^2 = x_1^2 + x_2^2$.

As we will show in the next section, one can also solve the more general problem of segmenting a union of n subspaces $\{S_i \subset \mathbb{R}^D\}_{i=1}^n$ of unknown and possibly different dimensions $\{d_i\}_{i=1}^n$ by polynomial fitting (Section III-C), differentiation (Section III-D) and division (Section III-E).

III. GENERALIZED PRINCIPAL COMPONENT ANALYSIS

In this section, we derive a constructive algebro-geometric solution to the subspace segmentation problem when the number of subspaces n is known. The case in which the number of subspaces is unknown will be discussed in Section IV-B. Our algebro-geometric solution is summarized in the following theorem.

Theorem 1 (Generalized Principal Component Analysis):

A union of n subspaces of \mathbb{R}^D can be represented with a set of homogeneous polynomials of degree n in D variables. These polynomials can be estimated linearly given enough sample points in general position in the subspaces. A basis for the complement of each subspace can be obtained from the derivatives of these polynomials at a point in each of the subspaces. Such points can be recursively selected via polynomial division. Therefore, the subspace segmentation problem is mathematically equivalent to fitting, differentiating and dividing a set of homogeneous polynomials.

A. Notation

Let \mathbf{x} be a vector in \mathbb{R}^D . A homogeneous polynomial of degree n in \mathbf{x} is a polynomial $p_n(\mathbf{x})$ such that $p_n(\lambda \mathbf{x}) = \lambda^n p_n(\mathbf{x})$ for all λ in \mathbb{R} . The space of all homogeneous polynomials of degree n in D variables is a vector space of dimension $M_n(D) = \binom{n+D-1}{D-1}$. A particular basis for this space is given by all the monomials of degree n in D variables, that is $\mathbf{x}^I = x_1^{n_1} x_2^{n_2} \dots x_D^{n_D}$ with $0 \leq n_j \leq n$ for $j = 1, \dots, D$, and $n_1 + n_2 + \dots + n_D = n$. Thus, each homogeneous polynomial can be written as a linear combination of a vector of coefficients $\mathbf{c}_n \in \mathbb{R}^{M_n(D)}$ as

$$p_n(\mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x}) = \sum c_{n_1, n_2, \dots, n_D} x_1^{n_1} x_2^{n_2} \dots x_D^{n_D}, \quad (1)$$

where $\nu_n: \mathbb{R}^D \rightarrow \mathbb{R}^{M_n(D)}$ is the Veronese map of degree n [7], also known as the polynomial embedding in machine learning, defined as $\nu_n: [x_1, \dots, x_D]^T \mapsto [\dots, \mathbf{x}^I, \dots]^T$ with I chosen in the degree-lexicographic order.

Example 1 (The Veronese map of degree 2 in 3 variables): If $\mathbf{x} = [x_1, x_2, x_3]^T \in \mathbb{R}^3$, the Veronese map of degree 2 is given by:

$$\nu_2(\mathbf{x}) = [x_1^2, x_1 x_2, x_1 x_3, x_2^2, x_2 x_3, x_3^2]^T \in \mathbb{R}^6. \quad (2)$$

B. Representing a union of n subspaces with a set of homogeneous polynomials of degree n

We represent a subspace $S_i \subset \mathbb{R}^D$ of dimension d_i , where $0 < d_i < D$, by choosing a basis

$$B_i \doteq [\mathbf{b}_{i1}, \dots, \mathbf{b}_{i(D-d_i)}] \in \mathbb{R}^{D \times (D-d_i)} \quad (3)$$

for its orthogonal complement S_i^\perp . One could also choose a basis for S_i directly, especially if $d_i \ll D$. Section IV-A will show that the problem can be reduced to the case $D = \max\{d_i\} + 1$, hence the orthogonal representation is more convenient if $\max\{d_i\}$ is small. With this representation, each subspace can be expressed as the set of points satisfying $D - d_i$ linear equations (polynomials of degree one), that is

$$S_i = \{\mathbf{x} \in \mathbb{R}^D : B_i^T \mathbf{x} = 0\} = \left\{ \mathbf{x} \in \mathbb{R}^D : \bigwedge_{j=1}^{D-d_i} (\mathbf{b}_{ij}^T \mathbf{x} = 0) \right\}. \quad (4)$$

For affine subspaces (which do not necessarily pass through the origin), we use homogeneous coordinates so that they become linear subspaces.

We now demonstrate that one can represent the union of n subspaces $\{S_i \subset \mathbb{R}^D\}_{i=1}^n$ with a set of polynomials whose degree is n rather than one. To see this, notice that $\mathbf{x} \in \mathbb{R}^D$ belongs to $\cup_{i=1}^n S_i$ if and only if it satisfies $(\mathbf{x} \in S_1) \vee \dots \vee (\mathbf{x} \in S_n)$. This is equivalent to

$$\bigvee_{i=1}^n (\mathbf{x} \in S_i) \Leftrightarrow \bigvee_{i=1}^n \bigwedge_{j=1}^{D-d_i} (\mathbf{b}_{ij}^T \mathbf{x} = 0) \Leftrightarrow \bigwedge_{\sigma} \bigvee_{i=1}^n (\mathbf{b}_{i\sigma(i)}^T \mathbf{x} = 0), \quad (5)$$

where the right hand side is obtained by exchanging ands and ors using De Morgan's laws, and σ is a particular choice of one normal vector $\mathbf{b}_{i\sigma(i)}$ from each basis B_i . Since each one of the $\prod_{i=1}^n (D - d_i)$ equations in (5) is of the form

$$\bigvee_{i=1}^n (\mathbf{b}_{i\sigma(i)}^T \mathbf{x} = 0) \Leftrightarrow \left(\prod_{i=1}^n (\mathbf{b}_{i\sigma(i)}^T \mathbf{x} = 0) \right) \Leftrightarrow (p_{n\sigma}(\mathbf{x}) = 0), \quad (6)$$

i.e. a homogeneous polynomial of degree n in D variables, we can write each polynomial as a superposition of monomials with the coefficient vector $\mathbf{c}_n \in \mathbb{R}^{M_n(D)}$, as in (1). Therefore, we have the following result.

Theorem 2 (Representing Subspaces with Polynomials): A union of n subspaces can be represented as the set of points satisfying a set of homogeneous polynomials of the form

$$p_n(\mathbf{x}) = \prod_{i=1}^n (\mathbf{b}_i^T \mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x}) = 0, \quad (7)$$

where $\mathbf{b}_i \in \mathbb{R}^D$ is a normal vector to the i th subspace.

The importance of Theorem 2 is that it allows us to solve the ‘‘chicken-and-egg’’ problem algebraically, because the polynomials in (7) are satisfied by *all* data points, regardless of which point belongs to which subspace. We can then use all the data to estimate all the subspaces, without prior segmentation, and without having to iterate between data segmentation and model estimation, as we will show in Sections III-C, III-D and III-E.

C. Fitting polynomials to data lying in multiple subspaces

Thanks to Theorem 2, the problem of identifying a union of n subspaces $\{S_i\}_{i=1}^n$ from a set of data points $\mathbf{X} \doteq \{\mathbf{x}_j\}_{j=1}^N$ lying in the subspaces is equivalent to solving for the normal bases $\{B_i\}_{i=1}^n$ from the set of *nonlinear* equations in (6). Although these polynomial equations are nonlinear in each data point \mathbf{x} , they are actually *linear* in the vector of coefficients \mathbf{c}_n . Indeed, since each polynomial $p_n(\mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x})$ must be satisfied by every data point, we have $\mathbf{c}_n^T \nu_n(\mathbf{x}_j) = 0$ for all $j = 1, \dots, N$. We use I_n to denote the space of coefficient vectors \mathbf{c}_n of all homogeneous polynomials that vanish on the n subspaces. Obviously, the coefficient vectors of the factorizable polynomials defined in (6) span a (possibly proper) subspace in I_n :

$$\text{span}_{\sigma} \{p_{n\sigma}\} \subseteq I_n. \quad (8)$$

As every vector \mathbf{c}_n in I_n represents a polynomial that vanishes on all the data points (on the subspaces), the vector must satisfy the system of linear equations

$$\mathbf{c}_n^T \mathbf{V}_n(D) \doteq \mathbf{c}_n^T [\nu_n(\mathbf{x}_1) \quad \dots \quad \nu_n(\mathbf{x}_N)] = \mathbf{0}^T. \quad (9)$$

$\mathbf{V}_n(D) \in \mathbb{R}^{M_n(D) \times N}$ is called the *embedded data matrix*. Obviously we have the relationship

$$I_n \subseteq \text{null}(\mathbf{V}_n(D)).$$

Although we know that the coefficient vectors \mathbf{c}_n of vanishing polynomials must lie in the left null space of $\mathbf{V}_n(D)$, we do not know if every vector in the null space corresponds to a polynomial that vanishes on the subspaces. Therefore, we would like to study under what conditions on the data points, we can solve for the unique $m_n \doteq \dim(I_n)$ independent polynomials that vanish on the subspaces from the null space of \mathbf{V}_n . Clearly, a necessary condition is to have $N \geq \sum_{i=1}^n d_i$ points in $\cup_{i=1}^n S_i$, with at least d_i points in general position within each subspace S_i , i.e. the d_i points must span S_i . However, because we are representing each polynomial $p_n(\mathbf{x})$ linearly via the vector of coefficients \mathbf{c}_n we need a number of samples such that a basis for I_n can be uniquely recovered from $\text{null}(\mathbf{V}_n(D))$. That is, the number of samples N must be such that

$$\text{rank}(\mathbf{V}_n(D)) = M_n(D) - m_n \leq M_n(D) - 1. \quad (10)$$

Therefore, if the number of subspaces n is known, we can recover I_n from $\text{null}(\mathbf{V}_n(D))$ given $N \geq M_n(D) - 1$ points in general position. A basis of I_n can be computed *linearly* as the set of m_n left singular vectors of $\mathbf{V}_n(D)$ associated with its m_n zero singular values. Thus, we obtain a basis of polynomials of degree n , say $\{p_{n\ell}\}_{\ell=1}^{m_n}$, that vanish on the n subspaces. Notice that the polynomials $p_{n\ell}$ do not necessarily factor as a product of linear forms. For example, $x_1^2 + x_1x_2$ and $x_2^2 - x_1x_2$ are factorizable but their sum $x_1^2 + x_2^2$ is not. As we will see shortly, this will not be a problem for us to use them to extract the subspaces.

Remark 1 (GPCA and Kernel PCA): Kernel PCA identifies a manifold from sample data by embedding the data into a higher-dimensional feature space \mathbf{F} such that the embedded data points lie in a linear subspace of \mathbf{F} . Unfortunately, there is no general methodology for finding the appropriate embedding for a particular problem, because the embedding naturally depends on the geometry of the manifold. The above derivation shows that the commonly used *polynomial embedding* ν_n is the appropriate embedding to use in KPCA when the original data lie in a union of subspaces, because the embedded data points $\{\nu_n(\mathbf{x}_j)\}_{j=1}^N$ lie in an subspace of $\mathbb{R}^{M_n(D)}$ of $M_n(D) - m_n$ dimension, where $m_n = \dim(I_n)$. Notice also that the matrix $\mathcal{C} = \mathbf{V}_n(D)\mathbf{V}_n(D)^T \in \mathbb{R}^{M_n(D) \times M_n(D)}$ is exactly the *covariance matrix* in the feature space and $\mathcal{K} = \mathbf{V}_n(D)^T \mathbf{V}_n(D) \in \mathbb{R}^{N \times N}$ is the *kernel matrix* associated with the N embedded samples.

Remark 2 (Estimation from Noisy Data): In the presence of moderate noise, we can still estimate the coefficients of each polynomial in a least-squares sense as the singular vectors of $\mathbf{V}_n(D)$ associated with its smallest singular values. However, we cannot directly estimate the number of polynomials from the rank of $\mathbf{V}_n(D)$, because $\mathbf{V}_n(D)$ may be of full rank. We use model selection to determine m_n as

$$m_n = \arg \min_m \frac{\sigma_{m+1}^2(\mathbf{V}_n(D))}{\sum_{j=1}^m \sigma_j^2(\mathbf{V}_n(D))} + \kappa m, \quad (11)$$

with $\sigma_j(\mathbf{V}_n(D))$ the j th singular vector of $\mathbf{V}_n(D)$ and κ a parameter. An alternative way of selecting the correct linear model (in feature space) for noisy data can be found in [11].

Remark 3 (Sub-Optimality in the Stochastic Case):

Notice that in the case of hyperplanes, the least-squares solution for \mathbf{c}_n is obtained by minimizing $\|\mathbf{c}^T \mathbf{V}_n(D)\|^2$ subject to $\|\mathbf{c}_n\| = 1$. However, when $n > 1$ the so-found \mathbf{c}_n does not minimize the sum of least-square errors $\sum_j \min_{i=1, \dots, n} (\mathbf{b}_i^T \mathbf{x}_j)^2$. Instead, it minimizes a “weighted version” of the least-square errors

$$\sum_j \alpha_j \min_{i=1, \dots, n} (\mathbf{b}_i^T \mathbf{x}_j)^2 \doteq \sum_j \prod_{i=1}^n (\mathbf{b}_i^T \mathbf{x}_j)^2 = \|\mathbf{c}^T \mathbf{V}_n(D)\|^2, \quad (12)$$

where the weight α_j is conveniently chosen so as to eliminate the minimization over $i = 1, \dots, n$. Such a “softening” of the objective function permits a global algebraic solution, because the softened error does not depend on the membership of one point to one of the hyperplanes. This least-squares solution for \mathbf{c}_n offers a sub-optimal approximation for the original stochastic objective when the variance of the noise is small. This solution can be used to initialize other iterative optimization schemes (such as EM) to further minimize the original stochastic objective.

D. Obtaining a basis and the dimension of each subspace by polynomial differentiation

In this section, we show that one can obtain a basis $\{B_i\}_{i=1}^n$ for the complement of each subspace and their dimensions $\{d_i\}_{i=1}^n$ by differentiating all the polynomials obtained from the left null space of the embedded data matrix $\mathbf{V}_n(D)$.

For the sake of simplicity, let us first consider the case of hyperplanes, i.e. subspaces of equal dimension $d_i = D - 1$, for $i = 1, \dots, n$. In this case, there is only one vector $\mathbf{b}_i \in \mathbb{R}^D$ normal to subspace S_i . Therefore, there is only one polynomial representing the n hyperplanes, namely $p_n(\mathbf{x}) = (\mathbf{b}_1^T \mathbf{x}) \cdots (\mathbf{b}_n^T \mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x})$, and its vector of coefficients \mathbf{c}_n can be computed as the unique vector in the left null space of $\mathbf{V}_n(D)$. Consider now the derivative of $p_n(\mathbf{x})$

$$Dp_n(\mathbf{x}) = \frac{\partial p_n(\mathbf{x})}{\partial \mathbf{x}} = \frac{\partial}{\partial \mathbf{x}} \prod_{i=1}^n (\mathbf{b}_i^T \mathbf{x}) = \sum_{i=1}^n (\mathbf{b}_i) \prod_{\ell \neq i} (\mathbf{b}_\ell^T \mathbf{x}), \quad (13)$$

at a point $\mathbf{y}_i \in S_i$, i.e. \mathbf{y}_i is such that $\mathbf{b}_i^T \mathbf{y}_i = 0$. Then all terms in (13), except the i th, vanish, because $\prod_{\ell \neq i} (\mathbf{b}_\ell^T \mathbf{y}_j) = 0$ for $j \neq i$, so that we can immediately obtain the normal vectors as

$$\mathbf{b}_i = \frac{Dp_n(\mathbf{y}_i)}{\|Dp_n(\mathbf{y}_i)\|}, \quad i = 1, \dots, n. \quad (14)$$

Therefore, in a *semi-supervised learning scenario* in which we are given only *one positive example per class*, the hyperplane segmentation problem can be solved *analytically* by evaluating the *derivatives* of $p_n(\mathbf{x})$ at the points with known labels.

As it turns out, the same principle applies to subspaces of arbitrary dimensions. This fact should come at no surprise. The zero set of each vanishing polynomial $p_{n\ell}$ is just a surface in \mathbb{R}^D , therefore the derivative of $p_{n\ell}$ at a point $\mathbf{y}_i \in S_i$, $Dp_{n\ell}(\mathbf{y}_i)$, gives a vector normal to the surface. Since a union

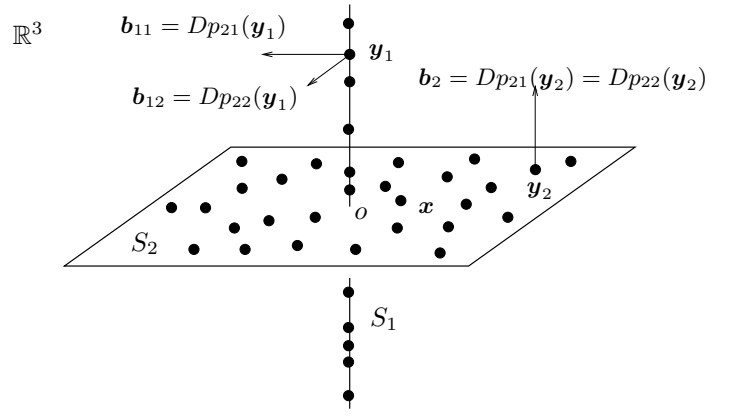


Fig. 2. The derivatives of the two polynomials x_1x_2 and x_1x_3 evaluated at a point \mathbf{y}_1 on the line S_1 give two normal vectors to the line. Similarly, the derivatives at a point \mathbf{y}_2 on the plane S_2 give the normal vector to the plane.

of subspaces is locally flat, i.e. in a neighborhood of \mathbf{y}_i the surface is merely the subspace S_i , then the derivative at \mathbf{y}_i lies in the orthogonal complement S_i^\perp of S_i . By evaluating the derivatives of *all* the polynomials in I_n at the same point \mathbf{y}_i , we obtain a set of normal vectors that span the orthogonal complement of S_i , as stated in Theorem 3. Figure 2 illustrates the theorem for the case of a plane and a line described in Section II.

Theorem 3 (Obtaining Subspace by Polynomial Differentiation):

Let I_n be (the space of coefficient vectors of) the set of polynomials of degree n that vanish on the n subspaces. If the data set \mathbf{X} is such that $\dim(\text{null}(\mathbf{V}_n(D))) = \dim(I_n) = m_n$ and one point $\mathbf{y}_i \in S_i$ but $\mathbf{y}_i \notin S_j$ for $j \neq i$ is given for each subspace S_i , then we have

$$S_i^\perp = \text{span} \left\{ \frac{\partial}{\partial \mathbf{x}} \mathbf{c}_n^T \nu_n(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{y}_i}, \forall \mathbf{c}_n \in \text{null}(\mathbf{V}_n(D)) \right\}. \quad (15)$$

Therefore, the dimensions of the subspaces are given by

$$d_i = D - \text{rank}(DP_n(\mathbf{y}_i)) \quad \text{for } i = 1, \dots, n, \quad (16)$$

with $P_n(\mathbf{x}) = [p_{n1}(\mathbf{x}), \dots, p_{nm_n}(\mathbf{x})] \in \mathbb{R}^{1 \times m_n}$ and $DP_n(\mathbf{x}) = [Dp_{n1}(\mathbf{x}), \dots, Dp_{nm_n}(\mathbf{x})] \in \mathbb{R}^{D \times m_n}$.

As a consequence of Theorem 3, we already have the sketch of an algorithm for segmenting subspaces of arbitrary dimensions in a semi-supervised learning scenario in which we are given *one positive example per class* $\{\mathbf{y}_i \in S_i\}_{i=1}^n$:

- 1) Compute a basis for the left null space of $\mathbf{V}_n(D)$ using, for example, SVD.
- 2) Evaluate the derivatives of the polynomial $\mathbf{c}_n^T \nu_n(\mathbf{x})$ at \mathbf{y}_i for each \mathbf{c}_n in the basis of $\text{null}(\mathbf{V}_n(D))$ to obtain a set of normal vectors in S_i^\perp .
- 3) Compute a basis B_i for S_i^\perp by applying PCA to the normal vectors obtained in step 2. PCA automatically gives the dimension of each subspace $d_i = \dim(S_i)$.
- 4) Cluster the data by assigning point \mathbf{x}_j to subspace i if

$$i = \arg \min_{\ell=1, \dots, n} \|\mathbf{B}_\ell^T \mathbf{x}_j\|. \quad (17)$$

Remark 4 (Estimating the Bases from Noisy Data Points): With a moderate level of noise in the data, we can still obtain a

basis for each subspace and cluster the data as above, because we are applying PCA to derivatives of the polynomials and both the coefficients of the polynomials and their derivatives depend continuously on the data. Notice also that we can obtain the dimension of each subspace by looking at the singular values of the matrix of derivatives, similarly to (11).

Remark 5 (Computing Derivatives of Homogeneous Polynomials): Notice that given \mathbf{c}_n the computation of the derivatives of $p_n(\mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x})$ does not involve taking derivatives of the (possibly noisy) data. For instance, one may compute the derivatives as $\frac{\partial p_n(\mathbf{x})}{\partial x_k} = \mathbf{c}_n^T \frac{\partial \nu_n(\mathbf{x})}{\partial x_k} = \mathbf{c}_n^T E_{nk} \nu_{n-1}(\mathbf{x})$, where $E_{nk} \in \mathbb{R}^{M_n(D) \times M_{n-1}(D)}$ is a constant matrix that depends on the exponents of the different monomials in the Veronese map $\nu_n(\mathbf{x})$.

E. Choosing one point per subspace by polynomial division

Theorem 3 demonstrates that one can obtain a basis for each S_i^\perp directly from the derivatives of the polynomials representing the union of subspaces. However, in order to proceed we need to have one point per subspace, i.e. we need to know the vectors $\{\mathbf{y}_i\}_{i=1}^n$.

In this section, we show how to select these n points in the *unsupervised learning scenario* in which we do not know the label for any of the data points. To this end, notice that we can always choose a point \mathbf{y}_n lying on one of the subspaces, say S_n , by checking that $P_n(\mathbf{y}_n) = \mathbf{0}^T$. Since we are given a set of data points $\mathbf{X} = \{\mathbf{x}_j\}_{j=1}^n$ lying on the subspaces, in principle we could choose \mathbf{y}_n to be any of the data points. However, in the presence of noise and outliers, a random choice of \mathbf{y}_n may be far from the true subspaces. In Section II we chose a point in the data set \mathbf{X} that minimizes $\|P_n(\mathbf{x})\|$. However, such a choice has the following problems:

- 1) The value $\|P_n(\mathbf{x})\|$ is merely an *algebraic* error, i.e. it does not represent the *geometric* distance from \mathbf{x} to its closest subspace. In principle, finding the geometric distance from \mathbf{x} to its closest subspace is a difficult problem, because we do not know the normal bases $\{B_i\}_{i=1}^n$.
- 2) Points \mathbf{x} lying close to the intersection of two or more subspaces could be chosen. However, at a point \mathbf{x} in the intersection of two or more subspaces, we often have $DP_n(\mathbf{x}) = \mathbf{0}$. Thus, one should avoid choosing such points, as they give very noisy estimates of the normal vectors.

As it turns out, one can avoid both of these problems thanks to the following lemma.

Lemma 1: Let $\tilde{\mathbf{x}}$ be the projection of $\mathbf{x} \in \mathbb{R}^D$ onto its closest subspace. The Euclidean distance from \mathbf{x} to $\tilde{\mathbf{x}}$ is

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| = n \sqrt{P_n(\mathbf{x}) (DP_n(\mathbf{x})^T DP_n(\mathbf{x}))^\dagger P_n(\mathbf{x})^T} + O(\|\mathbf{x} - \tilde{\mathbf{x}}\|^2),$$

where $P_n(\mathbf{x}) = [p_{n1}(\mathbf{x}), \dots, p_{nm_n}(\mathbf{x})] \in \mathbb{R}^{1 \times m_n}$, $DP_n(\mathbf{x}) = [Dp_{n1}(\mathbf{x}), \dots, Dp_{nm_n}(\mathbf{x})] \in \mathbb{R}^{D \times m_n}$, and A^\dagger is the Moore-Penrose inverse of A .

Proof: The projection $\tilde{\mathbf{x}}$ of a point \mathbf{x} onto the zero set of the polynomials $\{p_{n\ell}\}_{\ell=1}^{m_n}$ can be obtained as the solution of the following constrained optimization problem

$$\begin{aligned} \min \quad & \|\tilde{\mathbf{x}} - \mathbf{x}\|^2 \\ \text{subject to} \quad & p_{n\ell}(\tilde{\mathbf{x}}) = 0 \quad \ell = 1, \dots, m_n. \end{aligned} \quad (18)$$

By using Lagrange multipliers $\lambda \in \mathbb{R}^{m_n}$, we can convert this problem into the unconstrained optimization problem

$$\min_{\tilde{\mathbf{x}}, \lambda} \|\tilde{\mathbf{x}} - \mathbf{x}\|^2 + P_n(\tilde{\mathbf{x}})\lambda. \quad (19)$$

From the first order conditions with respect to $\tilde{\mathbf{x}}$ we have $2(\tilde{\mathbf{x}} - \mathbf{x}) + DP_n(\tilde{\mathbf{x}})\lambda = \mathbf{0}$. After multiplying on the left by $(\tilde{\mathbf{x}} - \mathbf{x})^T$ and $(DP_n(\tilde{\mathbf{x}}))^T$, respectively, we obtain

$$\|\tilde{\mathbf{x}} - \mathbf{x}\|^2 = \frac{1}{2} \mathbf{x}^T DP_n(\tilde{\mathbf{x}})\lambda, \quad \text{and} \quad (20)$$

$$\lambda = 2(DP_n(\tilde{\mathbf{x}})^T DP_n(\tilde{\mathbf{x}}))^\dagger DP_n(\tilde{\mathbf{x}})^T \mathbf{x}, \quad (21)$$

where we have used the fact that $(DP_n(\tilde{\mathbf{x}}))^T \tilde{\mathbf{x}} = nP_n(\tilde{\mathbf{x}}) = 0$, because $D\nu_n(\tilde{\mathbf{x}})^T \tilde{\mathbf{x}} = n\nu_n(\tilde{\mathbf{x}})$. After replacing (21) on (20), the squared distance from \mathbf{x} to its closest subspace is given by

$$\|\tilde{\mathbf{x}} - \mathbf{x}\|^2 = \mathbf{x}^T DP_n(\tilde{\mathbf{x}}) (DP_n(\tilde{\mathbf{x}})^T DP_n(\tilde{\mathbf{x}}))^\dagger DP_n(\tilde{\mathbf{x}})^T \mathbf{x}. \quad (22)$$

After expanding in Taylor series about $\tilde{\mathbf{x}} = \mathbf{x}$, and noticing that $DP_n(\mathbf{x})^T \mathbf{x} = nP_n(\mathbf{x})^T$ we obtain

$$\|\tilde{\mathbf{x}} - \mathbf{x}\|^2 \approx n^2 P_n(\mathbf{x}) (DP_n(\mathbf{x})^T DP_n(\mathbf{x}))^\dagger P_n(\mathbf{x})^T, \quad (23)$$

which completes the proof. \blacksquare

Thanks to Lemma 1, we can immediately choose a point \mathbf{y}_n lying in (close to) one of the subspaces and not in (far from) the other subspaces as

$$\mathbf{y}_n = \arg \min_{\mathbf{x} \in \mathbf{X}: DP_n(\mathbf{x}) \neq \mathbf{0}} P_n(\mathbf{x}) (DP_n(\mathbf{x})^T DP_n(\mathbf{x}))^\dagger P_n(\mathbf{x})^T, \quad (24)$$

and then compute the basis $B_n \in \mathbb{R}^{D \times (D-d_n)}$ for S_n^\perp by applying PCA to $DP_n(\mathbf{y}_n)$.

In order to find a point \mathbf{y}_{n-1} lying in (close to) one of the remaining $(n-1)$ subspaces but not in (far from) S_n , we find a new set of polynomials $\{p_{(n-1)\ell}(\mathbf{x})\}$ defining the algebraic set $\cup_{i=1}^{n-1} S_i$. In the case of hyperplanes, there is only one such polynomial, namely

$$p_{n-1}(\mathbf{x}) \doteq (\mathbf{b}_1 \mathbf{x}) \cdots (\mathbf{b}_{n-1}^T \mathbf{x}) = \frac{p_n(\mathbf{x})}{\mathbf{b}_n^T \mathbf{x}} = \mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x}).$$

Therefore, we can obtain $p_{n-1}(\mathbf{x})$ by *polynomial division*. Notice that dividing $p_n(\mathbf{x})$ by $\mathbf{b}_n^T \mathbf{x}$ is a *linear problem* of the form $\mathbf{c}_{n-1}^T R_n(\mathbf{b}_n) = \mathbf{c}_n^T$, where $R_n(\mathbf{b}_n) \in \mathbb{R}^{M_{n-1}(D) \times M_n(D)}$. This is because solving for the coefficients of $p_{n-1}(\mathbf{x})$ is equivalent to solving the equations $(\mathbf{b}_n^T \mathbf{x})(\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})) = \mathbf{c}_n^T \nu_n(\mathbf{x})$, where \mathbf{b}_n and \mathbf{c}_n are already known.

Example 2: If $n = 2$ and $\mathbf{b}_2 = [b_1, b_2, b_3]^T$, then the matrix $R_2(\mathbf{b}_2)$ is given by

$$R_2(\mathbf{b}_2) = \begin{bmatrix} b_1 & b_2 & b_3 & 0 & 0 & 0 \\ 0 & b_1 & 0 & b_2 & b_3 & 0 \\ 0 & 0 & b_1 & 0 & b_2 & b_3 \end{bmatrix} \in \mathbb{R}^{3 \times 6}.$$

In the case of subspaces of varying dimensions, in principle we cannot simply divide the entries of the polynomial vector $P_n(\mathbf{x})$ by $\mathbf{b}_n^T \mathbf{x}$ for any column \mathbf{b}_n of B_n , because the polynomials $\{p_{n\ell}(\mathbf{x})\}$ may not be factorizable. Furthermore, they do not necessarily have the common factor $\mathbf{b}_n^T \mathbf{x}$. The following theorem resolves this difficulty by showing how to compute the polynomials associated with the remaining subspaces $\cup_{i=1}^{n-1} S_i$.

Theorem 4 (Obtaining Points by Polynomial Division):

Let I_n be (the space of coefficient vectors of) the set of polynomials vanishing on n subspaces. If the data set \mathbf{X} is such that $\dim(\text{null}(\mathbf{V}_n(D))) = \dim(I_n)$, then the set of homogeneous polynomials of degree $(n-1)$ that vanish on the algebraic set $\cup_{i=1}^{n-1} S_i$ is spanned by $\{\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})\}$ where the vectors of coefficients $\mathbf{c}_{n-1} \in \mathbb{R}^{M_{n-1}(D)}$ must satisfy

$$\mathbf{c}_{n-1}^T R_n(\mathbf{b}_n) \mathbf{V}_n(D) = \mathbf{0}^T, \quad \text{for all } \mathbf{b}_n \in S_n^\perp. \quad (25)$$

Proof: We first show the necessity. That is, any polynomial of degree $n-1$, $\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})$, that vanishes on $\cup_{i=1}^{n-1} S_i$ satisfies the above equation. Since a point \mathbf{x} in the original algebraic set $\cup_{i=1}^{n-1} S_i$ belongs to either $\cup_{i=1}^{n-1} S_i$ or S_n , we have $\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x}) = 0$ or $\mathbf{b}_n^T \mathbf{x} = 0$ for all $\mathbf{b}_n \in S_n^\perp$. Hence $p_n(\mathbf{x}) \doteq (\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})) (\mathbf{b}_n^T \mathbf{x}) = 0$. If we denote $p_n(\mathbf{x})$ as $\mathbf{c}_n^T \nu_n(\mathbf{x})$, then the vector of coefficients \mathbf{c}_n must be in $\text{null}(\mathbf{V}_n(D))$. From $\mathbf{c}_n^T \nu_n(\mathbf{x}) = (\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})) (\mathbf{b}_n^T \mathbf{x})$, the relationship between \mathbf{c}_n and \mathbf{c}_{n-1} can be written as $\mathbf{c}_{n-1}^T R_n(\mathbf{b}_n) = \mathbf{c}_n^T$. Since $\mathbf{c}_n^T \mathbf{V}_n(D) = \mathbf{0}^T$, \mathbf{c}_{n-1} needs to satisfy the following linear system of equations $\mathbf{c}_{n-1}^T R_n(\mathbf{b}_n) \mathbf{V}_n(D) = \mathbf{0}^T$.

We now show the sufficiency. That is, if \mathbf{c}_{n-1} is a solution to (25), then for all $\mathbf{b}_n \in S_n^\perp$, $\mathbf{c}_n^T = \mathbf{c}_{n-1}^T R_n(\mathbf{b}_n)$ is in $\text{null}(\mathbf{V}_n(D))$. From the construction of $R_n(\mathbf{b}_n)$, we have $\mathbf{c}_n^T \nu_n(\mathbf{x}) = (\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})) (\mathbf{b}_n^T \mathbf{x})$. Then for every $\mathbf{x} \in \cup_{i=1}^{n-1} S_i$ but not in S_n , we have $\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x}) = 0$, because there is a \mathbf{b}_n such that $\mathbf{b}_n^T \mathbf{x} \neq 0$. Therefore, $\mathbf{c}_{n-1}^T \nu_{n-1}(\mathbf{x})$ is a homogeneous polynomial of degree $(n-1)$ that vanishes on $\cup_{i=1}^{n-1} S_i$. ■

Thanks to Theorem 4, we can obtain a collection of polynomials $\{p_{(n-1)\ell}(\mathbf{x})\}_{\ell=1}^{m_{n-1}}$ representing $\cup_{i=1}^{n-1} S_i$ from the intersection of the left null spaces of $R_n(\mathbf{b}_n) \mathbf{V}_n(D) \in \mathbb{R}^{M_{n-1}(D) \times N}$ for all $\mathbf{b}_n \in S_n^\perp$. We can then repeat the same procedure to find a basis for the remaining subspaces. We thus obtain the following *Generalized Principal Component Analysis* (GPCA) algorithm (Algorithm 1) for segmenting n subspaces of unknown and possibly different dimensions.

Remark 6 (Avoiding Polynomial Division): Notice that one may avoid computing P_i for $i < n$ by using a heuristic distance function to choose the points $\{\mathbf{y}_i\}_{i=1}^n$. Since a point in $\cup_{\ell=i}^n S_\ell$ must satisfy $\|B_i^T \mathbf{x}\| \cdots \|B_n^T \mathbf{x}\| = 0$, we can choose a point \mathbf{y}_{i-1} on $\cup_{\ell=1}^{i-1} S_\ell$ as:

$$\mathbf{y}_{i-1} = \arg \min_{\mathbf{x} \in \mathbf{X}: DP_n(\mathbf{x}) \neq 0} \frac{\sqrt{P_n(\mathbf{x})(DP_n(\mathbf{x})^T DP_n(\mathbf{x}))^\dagger P_n(\mathbf{x})^T} + \delta}{\|B_i^T \mathbf{x}\| \cdots \|B_n^T \mathbf{x}\| + \delta},$$

where a small number $\delta > 0$ is chosen to avoid cases in which both the numerator and the denominator are zero (e.g., with perfect data).

Remark 7 (Robustness and Outlier Rejection): In practice, there could be points in \mathbf{X} that are far away from any of the subspaces, i.e. outliers. By detecting and rejecting outliers we can typically ensure a much better estimate of the subspaces. Many methods from robust statistics can be deployed to detect and reject the outliers [5], [11]. For instance, the function

$$d^2(\mathbf{x}) = P_n(\mathbf{x})(DP_n(\mathbf{x})^T DP_n(\mathbf{x}))^\dagger P_n(\mathbf{x})^T$$

Algorithm 1 (GPCA: Generalized Principal Component Analysis)

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set  $\mathbf{V}_n = [\nu_n(\mathbf{x}_1), \dots, \nu_n(\mathbf{x}_N)] \in \mathbb{R}^{M_n(D) \times N}$ ;
for  $i = n : 1$  do
  solve  $\mathbf{c}^T \mathbf{V}_i = 0$  to obtain a basis  $\{\mathbf{c}_{i\ell}\}_{\ell=1}^{m_i}$  of  $\text{null}(\mathbf{V}_i)$ ,
  where the number of polynomials  $m_i$  is obtained as
  in (11);
  set  $P_i(\mathbf{x}) = [p_{i1}(\mathbf{x}), \dots, p_{im_i}(\mathbf{x})] \in \mathbb{R}^{1 \times m_i}$ , where
   $p_{i\ell}(\mathbf{x}) = \mathbf{c}_{i\ell}^T \nu_i(\mathbf{x})$  for  $\ell = 1, \dots, m_i$ ;
  do
     $\mathbf{y}_i = \arg \min_{\mathbf{x} \in \mathbf{X}: DP_i(\mathbf{x}) \neq 0} P_i(\mathbf{x})(DP_i(\mathbf{x})^T DP_i(\mathbf{x}))^\dagger P_i(\mathbf{x})^T$ ,
     $B_i = \text{PCA}(DP_i(\mathbf{y}_i))$ ,
     $\mathbf{V}_{i-1} = [R_i(\mathbf{b}_{i1}) \mathbf{V}_i, \dots, R_i(\mathbf{b}_{i, D-d_i}) \mathbf{V}_i]$ ,
    where  $\mathbf{b}_{ij}$  are columns of  $B_i$ ;
  end do
end for
for  $j = 1 : N$  do
  assign point  $\mathbf{x}_j$  to subspace  $S_i$  if  $i = \arg \min_\ell \|B_\ell^T \mathbf{x}_j\|$ ;
end for

```

approximates the squared distance of a point \mathbf{x} to the subspaces. From the d^2 -histogram of the sample set \mathbf{X} , we may exclude from \mathbf{X} all points that have unusually large d^2 values and use only the remaining sample points to re-estimate the polynomials before computing the normals. For instance, if we assume that the sample points are drawn around each subspace from independent Gaussian distributions with a small variance σ^2 , then $\frac{d^2}{\sigma^2}$ is approximately a χ^2 -distribution with $\sum_i (D - d_i)$ degrees of freedom. We can apply standard χ^2 -test to reject samples which deviate significantly from this distribution. Alternatively, one can detect and reject outliers using Random Sample Consensus (RANSAC) [5]. One can choose $M_n(D)$ data points at random, estimate a collection of polynomials passing through those points, determine their degree of support among the other points, and then choose the set of polynomials giving a large degree of support. This method is expected to be effective when $M_n(D)$ is small. An open problem is how to combine GPCA with methods from robust statistics in order to improve the robustness of GPCA to outliers.

IV. FURTHER ANALYSIS OF THE GPCA ALGORITHM

In this section, we discuss some extensions of GPCA that deal with practical situations such as low-dimensional subspaces of a high-dimensional space and unknown number of subspaces.

A. Projection and minimum representation

When the dimension of the ambient space D is large, the complexity of GPCA becomes prohibitive, because $M_n(D)$ is of the order n^D . However, in most practical situations we are interested in modeling the data as a union of subspaces of relatively small dimensions $\{d_i \ll D\}$. In such cases,

it seems rather redundant to use \mathbb{R}^D to represent such a low-dimensional linear structure. One way of reducing the dimensionality is to linearly project the data onto a lower-dimensional (sub)space. An example is shown in Figure 3, where two lines \mathcal{L}_1 and \mathcal{L}_2 in \mathbb{R}^3 are projected onto a plane \mathcal{P} . In this case, segmenting the two lines in the three-dimensional space \mathbb{R}^3 is equivalent to segmenting the two projected lines l_1 and l_2 in the plane \mathcal{P} .

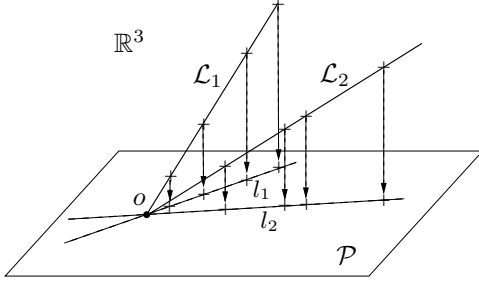


Fig. 3. A linear projection of two 1-dimensional subspaces $\mathcal{L}_1, \mathcal{L}_2$ in \mathbb{R}^3 onto a 2-dimensional plane \mathcal{P} preserves the membership of each sample and the dimension of the lines.

In general, we will distinguish between two different kinds of linear “projections.” The first kind corresponds to the case in which the span of all the subspaces is a proper subspace of the ambient space, i.e. $\text{span}(\cup_{i=1}^n S_i) \subset \mathbb{R}^D$. In this case, one may simply apply the classic PCA algorithm to the original data to eliminate the redundant dimensions. The second kind corresponds to the case in which the largest dimension of the subspaces, denoted by d_{\max} , is strictly less than $D - 1$. When d_{\max} is known, one may choose a $(d_{\max} + 1)$ -dimensional subspace \mathcal{P} such that, by projecting onto this subspace:

$$\pi_{\mathcal{P}} : \mathbf{x} \in \mathbb{R}^D \mapsto \mathbf{x}' = \pi_{\mathcal{P}}(\mathbf{x}) \in \mathcal{P},$$

the dimension of each original subspace S_i is preserved,² and the number of subspaces is preserved,³ as stated in the following theorem.

Theorem 5 (Segmentation-Preserving Projections): If a set of vectors $\{\mathbf{x}_j\}$ lie in n subspaces of dimensions $\{d_i\}_{i=1}^n$ in \mathbb{R}^D , and if $\pi_{\mathcal{P}}$ is a linear projection into a subspace \mathcal{P} of dimension D' , then the points $\{\pi_{\mathcal{P}}(\mathbf{x}_j)\}$ lie in $n' \leq n$ linear subspaces of \mathcal{P} of dimensions $\{d'_i \leq d_i\}_{i=1}^n$. Furthermore, if $D > D' > d_{\max}$, then there is an open and dense set of projections that preserve the number and dimensions of the subspaces, i.e. $n' = n$ and $d'_i = d_i$ for $i = 1, \dots, n$.

Thanks to Theorem 5, if we are given a data set \mathbf{X} drawn from a union of low-dimensional subspaces of a high-dimensional space, we can cluster the data set by first projecting \mathbf{X} onto a generic subspace of dimension $D' = d_{\max} + 1$ and then applying GPCA to the projected subspaces, as illustrated with the following sequence of steps:

$$\mathbf{X} \xrightarrow{\pi_{\mathcal{P}}} \mathbf{X}' \xrightarrow{\text{GPCA}} \cup_{i=1}^n \pi_{\mathcal{P}}(S_i) \xrightarrow{\pi_{\mathcal{P}}^{-1}} \cup_{i=1}^n S_i.$$

²This requires that \mathcal{P} be transversal to each S_i^{\perp} , i.e. $\text{span}\{\mathcal{P}, S_i^{\perp}\} = \mathbb{R}^D$ for every $i = 1, \dots, n$. Since n is finite, this transversality condition can be easily satisfied. Furthermore, the set of positions for \mathcal{P} which violate the transversality condition is only a zero-measure closed set [9].

³This requires that all $\pi_{\mathcal{P}}(S_i)$ be transversal to each other in \mathcal{P} , which is guaranteed if we require \mathcal{P} to be transversal to $S_i^{\perp} \cap S_j^{\perp}$ for $i, j = 1, \dots, n$. All \mathcal{P} 's which violate this condition form again only a zero-measure set.

Although we have shown that the set of $(d_{\max} + 1)$ -dimensional subspaces $\mathcal{P} \subset \mathbb{R}^D$ that preserve the number and dimensions of the subspaces is an open and dense set, it remains unclear what a “good” choice for \mathcal{P} is, especially when there is noise in the data. In practice, one may simply select a few random projections and choose the one that results in the smallest fitting error. Another alternative is to apply classic PCA to project onto a $(d_{\max} + 1)$ -dimensional affine subspace. The reader may refer to [1] for alternative ways of choosing a projection.

B. Identifying an unknown number of subspaces of unknown dimensions

The solution to the subspace segmentation problem proposed in Section III assumes prior knowledge of the number of subspaces n . In practice, however, the number of subspaces n may not be known beforehand, hence we cannot estimate the polynomials representing the subspaces directly.

For the sake of simplicity, let us first consider the problem of determining the number of subspaces from a generic dataset lying in a union of n different hyperplanes $S_i = \{\mathbf{x} : \mathbf{b}_i^T \mathbf{x} = 0\}$. From Section III, we know that in this case there is a *unique* polynomial of degree n that vanishes in $Z = \cup_{i=1}^n S_i$, namely $p_n(\mathbf{x}) = (\mathbf{b}_1^T \mathbf{x}) \cdots (\mathbf{b}_n^T \mathbf{x}) = \mathbf{c}_n^T \nu_n(\mathbf{x})$, and that its coefficient vector \mathbf{c}_n lives in the left null space of the embedded data matrix $\mathbf{V}_n(D)$ defined in (9), hence $\text{rank}(\mathbf{V}_n) = M_n(D) - 1$. Clearly, there cannot be a polynomial of degree $i < n$ that vanishes in Z , otherwise the data would lie in a union of $i < n$ hyperplanes. This implies that $\mathbf{V}_i(D)$ must be full rank for all $i < n$. In addition, notice that there is more than one polynomial of degree $i > n$ that vanishes on Z , namely any multiple of p_n , hence $\text{rank}(\mathbf{V}_i(D)) < M_i(D) - 1$ if $i > n$. Therefore, the number of hyperplanes can be determined as the minimum degree such that the embedded data matrix drops rank, i.e.

$$n = \min\{i : \text{rank}(\mathbf{V}_i(D)) < M_i(D)\}. \quad (26)$$

Consider now the case of data lying in subspaces of equal dimension $d_1 = d_2 = \dots = d_n = d < D - 1$. For example, consider a set of points $\mathbf{X} = \{\mathbf{x}_i\}$ lying in two lines in \mathbb{R}^3 , say

$$S_1 = \{\mathbf{x} : x_2 = x_3 = 0\} \quad \text{and} \quad S_2 = \{\mathbf{x} : x_1 = x_3 = 0\}. \quad (27)$$

If we construct the matrix of embedded data points $\mathbf{V}_n(D)$ for $n = 1$ we obtain $\text{rank}(\mathbf{V}_1(3)) = 2 < 3$, because all the points lie also in the plane $x_3 = 0$. Therefore, we cannot determine the number of subspaces as in (26), because we would obtain $n = 1$, which is not correct. In order to determine the correct number of subspaces, recall from Section IV-A that a linear projection onto a generic $(d+1)$ -dimensional subspace \mathcal{P} preserves the number and dimensions of the subspaces. Therefore, if we project the data onto \mathcal{P} , then the projected data lies in a union of n hyperplanes of \mathbb{R}^{d+1} . By applying (26) to the projected data, we can obtain the number of subspaces from the embedded (projected) data matrix $\mathbf{V}_i(d+1)$ as

$$n = \min\{i : \text{rank}(\mathbf{V}_i(d+1)) < M_i(d+1)\}. \quad (28)$$

Of course, in order to apply this projection we need to know the common dimension d of all the subspaces. Clearly, if we project onto a subspace of dimension $\ell + 1 < d + 1$, then the number and dimension of the subspaces are no longer preserved. In fact, the projected data points lie in one subspace of dimension $\ell + 1$, and $\mathbf{V}_i(\ell + 1)$ is of full rank for all i (as long as $M_i(D) < N$). Therefore, we can determine the dimension of the subspaces as the minimum integer ℓ such that there is a degree i for which $\mathbf{V}_i(\ell + 1)$ drops rank, that is

$$d = \min\{\ell : \exists i \geq 1 \text{ such } \text{rank}(\mathbf{V}_i(\ell + 1)) < M_i(\ell + 1)\}. \quad (29)$$

In summary, when the subspaces are of equal dimension d , both the number of subspaces n and their common dimension d can be retrieved from (28) and (29), and the subspace segmentation problem can be subsequently solved by first projecting the data onto a $(d + 1)$ -dimensional subspace and then applying GPCA (Algorithm 1) to the projected data points.

Remark 8: In the presence of noise, one may not be able to estimate d and n from (29) and (28), respectively, because the matrix $\mathbf{V}_i(\ell + 1)$ may be of full rank for all i and ℓ . Similarly to Remark 2, we use model selection techniques to determine the rank of $\mathbf{V}_i(\ell)$. However, in practice this requires to search for up to possibly $(D - 1)$ values for d and $\lceil N/(D - 1) \rceil$ values for n . One may refer to [11] for a more detailed discussion on selecting the best multiple-subspace model from noisy data, using model-selection criteria such as MML, MDL, AIC, and BIC.

Unfortunately, the situation is not so simple for subspaces of different dimensions. For instance, imagine that in addition to the two lines S_1 and S_2 we are also given data points on a plane $S_3 = \{\mathbf{x} : x_1 + x_2 = 0\}$, so that the overall configuration is similar to that shown in Figure 4. In this case we have $\text{rank}(\mathbf{V}_1(3)) = 3 \not< 3$, $\text{rank}(\mathbf{V}_2(3)) = 5 < 6$, and $\text{rank}(\mathbf{V}_3(3)) = 6 < 10$. Therefore, if we try to determine the number of subspaces as the degree of the embedding for which the embedded data matrix drops rank we would obtain $n = 2$, which is incorrect again. The reason for this is clear: we can fit the data either with one polynomial of degree $n = 2$, which corresponds to the plane S_3 and the plane \mathcal{P} spanned by the two lines, or with four polynomials of degree $n = 3$, which vanish precisely on the two lines S_1 , S_2 , and the plane S_3 .

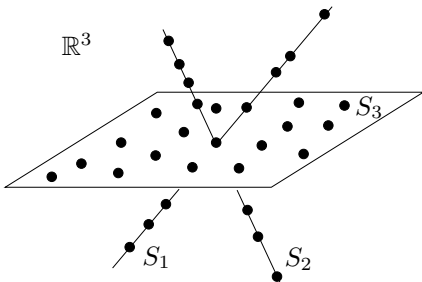


Fig. 4. A set of samples that can be interpreted as coming either from two lines and one plane or from two planes.

To resolve the difficulty in simultaneously determining the number and dimension of the subspaces, notice that the

algebraic set $Z = \cup_{j=1}^n S_j$ can be decomposed into irreducible subsets S_j 's – an irreducible algebraic set is also called a *variety*, and that the decomposition of Z into $\{S_j\}_{j=1}^n$ is always unique [8]. Therefore, as long as we are able to correctly determine from the given sample points the underlying algebraic set Z or the associated radical ideal $\mathcal{I}(Z)$,⁴ in principle, the number of subspaces n and their dimensions $\{d_j\}_{j=1}^n$ can always be uniquely determined in a purely algebraic fashion. In Figure 4, for instance, the first interpretation (2 lines and 1 plane) would be the right one and the second one (2 planes) would be incorrect, because the two lines, which span one of the planes, are not an irreducible algebraic set.

Having established that the problem of subspace segmentation is equivalent to decomposing the algebraic ideal associated with the subspaces, we are left with deriving a computable scheme to achieve the goal of decomposing algebraic sets into varieties. To this end, notice that the set of all homogeneous polynomials that vanish in Z can be graded by degree as

$$\mathcal{I}(Z) = \mathcal{I}_m \oplus \mathcal{I}_{m+1} \oplus \cdots \oplus \mathcal{I}_n \oplus \cdots, \quad (30)$$

where $m \leq n$ is the degree of the polynomial of minimum degree that fits all the data points. For each degree $i \geq m$, we can evaluate the derivatives of the polynomials in \mathcal{I}_i at points in subspace S_j and denote the collection of derivatives as

$$D_{i,j} \doteq \text{span}\{\cup_{\mathbf{x} \in S_j} \{\nabla f |_{\mathbf{x}}, \forall f \in \mathcal{I}_i\}\}, \quad j = 1, 2, \dots, n. \quad (31)$$

Obviously, we have the following relationship:

$$D_{i,j} \subseteq D_{i+1,j} \subseteq S_j^\perp, \quad \forall i \geq m. \quad (32)$$

Therefore, for each degree $i \geq m$, we may compute a union of i subspaces, Z_i ,

$$Z_i \doteq D_{i,1}^\perp \cup D_{i,2}^\perp \cup \cdots \cup D_{i,n}^\perp \supseteq Z, \quad (33)$$

which contains the original subspaces. Therefore, we can further partition Z_i to obtain the original subspaces. More specifically, in order to segment an unknown number of subspaces of unknown and possibly different dimensions, we can first search for the minimum degree i and dimension ℓ such that $\mathbf{V}_i(\ell + 1)$ drops rank. In our example in Figure 4, we obtain $i = 2$ and $\ell = 2$. By applying GPCA to the data set projected onto an $(\ell + 1)$ -dimensional space, we will partition the data into i subspaces Z_i which contain the original n subspaces. In our example, we partition the data into two planes \mathcal{P} and S_3 . Once the i subspaces have been estimated, we can re-apply the same process to each subspace. In our example, the plane \mathcal{P} will be separated into two lines S_1 and S_2 , while the plane S_3 will remain unchanged. This recursive process stops when every subspace obtained can no longer be separated into lower-dimensional subspaces.

We summarize the above derivation with the recursive GPCA algorithm (Algorithm 2).

⁴The ideal of an algebraic set Z is the set of all polynomials that vanish in Z . An ideal \mathcal{I} is called radical if $f \in \mathcal{I}$ whenever $f^s \in \mathcal{I}$ for some integer s .

Algorithm 2 Recursive GPCA Algorithm

```

n = 1;
repeat
  build a data matrix  $V_n(D) \doteq [\nu_n(\mathbf{x}_1), \dots, \nu_n(\mathbf{x}_N)] \in \mathbb{R}^{M_n(D) \times N}$  via the Veronese map  $\nu_n$  of degree  $n$ ;
  if  $\text{rank}(V_n(D)) < M_n(D)$  then
    compute the basis  $\{\mathbf{c}_{n\ell}\}$  of the left null space of  $V_n(D)$ ;
    obtain polynomials  $\{p_{n\ell}(\mathbf{x}) \doteq \mathbf{c}_{n\ell}^T \nu_n(\mathbf{x})\}$ ;
     $Y = \emptyset$ ;
    for  $j = 1 : n$  do
      select a point  $\mathbf{x}_j$  from  $X \setminus Y$  (similar to Algorithm 1);
      obtain the subspace  $S_j^\perp$  spanned by the derivatives  $\text{span}\{Dp_{n\ell}(\mathbf{x}_j)\}$ ;
      find the subset of points  $X_j \subset X$  that belong to the subspace  $S_j$ ;
       $Y \leftarrow Y \cup X_j$ ;
      Recursive-GPCA( $X_j$ ); (with  $S_j$  now as the ambient space)
    end for
     $n \leftarrow n_{max}$ ;
  else
     $n \leftarrow n + 1$ ;
  end if
until  $n \geq n_{max}$ .
```

V. EXPERIMENTAL RESULTS AND APPLICATIONS IN COMPUTER VISION

In this section, we evaluate the performance of GPCA on synthetically generated data by comparing and combining it with the following approaches:

- 1) *Polynomial Factorization Algorithm (PFA)*: this algorithm is only applicable to the case of hyperplanes. It computes the normal vectors $\{\mathbf{b}_i\}_{i=1}^n$ to the n hyperplanes by factorizing the homogeneous polynomial $p_n(\mathbf{x}) = (\mathbf{b}_1^T \mathbf{x})(\mathbf{b}_2^T \mathbf{x}) \cdots (\mathbf{b}_n^T \mathbf{x})$ into a product of linear factors. See [24] for further details.
- 2) *K-subspace*: given an initial estimate for the subspace bases, this algorithm alternates between clustering the data points using the distance residual to the different subspaces, and computing a basis for each subspace using standard PCA. See [10] for further details.
- 3) *Expectation Maximization (EM)*: this algorithm assumes that the data is corrupted with zero-mean Gaussian noise in the directions orthogonal to the subspace. Given an initial estimate for the subspace bases, EM alternates between clustering the data points (E-step) and computing a basis for each subspace (M-step) by maximizing the log-likelihood of the corresponding probabilistic model. See [19] for further details.

We also apply GPCA to solve various problems in computer vision such as face clustering under varying illumination, temporal video segmentation, two-view segmentation of linear motions and multi-view segmentation of rigid-body motions. However, it is *not* our intention to convince the reader that

the proposed GPCA algorithm offers an optimal solution to each of these problems. In fact, one can easily obtain better segmentation results by using algorithms/systems specially designed for these tasks. We merely wish to point out that GPCA provides an effective tool to automatically detect the multiple-subspace structure present in these data sets in a non-iterative fashion and that it provides a good initial estimate for any iterative algorithm.

A. Experiments on synthetic data

The experimental setup consists of choosing $n = 2, 3, 4$ collections of $N = 200n$ points in randomly chosen planes in \mathbb{R}^3 . Zero-mean Gaussian noise with s.t.d. σ from 0% to 5% along the subspace normals is added to the sample points. We run 1000 trials for each noise level. For each trial the error between the true (unit) normal vectors $\{\mathbf{b}_i\}_{i=1}^n$ and their estimates $\{\hat{\mathbf{b}}_i\}_{i=1}^n$ is computed as the mean angle between the normal vectors:

$$\text{error} \doteq \frac{1}{n} \sum_{i=1}^n \text{acos} \left(\mathbf{b}_i^T \hat{\mathbf{b}}_i \right) \text{ (degrees)}. \quad (34)$$

Figure 5 (a) plots the mean error as a function of noise for $n = 4$. Similar results were obtained for $n = 2, 3$, though with smaller errors. Notice that the estimates of GPCA with the choice of $\delta = 0.02$ (see Remark 6) have an error that is only about 50% the error of the PFA. This is because GPCA deals automatically with noisy data by choosing the points $\{\mathbf{y}_i\}_{i=1}^n$ in an optimal fashion. The choice of δ was not important (results were similar for $\delta \in [0.001, 0.1]$). Notice also that both the K-subspace and EM algorithms have a nonzero error in the noiseless case, showing that they frequently converge to a local minimum when a single randomly chosen initialization is used. When initialized with GPCA, both the K-subspace and EM algorithms reduce the error to approximately 35-50% with respect to random initialization. The best performance is achieved by using GPCA to initialize the K-subspace and EM algorithms.

Figure 5 (b) plots the estimation error of GPCA as a function of the number of subspaces n , for different levels of noise. As expected, the error increases rapidly as a function of n , because GPCA needs a minimum of $O(n^2)$ data points to linearly estimate the polynomials (see Section IV-A).

Table I shows the mean computing time and the mean number of iterations for a MATLAB implementation of each one of the algorithms over 1000 trials. Among the algebraic algorithms, the fastest one is PFA which directly factors $p_n(\mathbf{x})$ given \mathbf{c}_n . The extra cost of GPCA relative to the PFA is to compute the derivatives $Dp_n(\mathbf{x})$ for all $\mathbf{x} \in X$ and to divide the polynomials. Overall, GPCA gives about half the error of PFA in about twice as much time. Notice also that GPCA reduces the number of iterations of K-subspace and EM to approximately 1/3 and 1/2, respectively. The computing times for K-subspace and EM are also reduced including the extra time spent on initialization with GPCA or GPCA+K-subspace.

B. Face clustering under varying illumination

Given a collection of unlabeled images $\{I_j \in \mathbb{R}^D\}_{j=1}^N$ of n different faces taken under varying illumination, we would

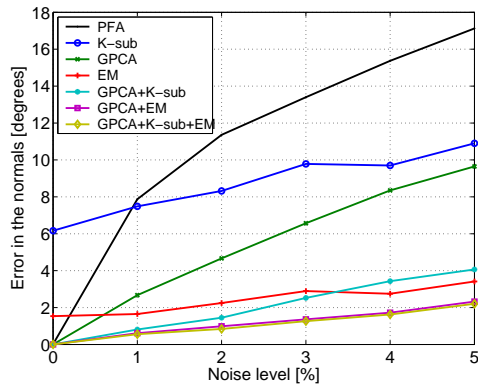
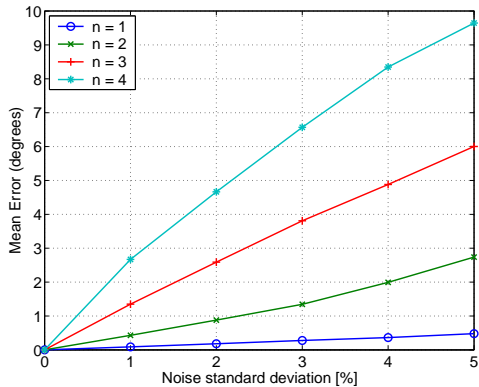
(a) Error versus noise for $n = 4$ (b) Error versus noise for $n = 1, \dots, 4$

Fig. 5. Error versus noise for data lying on two-dimensional subspaces of \mathbb{R}^3 . (a) A comparison of PFA, GPCA ($\delta = 0.02$), K-subspace and EM randomly initialized, K-subspace and EM initialized with GPCA, and EM initialized with K-subspace initialized with GPCA for $n = 4$ subspaces. (b) GPCA for $n = 1, \dots, 4$ subspaces.

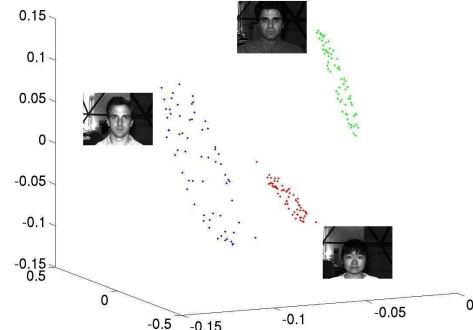
TABLE I

MEAN COMPUTING TIME AND MEAN NUMBER OF ITERATIONS FOR VARIOUS SUBSPACE SEGMENTATION ALGORITHMS.

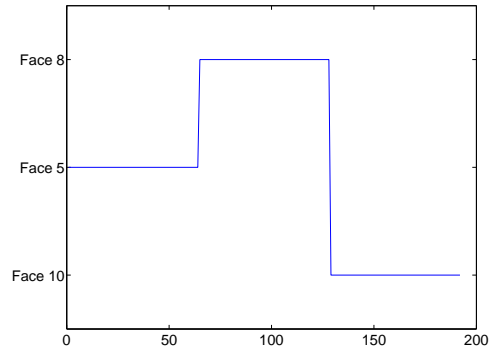
Algorithms	$c^T V_n = 0^T$	PFA	GPCA	K-sub
Time (sec.)	0.0854	0.1025	0.1818	0.4637
# Iterations	none	none	none	19.7
Algorithms	GPCA +K-sub	EM	GPCA+EM	GPCA+K-sub+EM
Time (sec.)	0.2525	1.0408	0.6636	0.7528
# Iterations	7.1	30.8	17.1	15.0

like to cluster the images corresponding to the face of the same person. For a Lambertian object, it has been shown that the set of all images taken under all lighting conditions forms a cone in the image space, which can be well approximated by a low-dimensional subspace [10]. Therefore, we can cluster the collection of images by estimating a basis for each one of those subspaces, because images of different faces will lie in different subspaces. Since in practice the number of pixels D is large compared with the dimension of the subspaces, we first apply PCA to project the images onto $\mathbb{R}^{D'}$ with $D' \ll D$ (see Section IV-A). More specifically, we compute the SVD of the data $[I_1 I_2 \dots I_N]_{D \times N} = U \Sigma V^T$ and consider a matrix $X \in \mathbb{R}^{D' \times N}$ consisting of the first D' columns of V^T . We obtain a new set of data points in $\mathbb{R}^{D'}$ from each one of the columns of X . We use homogeneous coordinates $\{x_j \in \mathbb{R}^{D'+1}\}_{j=1}^N$

so that each projected subspace goes through the origin. We consider a subset of the Yale Face Database B consisting of $N = 64n$ frontal views of $n = 3$ faces (subjects 5, 8 and 10) under 64 varying lighting conditions. For computational efficiency, we down-sampled each image to $D = 30 \times 40$ pixels. Then we projected the data onto the first $D' = 3$ principal components, as shown in Figure 6. We applied GPCA to the data in homogeneous coordinates and fitted three linear subspaces of dimensions 3, 2, and 2. GPCA obtained a perfect segmentation as shown in Figure 6.



(a) Image data projected onto the three principal components

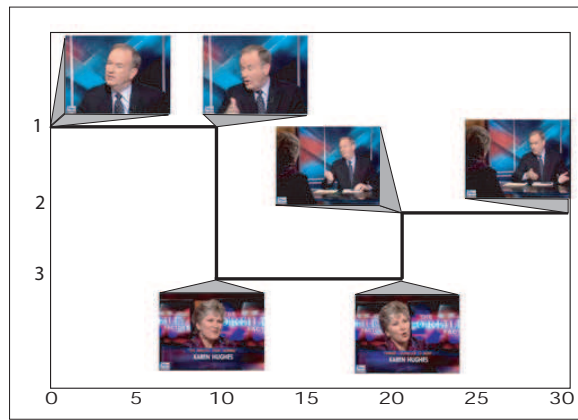


(b) Clustering results given by GPCA

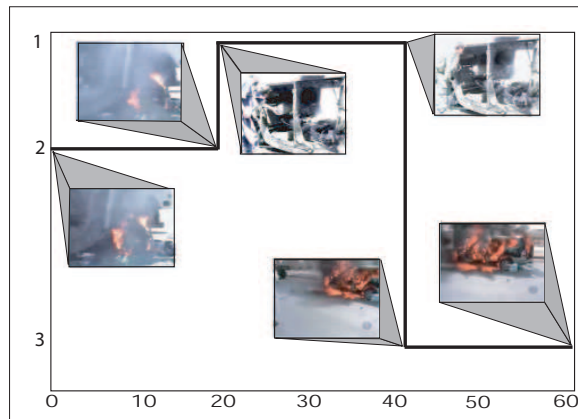
Fig. 6. Clustering a subset of the Yale Face Database B consisting of 64 frontal views under varying lighting conditions for subjects 2, 5 and 8.

C. Segmentation of news in video sequences

Consider a news video sequence in which the camera is switching among a small number of scenes. For instance, the host could be interviewing a guest and the camera may be switching between the host, the guest and both of them, as shown in Figure 7(a). Given the frames $\{I_j \in \mathbb{R}^D\}_{j=1}^N$, we would like to cluster them according to the different scenes. We assume that all the frames corresponding to the same scene live in a low-dimensional subspace of \mathbb{R}^D and that different scenes correspond to different subspaces. As in the case of face clustering, we may segment the video sequence into different scenes by applying GPCA to the image data projected onto the first few principal components. Figure 7(b) shows the segmentation results for two video sequences. In both cases, a perfect segmentation is obtained.



(a) 30 frames of a news video sequence clustered into 3 groups: host, guest and both of them



(b) 60 frames clustered into 3 groups: rear of a car with a burning wheel, a burnt car with people and a burning car

Fig. 7. Clustering frames of a news video sequence into groups of scenes using GPCA.

D. Segmentation of linearly moving objects

In this section, we apply GPCA to the problem of segmenting the 3-D motion of multiple objects undergoing a purely translational motion. We refer the reader to [25] for the case of arbitrary rotation and translation via the segmentation of a mixture of fundamental matrices.

We assume that the scene can be modeled as a mixture of purely translational motion models, $\{T_i\}_{i=1}^n$, where $T_i \in \mathbb{R}^3$ represents the translation of object i relative to the camera between the two consecutive frames. Given the images \mathbf{x}_1 and \mathbf{x}_2 of a point in object i in the first and second frame, respectively, the rays \mathbf{x}_1 , \mathbf{x}_2 and T_i are coplanar. Therefore \mathbf{x}_1 , \mathbf{x}_2 and T_i must satisfy the well-known epipolar constraint for linear motions

$$\mathbf{x}_2^T(T_i \times \mathbf{x}_1) = 0. \quad (35)$$

In the case of an uncalibrated camera, the epipolar constraint reads $\mathbf{x}_2^T(\mathbf{e}_i \times \mathbf{x}_1) = 0$, where $\mathbf{e}_i \in \mathbb{R}^3$ is known as the *epipole* and is linearly related to the translation vector $T_i \in \mathbb{R}^3$. Since the epipolar constraint can be conveniently rewritten as

$$\mathbf{e}_i^T(\mathbf{x}_2 \times \mathbf{x}_1) = 0, \quad (36)$$

where $\mathbf{e}_i \in \mathbb{R}^3$ represents the epipole associated with the i th motion, $i = 1, \dots, n$, if we define the *epipolar line*

$\ell = (\mathbf{x}_2 \times \mathbf{x}_1) \in \mathbb{R}^3$ as a data point, then we have that $\mathbf{e}_i^T \ell = 0$. Therefore, the segmentation of a set of images $\{(\mathbf{x}_1^j, \mathbf{x}_2^j)\}_{j=1}^N$ of a collection of N points in 3D undergoing n distinct linear motions $\mathbf{e}_1, \dots, \mathbf{e}_n \in \mathbb{R}^3$, can be interpreted as a subspace segmentation problem with $d = 2$ and $D = 3$, where the epipoles $\{\mathbf{e}_i\}_{i=1}^n$ are the normal to the planes and the epipolar lines $\{\ell^j\}_{j=1}^N$ are the data points. One can use equation (26) and Algorithm 1 to determine the number of motions n and the epipoles \mathbf{e}_i , respectively.

Figure 8(a) shows the first frame of a 320×240 video sequence containing a truck and a car undergoing two 3-D translational motions. We applied GPCA with $D = 3$, and $\delta = 0.02$ to the epipolar lines obtained from a total of $N = 92$ features, 44 in the truck and 48 in the car. The algorithm obtained a perfect segmentation of the features, as shown in Figure 8(b), and estimated the epipoles with an error of 5.9° for the truck and 1.7° for the car.

We also tested the performance of GPCA on synthetic point correspondences corrupted with zero-mean Gaussian noise with s.t.d. between 0 and 1 pixels for an image size of 500×500 pixels. For comparison purposes, we also implemented the PFA and the EM algorithm for segmenting hyperplanes in \mathbb{R}^3 . Figures 8(c) and (d) show the performance of all the algorithms as a function of the level of noise for $n = 2$ moving objects. The performance measures are the mean error between the estimated and the true epipoles (in degrees), and the mean percentage of correctly segmented feature points using 1000 trials for each level of noise. Notice that GPCA gives an error of less than 1.3° and a classification performance of over 96%. Thus GPCA gives approximately 1/3 the error of PFA, and improves the classification performance by about 2%. Notice also that EM with the normal vectors initialized at random (EM) yields a nonzero error in the noise free case, because it frequently converges to a local minimum. In fact, our algorithm outperforms EM. However, if we use GPCA to initialize EM (GPCA+EM), the performance of both algorithms improves, showing that our algorithm can be effectively used to initialize iterative approaches to motion segmentation. Furthermore, the number of iterations of GPCA+EM is approximately 50% with respect to EM randomly initialized, hence there is also a gain in computing time. Figures 8(e) and (f) show the performance of GPCA as a function of the number of moving objects for different levels of noise. As expected, the performance deteriorates as the number of moving objects increases, though the translation error is still below 8° and the percentage of correct classification is over 78%.

E. 3-D motion segmentation from multiple affine views

Let $\{\mathbf{x}_{fp} \in \mathbb{R}^2\}_{f=1, \dots, F}^{p=1, \dots, N}$ be a collection of F images of N 3-D points $\{\mathbf{X}_p \in \mathbb{R}^3\}_{j=1}^N$ taken by a moving affine camera. Under the affine camera model, which generalizes orthographic, weak perspective, and paraperspective projection, the images satisfy the equation

$$\mathbf{x}_{fp} = A_f \mathbf{X}_p, \quad (37)$$

where $A_f \in \mathbb{R}^{2 \times 4}$ is the affine camera matrix for frame f , which depends on the position and orientation of the camera

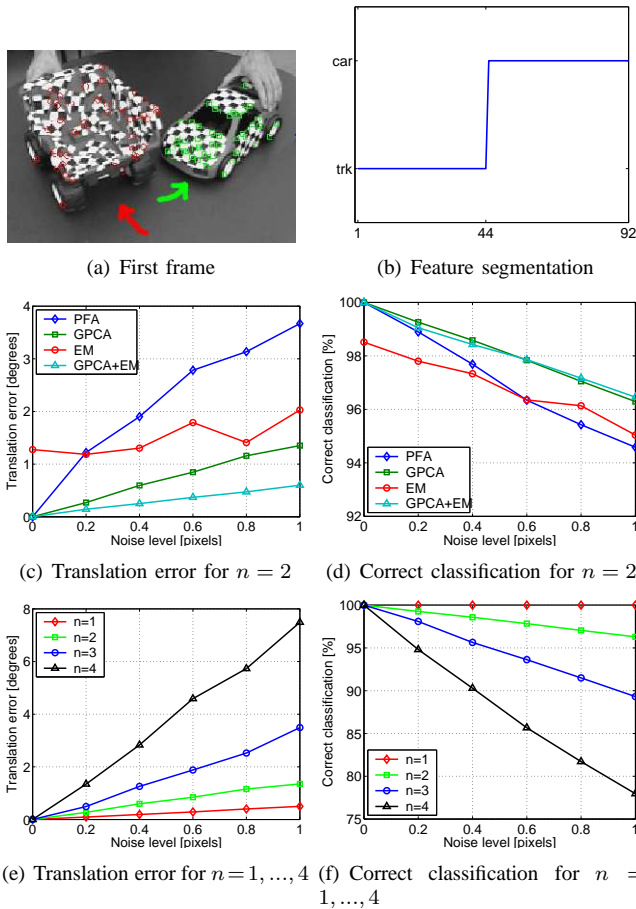


Fig. 8. Segmenting 3-D translational motions by segmenting planes in \mathbb{R}^3 . (a)-(b) segmenting a real sequence with 2 moving objects. (c)-(d) comparing GPCA with PFA and EM as a function of noise in the image features. (e)-(f) performance of GPCA as a function of the number of motions.

as well as the internal calibration parameters. Therefore, if we stack all the image measurements into a $2F \times N$ matrix W , we obtain

$$W = MS^T$$

$$\begin{bmatrix} \mathbf{x}_{11} & \cdots & \mathbf{x}_{1N} \\ \vdots & & \vdots \\ \mathbf{x}_{F1} & \cdots & \mathbf{x}_{FN} \end{bmatrix}_{2F \times N} = \begin{bmatrix} \mathbf{A}_1 \\ \vdots \\ \mathbf{A}_F \end{bmatrix}_{2F \times 4} \begin{bmatrix} \mathbf{X}_1 & \cdots & \mathbf{X}_N \end{bmatrix}_{4 \times N}. \quad (38)$$

It follows from equations (37) and (38) that $\text{rank}(W) \leq 4$, hence the 2-D trajectories of the image points across multiple frames, that is the columns of W , live in a subspace of \mathbb{R}^{2F} of dimension 2, 3 or 4 spanned by the columns of the motion matrix $M \in \mathbb{R}^{2F \times 4}$.

Consider now the case in which the set of points $\{\mathbf{X}_p\}_{p=1}^N$ corresponds to n moving objects undergoing n different motions. In this case, each moving object spans a different d -dimensional subspace of \mathbb{R}^{2F} , where $d = 2, 3$ or 4. Therefore, solving the motion segmentation problem is equivalent to finding a basis for each one of such subspaces without knowing which points belong to which subspace. When the image points are such that the motion subspaces are four dimensional and independent (this implies that $F \geq 2n$ and $N \geq 4n$), one can apply the Costeira and Kanade (CK) algorithm [3],

[13] to segment the subspaces. The CK algorithm is based on thresholding the entries of the so-called *shape interaction matrix*

$$Q = VV^T, \quad (39)$$

which is built from the SVD of the measurement matrix $W = U\Sigma V^T$ and has the property that

$$Q_{ij} = 0 \quad \text{if } i \text{ and } j \text{ correspond to different motions.} \quad (40)$$

However, in most practical sequences the motion subspaces have a nontrivial intersection, e.g., motions with common translation and different rotation, or motion subspaces that are not fully dimensional, e.g., purely translating motions. As reported in [27], [14], [22], most existing algorithms show poor performance in the presence of degenerate motions, because they cannot deal with intersecting motion subspaces.

In this section, we demonstrate that GPCA gives a closed form solution to the multiframe motion segmentation problem both in the case of degenerate and nondegenerate motions. This is because GPCA does not impose any restriction on either the intersection or the dimensionality of the subspaces. In essence, the motion segmentation problem is a subspace segmentation problem with $d_1, \dots, d_n \leq d_{\max} = 4$. Therefore, we can apply GPCA to the image measurements projected onto a subspace of \mathbb{R}^{2F} of dimension $D = d_{\max} + 1 = 5$. That is, if $W = U\Sigma V^T$ is the SVD of the data matrix, then we can solve the motion segmentation problem by applying GPCA to the first 5 columns of V^T .

We tested GPCA on two outdoor sequences taken by a moving camera tracking a car moving in front of a parking lot and a building (sequences A and B), and one indoor sequence taken by a moving camera tracking a person moving his head (sequence C), as shown in Figure 9. The data for these sequences are taken from [14] and consists of point correspondences in multiple views, which are available at <http://www.suri.it.okayama-u.ac.jp/data.html>. For all sequences the number of motions is correctly estimated from (11) as $n = 2$ for all values of $\kappa \in [2, 20] 10^{-7}$. Also, GPCA gives a percentage of correct classification of 100.0% for all three sequences as shown in Table II. The table also shows results reported in [14] from existing *multiframe* algorithms for motion segmentation. The comparison is somewhat unfair, because our algorithm is purely algebraic, while the others use iterative refinement to deal with noise. Nevertheless, the only algorithm having a comparable performance to ours is Kanatani's multi-stage optimization algorithm, which is based on solving a series of EM-like iterative optimization problems, at the expense of a significant increase in computation.

VI. CONCLUSIONS AND OPEN ISSUES

We have proposed an algebro-geometric approach to subspace segmentation called *Generalized Principal Component Analysis* (GPCA). Our approach is based on estimating a collection of polynomials from data and then evaluating their derivatives at a data point in order to obtain a basis for the subspace passing through that point. Our experiments showed that GPCA gives about half of the error with respect to existing algebraic algorithms based on polynomial factorization, and

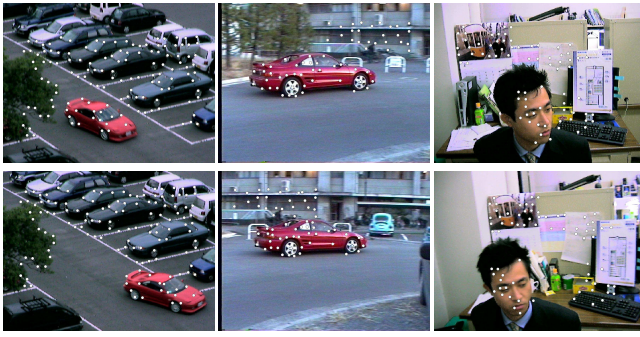


Fig. 9. Segmenting the point correspondences of sequences A (left), B (center) and C (right) in [14] for each pair of consecutive frames by segmenting subspaces in \mathbb{R}^5 . First row: first frame of the sequence with point correspondences superimposed. Second row: last frame of the sequence with point correspondences superimposed.

TABLE II

CLASSIFICATION RATES GIVEN BY VARIOUS SUBSPACE SEGMENTATION ALGORITHMS FOR SEQUENCES A, B, C IN [14].

Sequence	A	B	C
Number of points	136	63	73
Number of frames	30	17	100
Costeira-Kanade	60.3%	71.3%	58.8%
Ichimura	92.6%	80.1%	68.3%
Kanatani: subspace separation	59.3%	99.5%	98.9%
Kanatani: affine subspace separation	81.8%	99.7%	67.5%
Kanatani: multi-stage optimization	100.0%	100.0%	100.0%
GPCA	100.0%	100.0%	100.0%

significantly improves the performance of iterative techniques such as K-subspace and EM. We also demonstrated the performance of GPCA on the estimation of face clustering and video/motion segmentation.

At present, GPCA works well when the number and the dimensions of the subspaces are small, but the performance deteriorates as the number of subspaces increases. This is because all the algorithms start by estimating a collection of polynomials in a linear fashion, thus neglecting the nonlinear constraints among the coefficients of those polynomials, the so-called Brill's equations [6]. Another open issue has to do with the estimation of the number of subspaces n and their dimensions $\{d_i\}_{i=1}^n$ by harnessing additional algebraic properties of the vanishing ideals of subspace arrangements (e.g., the Hilbert function of the ideals). Throughout the paper we hinted connections of GPCA with Kernel Methods, e.g., the Veronese map gives an embedding that satisfies the modeling assumptions of KPCA (see Remark 1). Further connections between GPCA and KPCA are worthwhile investigating. Finally, the current GPCA algorithm does not assume the existence of outliers in the given sample data, though one can potentially incorporate statistical methods such as influence theory and random sampling consensus to improve its robustness. We will investigate these problems in future research.

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