A Convex Approach to Subspace Clustering

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Abstract—The identification of multiple affine subspaces from a set of data is of interest in fields such as system identification, data compression, image processing and signal processing and in the literature referred to as subspace clustering. If the origin of each sample would be known, the problem would be trivially solved by applying principal component analysis to samples originated from the same subspace. Now, not knowing what samples that originates from what subspace, the problem becomes considerably more difficult.

We present a novel convex formulation for subspace clustering. The proposed method takes the shape of a least-squares problem with sum-of-norms regularization over optimization parameter differences, a generalization of the $\ell_1$-regularization. The regularization constant is used to trade off fit and the identified number of affine subspaces.

I. INTRODUCTION

Principal Component Analysis (PCA, [22], [15], also referred to as the Karhunen-Loève transform) is a fundamental tool in areas such as image and signal processing and maybe the most commonly used method for data analysis. PCA finds the linear subspace that maximizes the variance of the projected samples. It can also be shown that this is the linear subspace which minimizes the sum of squared distances between the samples and the projections. In a least squares sense, the projection onto the linear subspace which minimizes the sum of squared distances between the samples and the projections. It can also be shown that this is the linear subspace that maximizes the variance of the projected samples. This is of course a useful property if one seeks a low-dimensional representation of a set of data and the reason for PCA’s popularity as a compression method.

PCA assumes that the data is confined to, or in the vicinity of, a single subspace. Now, if data originates from multiple linear subspaces, PCA will not give a satisfying result. The problem also becomes considerably more complex since it is not known what samples that originates from what subspace. If the origin of each sample would be known, the problem would be trivially solved by PCA. We hence need to estimate the subspaces and decide the origin of samples simultaneously. Methods dealing with the estimation of multiple subspaces are in the literature referred to as subspace clustering methods. For an excellent recent survey of subspace clustering see [28].

Subspace clustering methods can be divided into algebraic methods, iterative methods, statistical methods and spectral clustering methods. Most subspace clustering methods (see e.g., [28]) require a careful initialization. The main reason being that most subspace clustering methods lead to non-convex optimization problems and can get stuck in local optima leading to poor solutions.

This paper presents a novel approach to subspace clustering. The proposed method resembles in a convex optimization problem with a performance that is comparable to state of the art subspace clustering methods (when they manage to find a “good” solution and not get stuck in a “bad” local optima).

II. PROBLEM FORMULATION

An affine subspace can be defined as the set of points

$$S = \{ x \in R^D : b^T(x + \mu) = 0, \ b \in R^{D \times d}, \ \mu \in R^D \}. \ (1)$$

The $d$ columns of $b$ span the orthogonal space $S^\perp$. For example, if $D = 3$, $d = 1$ and $\mu = 0$, $b$ is the normal to a 2-dimensional linear subspace. Given a set of points $\{x_i\}_{i=1}^N$ on some affine subspace, PCA can be used to estimate $b$. With a sufficient number of points ($\geq D - d + 1$) and no noise, PCA will recover the true $b$.

Now, consider a data set $\{x_i\}_{i=1}^N$ sampled from $n$ affine subspaces. That is, $\{x_i\}_{i=1}^N$ satisfy

$$x_j \in \bigcup_i S_i, \quad j = 1, \ldots, N, \quad (2a)$$

with

$$S_i = \{ x \in R^D : b_i^T(x + \mu_i) = 0, \ b_i \in R^{D \times d_i}, \ \mu_i \in R^{D} \}, \quad (2b)$$

for $i = 1, \ldots, n$. If the origin of each of the samples $\{x_t\}_{t=1}^N$ was known i.e., if the function $c(\cdot)$ such that $x_j \in S_{c(j)}, \ j = 1, \ldots, N$ was known, PCA could be applied to identify $b_i$ by applying PCA to $\{x_t\}_{t \in c(i)}$. With $c(\cdot)$ unknown, the problem becomes considerably more difficult. One then has to, simultaneously, identify to what subspace a sample belongs and at the same time estimate $b$ and $\mu$ of the subspaces. Note that PCA would not do any good on this data set. The later, when nor the subspaces or the origin of the samples are known, is referred to as subspace clustering and the topic of this paper.

Remark 1 (Noisy data): Data are seldom situated on a low number of affine subspaces but rather in a vicinity of a low number of affine subspaces. (2) will therefore never be satisfied for other than $n \geq N/(D - d + 1)$ in reality. This is handled in PCA by seeking the linear subspace that minimizes the sum of squared distances between the samples and the projections of the samples onto the subspace.

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III. Previous Work

As stated in the introduction, subspace clustering methods can be divided into algebraic, iterative, statistical and spectral clustering methods.

Algebraic methods use algebraic properties of the unions of subspaces. Of rather recent date, compared to PCA, is the Generalized Principal Component Analysis (GPCA, [30], [31]). GPCA has the ability to identify multiple affine subspaces and is built around the fact that GPCA has attained quite some interest since its introduction.

Statistical methods are based on a model for the data in subspace $i$ of the form

$$x = A_is + a_i + \varepsilon, \quad s \sim N(0,1), \varepsilon \sim N(0, \sigma_i^2I). \quad (7)$$

To find the maximum likelihood solution for $\{A_i\}$ and $\{a_i\}$, the Expectation Maximization Algorithm (EM, [5]) is often used. Statistical methods for subspace clustering are also known to be sensitive to initialization.

Finally, spectral clustering methods. For this type of method, an affinity matrix or similarity matrix is a central concept. The entry $ij$ in this $N \times N$ matrix is desired to be 1 if $x_i$ and $x_j$ belong to the same subspace and otherwise small. Spectral clustering methods proceed by seeking for clusters in the set of eigenvectors to the affinity matrix, typically using non convex clustering methods such as k-means clustering (see e.g., [28]).

For a more detailed discussion on algebraic, iterative, statistical and spectral clustering methods, see [28].

In the following we will take an optimization approach to the subspace clustering problem. Something that will be used is a concept called regularization. Regularization has gained a lot of publicity through methods such as the lasso method [26] and Compressed Sensing (CS, [6], [4]). Both these methods use a $\ell_1$-regularization to find sparse solutions. A slightly more general type of regularization is the sum-of-norms regularization. In a statistical linear regression framework, sum-of-norms regularization is called group-lasso [33], since it results in estimates in which many groups of variables are zero. Sum-of-norms regularization has previously been applied to the identification of segmented ARX models [21], piecewise affine systems [20] and to clustering [16].

IV. Subspace Clustering Through Overparametrization and Sum-of-Norms Regularization

Consider the case where $b \in R^{D \times 1}$ and $n = 1$. Let \(\{x_i\}_{i=1}^N\) be a set of data situated on a $D-1$-dimensional linear subspace. Let $b^0$ be the true $b$-vector. To find the linear subspace, we could consider the convex optimization problem

$$\min_b \sum_{t=1}^N \|b^T x_t\|^2_2, \text{ s.t. } a^T b = 1. \quad (8)$$

This optimization will perfectly recover the linear subspace if $a$ is such that $a^T b^0 \neq 0$. To see this, let $b$ be $\frac{b^0}{a^Tb^0}$; note that $b^T x_1 = 0$, $t = 1, \ldots, N$, and that $a^T b = 1$. $b$ is hence the solution to (8). In practice, $a$ can be sampled from a $D$-dimensional unit Gaussian distribution, making the probability that $a^T b^0 = 0$ equal to zero.

Example 1 (Comparison to PCA): To examine the ability of the convex formulation (8) to recover the linear subspace of a set of data, we let

$$b^0 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad (9)$$

and sample 100 data points from

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} s + \varepsilon, \quad s \sim U(-0.5, 0.5), \varepsilon \sim N(0, 0.011). \quad (10)$$
The data is shown with black dots in the left plot of Figure 1. PCA and (6) (a in (6) was sampled from a unit Gaussian) were now applied to the data to get an estimate of $b^0$. The left plot of Figure 1 shows the $b^0$-estimates from PCA with dashed line and that of (6) with solid line. Since the data has been disturbed off the one dimensional linear subspace by noise, neither PCA nor (6) give the true $b^0$. However, we see that the convex optimization approach to estimate $b^0$ (6) is doing fairly well. In the right plot of Figure 1, the resulting estimates and data from 100 runs have been plotted on top of each other (new x’s and a new a in each run).

![Left plot: Data shown with black dots, estimate of $b^0$ given by PCA showed using dashed line and by (6) by solid black line. Right plot: The same as in the left plot but the result from 100 runs plotted on top of each other. For visualization purposes, a rotation of 180° was applied to some of the b-estimates so that the PCA estimate are all between 180° and 360° and the estimate from (6) between 0° and 180°.](image)

**Remark 2 (Convex optimization formulations of PCA):** (6) has the advantage of being a convex optimization problem. Some convex optimization formulations of PCA has been proposed in the literature [24], [25], [3]. We do not believe that (6) can perform better than these but the simplicity made (6) an attractive approach for what is coming. However, any of the methods developed in [24], [25], [3] could potentially also be used in the coming derivations. This has not been exploited.

**Remark 3 (Subspace of less dimensions than $D − 1$):** Let say that \{x\}_i=1^N is a set of data situated on a linear subspace of less dimension that $D − 1$, $b^0$ is then a matrix. If we still seek a $b \in R^{D \times 1}$ by (6), the found $b$ will be in the orthogonal space to the linear subspace that the data is in (as long as $a^T b^0 \neq 0$). Having found the $D − 1$-dimensional subspace containing the data, (6) could now be applied in this $D − 1$-dimensional space to find the $D − 2$-dimensional space containing the data, and so on. One could continue this procedure as long as the sum of squared distances between the samples and the projections of the samples onto the subspace is below some threshold.

We now turn to the considerably more difficult problem of identifying multiple linear subspaces from a set of samples \{x\}_i=1^N. Assume for now that the µ’s are zero i.e., we consider linear subspaces. Also, we will assume that subspaces are $D − 1$-dimensional. Subspaces of lower dimension can be handled as discussed in Remark 3 and not further discussed. Since it is unknown what sample that originates from what subspace, we overparametrize and estimate a parameter $b$ for each sample. To avoid a severe over fit, a regularization that aims at making $b$’s identical if there is “no need” for them to be different is used. We denote the $b$ associated with $x_j$ with $b^j$. The proposed criterion now takes the form

$$\min_{b, j=1,...,N} \sum_{j=1}^N \| (b^j)^T x_j \|_2^2 + \lambda \sum_{k,l=1}^N k(x_k,x_l)\|b^k - b^l\|_2,$$

s.t. $a^T b^j = 1, \ j = 1,\ldots, N$ \hfill (11)

$k(\cdot,\cdot) : R^D \times R^D \rightarrow R^+$ is a kernel. This kernel can be used to introduce prior information and should ideally be positive if $x_k$ and $x_l$ belongs to the same subspace and 0 otherwise. Also in spectral clustering-based methods, this type of similarity kernel is used and there is therefore a whole literature on how to find $k(\cdot,\cdot)$, see e.g., [7], [17], [28] for interesting choices.

The first term in the objective of (11) can be seen as a fit term and the second a regularization. The fit term will be zero if $(b^j)^T x_j = 0, \ j = 1,\ldots, N$, that is, if $b^j$ is orthogonal to $x_j$ for all $j = 1,\ldots, N$. Note that as long as $a^T x_j \neq 0, \ j = 1,\ldots, N$, there is $b^j, \ j = 1,\ldots, N$, that makes the fit term equal to zero and satisfies the constraint $a^T b^j = 1, \ j = 1,\ldots, N$ (also for noisy data). The vector $a \in R^D$ is in the coming assumed sampled from a unit Gaussian.

The regularization term is a Sum-Of-Norms regularization (SON regularization). Note that there is no square on the norm in the regularization, this is hence not a sum of squared norms. Sum-of-norms regularization is a well known sparsity regularization, see e.g., [33]. Hence, at the optimum, several of the terms $\|b^j - b^l\|_2$ will (typically) be exactly zero. Equivalently, several of the $\{b^j\}_{j=1}^N$ will be identical, and associated $x$’s can be seen as belonging to the same linear subspace.

**Remark 4 (Sum-of-norms regularization):** The SON regularization used in (11) is an $\ell_1$-regularization of the 2-norm of differences $b^k - b^l, \ k, l = 1,\ldots, N$. That is, the SON term is the $\ell_1$-norm of the vector obtained by stacking $\|b^k - b^l\|_2$, for $k, l = 1,\ldots, N$. Hence, this stacked vector, and not the individual $b$-vectors, will become sparse.

The regularization parameter $\lambda > 0$ is a parameter that will control the tradeoff between fit and the number of subspaces. This parameter can be chosen by considering how the sum of squared distances between the samples and the projections of the samples onto the subspaces changes with $\lambda$. We will use this in the coming examples to choose $\lambda$.

Another key property of the proposed criterion for subspace clustering is that the criterion (11) is convex. That means that the global optimum can be found independently of initialization. Many existing subspace clustering methods are dependent of a good initialization for a good result (see e.g., [28]). The convexity also implies that convex constraints easily can be added.

The estimated $b$’s of (11) will be biased due to the regularization and to obtain unbiased estimates, PCA is applied to $x$’s having the same $b$’s.
Example 2 (Multiple Linear Subspaces): Let \( n = 2, D = 2, d = 1 \) and sample 120 samples from
\[
(\alpha(b^0_1) + (1 - \alpha)(b^0_2) + s + \varepsilon),
\]
with \( s \) sampled from a uniform distribution, \( s \sim U(-0.5, 0.5), \alpha = 1 \) with probability 0.5 and 0 with probability 0.5, \( \varepsilon \sim N(0, 0.0049) \) and
\[
b_1^0 = \begin{bmatrix} -1 \\ -0.5 \end{bmatrix},
b_2^0 = \begin{bmatrix} -1 \\ 0.5 \end{bmatrix}.
\]
The data is shown in Figure 2. Motivated by the discussion following (11), we chose
\[
k(x_k, x_l) = e^{-\frac{\|x_k^T x_l\|}{2\sigma^2}}.
\]
Now apply (11) for a number of \( \lambda \)'s, see Figure 3. As seen, the sum of squared differences is rather flat for \( \lambda < 0.002 \), indicating that two subspaces (two distinct values in the estimated \( \{b^j, j = 1, \ldots, N\} \)) is a good choice. We chose \( \lambda = 0.001 \). The members of the two groups are visualized in Figure 2 by the use of a 'o'-symbol for members of the first group and a '*'-symbol for members of the second group. The resulting estimates of \( b_0^1 \) after using PCA on the \( x \)'s of the first group is given by a dashed line in Figure 2. The solid line in Figure 2 gives the estimate of \( b_0^2 \) obtained by using PCA on the \( x \)'s of the second group.

Example 3 (Larger \( D, n \) and \( N \)): To demonstrate that the proposed method (11) is also practical to use on larger problems, the same \( \lambda \) and kernel as in the previous example was used (a threshold was however applied to set \( k(x_k, x_l) \) to zero if not large enough) on a data set with 40 samples from 10 99-dimensional linear subspaces in 100 dimensions. That is \( D = 100, n = 10, N = 400 \) and \( d = 1 \). The true \( b \)'s were generated by sampling from a zero mean Gaussian distribution. Data was made noisy by adding zero mean Gaussian noise with a variance of 0.25. One simulation (see also Section IV-A) took \( \sim 4 \) minutes on a standard desktop machine. Over 10 runs, no samples were associated with the wrong subspace and the number of subspace were correctly found.

So far we have only discussed multiple linear subspaces. Its however straightforward to also handle affine subspaces by a small modification of (11). For affine subspace we propose to consider
\[
\min_{b^j, \mu^j, j = 1, \ldots, N} \sum_{j=1}^{N} \| (b^j)^T x_j - \mu^j \|_2^2 \\
+ \lambda \sum_{k,j=1}^{N} k(x_k, x_l) \| \mu^b_k - \mu^b_j \|_2, \\
\text{s.t. } a^T b^j = 1, j = 1, \ldots, N.
\]

Example 4 (Multiple Affine Subspaces): Let \( n = 3, D = 2, d = 1 \) and sample 120 samples from
\[
\begin{align*}
\alpha(b_1^0) + s + \mu_1 + \varepsilon, & \quad \text{with probability } 1/3, \\
\alpha(b_2^0) + s + \mu_2 + \varepsilon, & \quad \text{with probability } 1/3, \\
\alpha(b_3^0) + s + \mu_3 + \varepsilon, & \quad \text{with probability } 1/3,
\end{align*}
\]
with \( s \sim U(-0.5, 0.5), \varepsilon \sim N(0, 0.0049) \) and
\[
\begin{align*}
b_1^0 &= \begin{bmatrix} 0 \\ 1 \end{bmatrix},
b_2^0 &= \begin{bmatrix} -1 \\ -0.5 \end{bmatrix},
b_3^0 &= \begin{bmatrix} -1 \\ 0.5 \end{bmatrix}, \\
\mu_1 &= \begin{bmatrix} 0 \\ -0.7 \end{bmatrix},
\mu_2 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix},
\mu_3 &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
\end{align*}
\]
We now apply (15) with
\[
k(x_k, x_l) = e^{-\frac{\|x_k^T x_l\|}{2\sigma^2}} + \frac{|x_k^T x_l|}{\|x_k^T x_l\|}
\]
and for a number of different \( \lambda \)'s, see Figure 5. As seen, the sum of squared differences is rather flat for \( \lambda < 2 \), indicating that four subspaces is a good choice, \( \lambda = 0.2 \) was therefore chosen. The data associated with the first group is visualized with '*'-symbol in Figure 4. Data associated with the second group, with 'o' and so on. The resulting estimates after having applied PCA to the data of each group is also
showed in Figure 4. As seen, one of the three affine subspaces has been divided into two. This could possibly have been avoided by a better choice of kernel $k$.

Fig. 4. Data sampled with noise from three affine subspaces. (15) groups the optimization variables into four groups. The associated points of different groups are shown with different symbols while points of the same group with the same symbol. The figure also shows the computed estimates of the $b$'s and the $\mu$'s.

The number of distinct $b$’s (or estimated # of subspaces, dashed line) and the sum of squared distances between the samples and the projections of the samples onto the subspaces (solid line) as a function of $\lambda$.

Fig. 5. The number of distinct $b$’s (or estimated # of subspaces, dashed line) and the sum of squared distances between the samples and the projections of the samples onto the subspaces (solid line) as a function of $\lambda$.

V. COMPARISON WITH CONVENTIONAL SUBSPACE CLUSTERING METHODS

In this section we apply generalized PCA with polynomial differentiation and spectral clustering (see [28], Sect. 2.4) and sparse subspace clustering [7] using implementations kindly provided by the Vision Lab at Johns Hopkins University. The same data that was used in Examples 2 and 4 were used. GPCA with polynomial differentiation and spectral clustering (using homogeneous coordinates, see [28], and the default for the input parameters) was first applied. The data used in Example 2 resulted in the same plot as Figure 2 and hence an identical result to that of the proposed approach. The data used in Example 4 resulted in the left plot of Figure 6 (cf. Figure 4). Generalized PCA with polynomial differentiation and spectral clustering has some problems finding the true subspaces that the data belongs to but it does a fairly good job in finding the $b$’s and $\mu$’s.

Also sparse subspace clustering ($\lambda = 0.001$) recover a result identical to that of the proposed method for the data of Example 2. Data used in Example 4 resulted in the right plot of Figure 6 (cf. Figure 4). As seen, sparse subspace clustering has some problems to recover the affine subspaces. $\lambda = 0.0001$ gave the best result in sparse subspace clustering and was used in the right plot of Figure 6.

Fig. 6. Data sampled with noise from three affine subspaces. The results should be compared to those shown in Figure 4. Left plot: Results using generalized PCA with polynomial differentiation and spectral clustering. Right plot: Results using sparse subspace clustering.

VI. EXTENSIONS

Many subspace clustering methods can be extended to handle the identification of hybrid systems and so also the proposed scheme. In fact, it has been shown [20] that the criterion

$$\min_{\theta_k, k=1,\ldots,N} \sum_{k=1}^{N} \left| y_k - \theta_k^T \left[ \frac{x_k}{1} \right] \right|^2 + \lambda \sum_{k,j=1}^{N} k(x_k, x_j) \| \theta_k - \theta_j \|_p$$

is very suitable for the identification of piecewise affine systems. $y$ is here the measured output of a hybrid system and $x$ the regressor. The $\theta$’s are the sought system parameters associated with the different subsystems. Since $\{y_k\}_{k=1}^{N}$ now hinders the optimization variables $\theta_k$ from becoming

\footnote{http://www.vision.jhu.edu/gpca.htm, code version: April 19th, 2010 for GPCA with polynomial differentiation and spectral clustering.}

Many standard methods of convex optimization can be used to solve the problem (11) and (15). Systems such as CVX [13], [12] or YALMIP [19] can readily handle the sum-of-norms regularization, by converting the problem to a cone problem and calling a standard interior-point method. Recently, many authors have developed fast, first order methods of-norms regularization, by converting the problem to a cone

A. Solution Algorithms and Software

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identical to zero, a constraint like in (11) and (15) is not needed. See [20] for details.

The proposed framework could also be used to estimate nonlinear surfaces or manifolds using kernelization techniques developed in [9].

VII. CONCLUSIONS AND FUTURE WORKS

This paper presents a novel intuitive method to subspace clustering. The formulation takes the form of a convex optimization problem and does hence not need a careful initialized, like many other subspace clustering methods. The regularization parameter regulates the number of subspaces identified and is relatively easy to find a good value for. The similarity kernel can be used to introduce prior information. The method’s simplicity together with that it performs well in comparison to state of the art subspace clustering methods should make the method into an attractive choice.

A proper evaluation on large scale real data sets is important and something that is to be done. For this purpose, an implementation using Alternating Direction Method of Multipliers (ADMM, [10], [11], see also [1]) is in preparation.

Some convex optimization formulations of PCA have been proposed in the literature [24], [25], [3]. These could potentially be used to develop subspace clustering methods in a very similar way as presented in this paper. This has not been exploited but seen as interesting future work.

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