

A Simple Approach to Sparse Clustering

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Abstract. We consider the problem of sparse clustering, where it is assumed that only a subset of the features are useful for clustering purposes. In the framework of the COSA method of [Friedman and Meulman \(2004\)](#), subsequently improved in the form of the Sparse K-means method of [Witten and Tibshirani \(2010\)](#), we propose a very natural and simpler hill-climbing approach that is competitive with these two methods.

Reproducible research. The R code for the numerical experiments is publicly available at https://github.com/victorpu/SAS_Hill_Climb

1 Introduction

Consider a typical setting for clustering n items based on pairwise dissimilarities, with $\delta(i, j)$ denoting the dissimilarity between items $i, j \in [n] := \{1, \dots, n\}$. For concreteness, we assume that $\delta(i, j) \geq 0$ and $\delta(i, i) = 0$ for all $i, j \in [n]$. In principle, if we want to delineate κ clusters, the goal is (for example) to minimize the average within-cluster dissimilarity. In detail, a clustering into κ groups may be expressed as an assignment function $C : [n] \mapsto [\kappa]$, meaning that $C(i)$ indexes the cluster that observation $i \in [n]$ is assigned to. Let \mathcal{C}_κ^n denote the class of clusterings of n items into κ groups. For $C \in \mathcal{C}_\kappa^n$, its average within-cluster dissimilarity is defined as

$$\Delta[C] := \sum_{k \in [\kappa]} \frac{1}{|C^{-1}(k)|} \sum_{i, j \in C^{-1}(k)} \delta(i, j). \quad (1)$$

The resulting optimization problem is the following:

$$\text{Given } (\delta(i, j) : i, j \in [n]), \text{ minimize } \Delta[C] \text{ over } C \in \mathcal{C}_\kappa^n. \quad (2)$$

This problem is combinatorial and quickly becomes computationally too expensive, even for small datasets. A number of proposals have been suggested ([Hastie et al., 2009](#)), ranging from hierarchical clustering approaches to K-medoids.

Following in the footsteps of [Friedman and Meulman \(2004\)](#), we consider a situation where we have at our disposal not 1 but $p \geq 2$ measures of pairwise dissimilarities on the same set of items, with $\delta_a(i, j)$ denoting the a -th dissimilarity between items $i, j \in [n]$. Obviously, these measures of dissimilarity could be combined into a single measure of dissimilarity, for example,

$$\delta(i, j) = \sum_a \delta_a(i, j). \quad (3)$$

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This work was partially supported by a grant from the US Office of Naval Research (N00014-13-1-0257).

Our working assumption, however, is that only a few of these measures of dissimilarity are useful for clustering purposes, but we do not know which ones. This is the setting of sparse clustering, where the number of useful measures is typically small compared to the whole set of available measures.

We assume henceforth that all dissimilarity measures are equally important (for example, when we do not have any a priori on the relative importance of these measures) and that they all satisfy

$$\sum_{i,j \in [n]} \delta_a(i,j) = 1, \quad \forall a \in [p], \quad (4)$$

which, in practice, can be achieved via normalization, meaning,

$$\delta_a(i,j) \leftarrow \frac{\delta_a(i,j)}{\sum_{i,j} \delta_a(i,j)}. \quad (5)$$

This assumption is important when combining measures in the standard setting (3) and in the sparse setting (6) below.

Suppose for now that we know that at most s measures are useful among the p measures that we are given. For $S \subset [p]$, define the S -dissimilarity as

$$\delta_S(i,j) = \sum_{a \in S} \delta_a(i,j), \quad (6)$$

and the corresponding average within-cluster S -dissimilarity for the cluster assignment C as

$$\Delta_S[C] := \sum_{k \in [\kappa]} \frac{1}{|C^{-1}(k)|} \sum_{i,j \in C^{-1}(k)} \delta_S(i,j). \quad (7)$$

If the goal is to delineate κ clusters, then a natural objective is the following:

$$\text{Given } (\delta_a(i,j) : a \in [p], i, j \in [n]), \text{ minimize } \Delta_S[C] \text{ over } S \subset [p] \text{ of size } s \text{ and over } C \in \mathcal{C}_\kappa^n. \quad (8)$$

In words, the goal is to find the s measures (which play the role of features in this context) that lead to the smallest optimal average within-cluster dissimilarity. The problem stated in (8) is at least as hard as the problem stated in (2), and in particular, is computationally intractable even for small item sets.

Remark 1. In many situations, but not all, p measurements of possibly different types are taken from each item i , resulting in a vector of measurements $x_i = (x_{ia} : a \in [p])$. This vector is not necessarily in a Euclidean space, although this is an important example — see Section 2.2 below. We recover our setting when we have available a dissimilarity measure $\delta_a(i,j)$ between x_{ia} and x_{ja} . This special case justifies our using the terms ‘feature’ and ‘attribute’ when referring to a dissimilarity measure.

2 Related work

The literature on sparse clustering is much smaller than that of sparse regression or classification. Nonetheless, it is substantial and we review some of the main proposals in this section. We start with the contributions of Friedman and Meulman (2004) and Witten and Tibshirani (2010), which inspired the present work.

2.1 COSA and Sparse K-Means

Friedman and Meulman (2004) propose clustering objects on subsets of attributes (COSA), which (in its simplified form) amounts to the following optimization problem

$$\text{minimize } \sum_{k \in [\kappa]} \alpha(|C^{-1}(k)|) \sum_{i, j \in C^{-1}(k)} \sum_{a \in [p]} (w_a \delta_a(i, j) + \lambda w_a \log w_a), \quad (9)$$

$$\text{over any clustering } C \text{ and any weights } w_1, \dots, w_p \geq 0 \text{ subject to } \sum_{a \in [p]} w_a = 1. \quad (10)$$

Here α is some function and $\lambda \geq 0$ is a tuning parameter. When $\alpha(u) = 1/u$, the objective function can be expressed as

$$\sum_{a \in [p]} (w_a \Delta_a[C] + \lambda w_a \log w_a). \quad (11)$$

When $\lambda = 0$, the minimization of (11) over (10) results in any convex combination of attributes with smallest average within-cluster dissimilarity. In general, $\lambda > 0$, and the term it multiplies is the negative entropy of the weights ($w_a : a \in [p]$) seen as a distribution on $\{1, \dots, p\}$. This penalty term encourages the weights to spread out over the attributes. Minimizing over the weights first leads to

$$\text{minimize } \Delta_{\text{cosa}}[C] := \min_w \sum_{a \in [p]} (w_a \Delta_a[C] + \lambda w_a \log w_a) \quad (12)$$

$$\text{over any clustering } C. \quad (13)$$

where the minimum is over the w 's satisfying (10). (Note that the λ needs to be tuned.) The minimization is carried out using an alternating strategy where, starting with an initialization of the weights w (say all equal, $w_a = 1/p$ for all $a \in [p]$), the procedure alternates between optimizing with respect to the clustering assignment C and optimizing with respect to the weights. (There is a closed-form expression for that derived in that paper.) The procedure stops when achieving a local minimum.

Witten and Tibshirani (2010) observe that an application of COSA rarely results in a sparse set of features, meaning that the weights are typically spread out. They propose an alternative method, which they call Sparse K-means, which, under (4), amounts to the following optimization problem

$$\text{maximize } \sum_{a \in [p]} w_a \left(\frac{1}{n} - \Delta_a[C] \right), \quad (14)$$

$$\text{over any clustering } C \text{ and any weights } w_1, \dots, w_p \geq 0 \text{ subject to } \|w\|_2 \leq 1, \|w\|_1 \leq s. \quad (15)$$

The ℓ_1 penalty on w results in sparsity for small values of the tuning parameter s , which is tuned by the gap statistic of Tibshirani et al. (2001). The ℓ_2 penalty is also important, as without it, the solution would put all the weight on only one the attribute with smallest average within-cluster dissimilarity. A similar minimization strategy is proposed, which also results in a local optimum.

2.2 Some methods for the Euclidean setting

Consider points in space (denoted x_1, \dots, x_n in \mathbb{R}^p) that we want to cluster. A typical dissimilarity is the Euclidean metric, denoted by $\delta(i, j) = \|x_i - x_j\|^2$. Decomposing this into coordinate components, with $x_i = (x_{ia} : a \in [p])$, and letting $\delta_a(i, j) = (x_{ia} - x_{ja})^2$, we have

$$\delta(i, j) = \sum_{a \in [p]} \delta_a(i, j). \quad (16)$$

A normalization would lead us to consider a weighted version of these dissimilarities. But assuming that the data has been normalized to have (Euclidean) norm 1 along each coordinate, (4) holds and we are within the framework described above.

This Euclidean setting has drawn most of the attention. Some papers propose to perform clustering after reducing the dimensionality of the data (Ghosh and Chinnaiyan, 2002; Liu et al., 2003; Tamayo et al., 2007). However, the preprocessing step of dimensionality reduction is typically independent of the end goal of clustering, making such approaches non-competitive.

A model-based clustering approach is based maximizing the likelihood. Under the sparsity assumption made here, the likelihood is typically penalized. Most papers assume a Gaussian mixture model. Let $f(x; \mu, \Sigma)$ denote the density of the normal distribution with mean μ and covariance matrix Σ . The penalized negative log-likelihood (when the goal is to obtain κ clusters) is of the form

$$- \sum_{i \in [n]} \log \left[\sum_{k \in [\kappa]} \pi_k f_k(x_i; \mu_k, \Sigma_k) \right] + p_\lambda(\Theta), \quad (17)$$

where Θ gathers all the parameters, meaning, the mixture weights π_1, \dots, π_p , the group means μ_1, \dots, μ_p , and the group covariance matrices $\Sigma_1, \dots, \Sigma_p$. For instance, assuming that the data has been standardized so that each feature has sample mean 0 and variance 1, Pan and Shen (2007) use

$$p_\lambda(\Theta) = \lambda \sum_{k \in [\kappa]} \|\mu_k\|_1. \quad (18)$$

This may be seen as a convex relaxation of

$$p_\lambda(\Theta) = \lambda \sum_{a \in [p]} \sum_{k \in [\kappa]} \mathbb{I}\{\mu_{ka} \neq 0\} = \lambda \sum_{k \in [\kappa]} \|\mu_k\|_0. \quad (19)$$

Typically, this optimization will result in some coordinates set to zero and thus deemed not useful for clustering purposes. In another variant, Wang and Zhu (2008) use

$$p_\lambda(\Theta) = \lambda \sum_{a \in [p]} \max_{k \in [\kappa]} |\mu_{ka}|. \quad (20)$$

Taking into account the covariance matrices, and assuming they are diagonal, Xie et al. (2008) use

$$p_\lambda(\Theta) = \lambda_1 \sum_{k \in [\kappa]} \sum_{a \in [p]} |\mu_{ka}| + \lambda_2 \sum_{k \in [\kappa]} \sum_{a \in [p]} |\sigma_{ka}^2 - 1|. \quad (21)$$

The assumption that the covariance matrices are diagonal is common in high-dimensional settings and was demonstrated to be reasonable in the context of clustering (Fraley and Raftery, 2006). Note that none of these proposals make the optimization problem (17) convex or otherwise tractable. The methods are implemented via an EM-type approach.

Another line of research on sparse clustering is based on coordinate-wise testing for mixing. This constitutes the feature selection step. The clustering step typically amounts to applying a clustering algorithm to the resulting feature space. For example, Jin and Wang (2014) use a Kolmogorov-Smirnov test against the normal distribution, while Jin et al. (2015) use a (chi-squared) variance test. The latter is also done in (Azizyan et al., 2013) and in (Verzelen and Arias-Castro, 2014). This last paper also studies the case where the covariance matrix is unknown and proposes an approach via moments. In a nonparametric setting, Chan and Hall (2010) use coordinate-wise mode testing.

3 Our method: Sparse Alternate Sum (SAS) Clustering

Hill-climbing methods are iterative in nature, making ‘local’, that is, ‘small’ changes at each iteration. They have been studied in the context of graph partitioning, e.g., by Kernighan and Lin (1970) and Carson and Impagliazzo (2001), among others. In the context of sparse clustering, we find the K-medoids variant of Aggarwal et al. (1999), which includes a hill-climbing step.

Many of the methods cited in Section 2 use alternate optimization in some form (e.g., EM), which can be interpreted as hill-climbing. Our method is instead directly formulated as a hill-climbing approach, making it simpler and, arguably, more principled than COSA or Sparse K-means.

3.1 Our approach: SAS Clustering

Let \hat{C} be an algorithm for clustering based on dissimilarities. Formally, $\hat{C} : \mathbb{D} \times \mathbb{N} \mapsto \mathcal{C}$, where \mathbb{D} is a class of dissimilarity matrices and $\mathcal{C} := \bigcup_n \bigcup_\kappa \mathcal{C}_\kappa^n$, and for $(d, \kappa) \in \mathbb{D} \times \mathbb{N}$ with d of dimension n , $\hat{C}(d, \kappa) \in \mathcal{C}_\kappa^n$. Note that \hat{C} could be a hill-climbing method for graph partitioning, or K-medoids (or K-means if we are provided with points in a vector space rather than dissimilarities), or a spectral method, namely, any clustering algorithm that applies to dissimilarities. (In this paper, we will use K-means for numerical data and K-medoids for categorical data using hamming distances as dissimilarities.) For $S \subset [p]$, define

$$\delta_S = (\delta_a(i, j) : a \in S; i, j \in [n]) \quad \text{and} \quad \delta = \delta_{[p]}. \quad (22)$$

Our procedure is described in Algorithm 1. The use of algorithm \hat{C} in Step 1 is an attempt to

Algorithm 1 Sparse Alternate Similarity (SAS) Clustering

Input: dissimilarities $(\delta_a(i, j) : a \in [p], i, j \in [n])$, number of clusters κ , number of features s

Output: feature set S , group assignment function C

Initialize: For each $a \in [p]$, compute $C_a \leftarrow \hat{C}(\delta_a, \kappa)$ and then $\Delta_a[C_a]$. Let $S \subset [p]$ index the smallest s among these.

Alternate between the following steps until ‘convergence’:

1: Keeping S fixed, compute $C \leftarrow \hat{C}(\delta_S, \kappa)$.

2: Keeping C fixed, compute $S \leftarrow \arg \min_{|S|=s} \Delta_S[C]$.

minimize $C \mapsto \Delta_S[C]$ over $C \in \mathcal{C}_\kappa^n$. The minimization in Step 2 is over $S \subset [p]$ of size s and it is trivial. Indeed, the minimizing S is simply made of the s indices $a \in [p]$ corresponding to the smallest $\Delta_a[C]$. For the choice of parameters κ and s , any standard method for tuning parameters of a clustering algorithm applies, for example, by optimization of the gap statistic of Tibshirani et al. (2001). We note that the initialization phase, by itself, is a pure coordinate-wise approach that has analogs in the Euclidean setting as mentioned Section 2.2. The hill-climbing process is the iteration phase.

Remark 2. We tried another initialization in Algorithm 1 consisting of drawing a feature set S at random. We found that the algorithm behaved similarly. (Results not reported here.)

3.2 Number of iterations needed

A first question of interest is whether the iterations improve the purely coordinate-wise method, defined as the method that results from stopping after one pass through Steps 1-2 in Algorithm 1 (no iteration). Although this is bound to vary with each situation, we examine an instance where

the data come from the mixture of three Gaussians with sparse means. In detail, the setting comprises 3 clusters with 30 observations each and respective distributions $\mathcal{N}(\boldsymbol{\mu}, \mathbf{I})$, $\mathcal{N}(\mathbf{0}, \mathbf{I})$ and $\mathcal{N}(-\boldsymbol{\mu}, \mathbf{I})$, with $\boldsymbol{\mu} = (\mu, \dots, \mu, 0, \dots, 0)$ having 50 μ 's and 450 zeros. We assume that $\kappa = 3$ and $s = 50$ are both given, and we run the SAS algorithm and record the Rand indexes (Rand, 1971) and symmetric differences $|S_* \Delta \hat{S}|$ as the end of each iteration of Steps 1-2. The setting is repeated 400 times. The means and confidence intervals under different regimes ($\mu = 0.6$, $\mu = 0.7$, $\mu = 0.8$, $\mu = 0.9$) are shown in Figure 1. At least in this setting, the algorithm converges in a few iterations and, importantly, these few iterations bring significant improvements, particularly over the purely coordinate-wise algorithm.

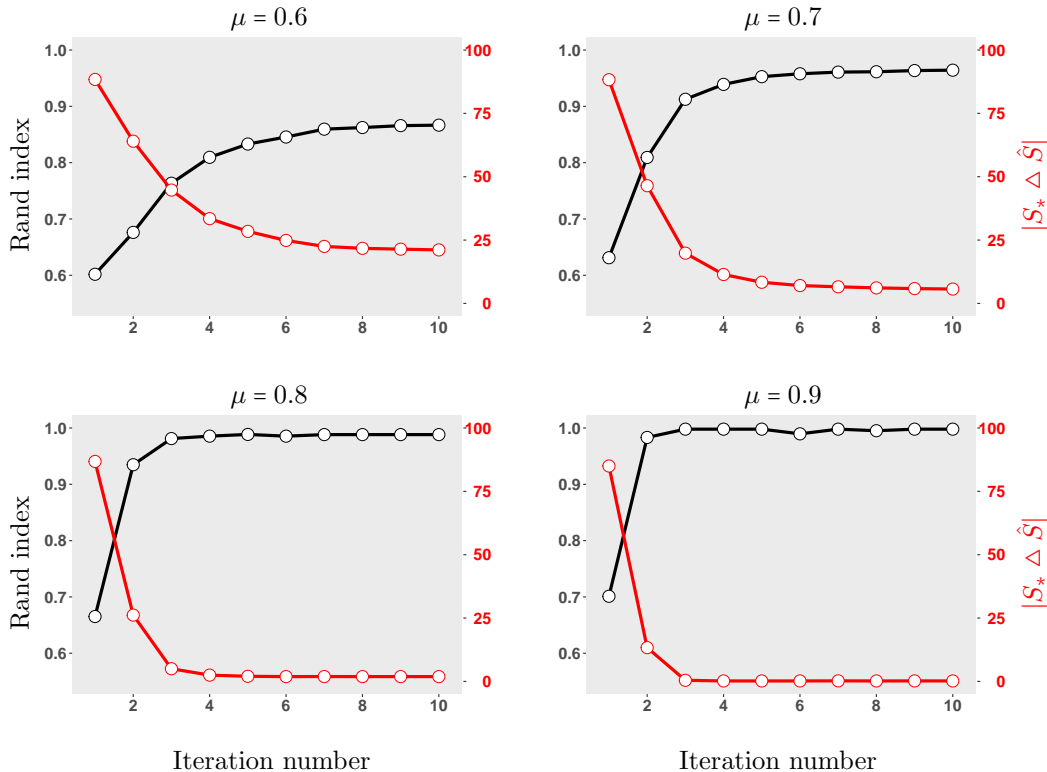


Figure 1: Means of Rand indexes and symmetric differences.

3.3 Selection of the sparsity parameter

We consider the problem of selecting κ , the number of clusters, as outside of the scope of the present paper, as it is intrinsic to the problem of clustering and has been discussed extensively in the literature — see (Kou, 2014; Tibshirani et al., 2001) and references therein. Thus we assume that κ is given. Besides κ , our algorithm has one tuning parameter, the sparsity parameter s , which is the number of useful features for clustering, meaning, the cardinality of set S in (8).

Inspired by the gap statistic of Tibshirani et al. (2001), which was designed for selecting the number of clusters κ in standard K-means clustering, we propose a permutation approach for selecting s . Let Δ_s^{obs} denote the average within-cluster dissimilarity of the clustering computed by the algorithm on the original data with input number of features s . Let Δ_s^{perm} denote the same quantity but obtained from a random permutation of the data — a new sample is generated by

independently permuting the observations within each feature. The gap statistic (for s) is then defined as

$$\text{gap}(s) = \log \Delta_s^{\text{obs}} - \mathbb{E}(\log \Delta_s^{\text{perm}}). \quad (23)$$

In practice, the expectation is estimated by Monte Carlo, generating B random permuted datasets. A large gap statistic indicates a large discrepancy between the observed amount of clustering and that expected of a null model (here a permutation of the data) with no salient clusters.

The optimization of the gap statistics over $s \in [p]$ is a discrete optimization problem. An exhaustive search for s would involve computing p gap statistics, each requiring B runs of the SAS algorithm. This is feasible when p and B are not too large.¹ See Algorithm 2, which allows for coarsening the grid.

Algorithm 2 SAS Clustering with Grid Search

Input: Dissimilarities $(\delta_a(i, j) : a \in [p], i, j \in [n])$, number of clusters κ , step size h , number of Monte Carlo permutations B

Output: Number of useful features \hat{s} , feature set S , group assignment C

for $s = 1$ to p with step size h **do**

 Run **Algorithm 1** to get the feature set S_s and group assignment C_s

 Run **Algorithm 1** on B permuted datasets to get the gap statistic G_s

end for

return Let $\hat{s} = \arg \max_s G_s$ and return $S_{\hat{s}}$ and $C_{\hat{s}}$

To illustrate the effectiveness of choosing s using the gap statistic, we computed the gap statistic for all $s \in [p]$ in the same setting as that of Section 3.2 with $\mu = 1$. The result of the experiment is reported in Figure 2. Note that, in this relatively high SNR setting, the gap statistic achieves its maximum at the correct number of features.

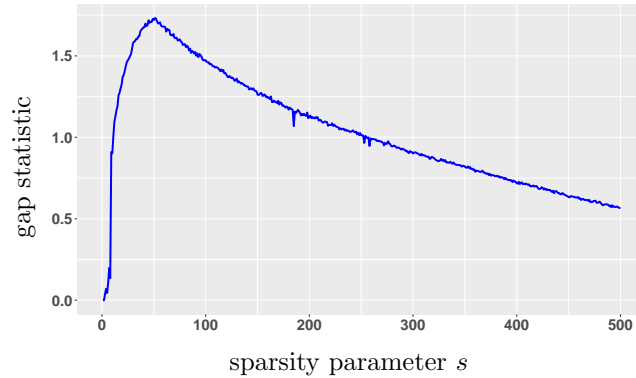


Figure 2: A plot of the gap statistic for each $s \in [p]$ for a Gaussian mixture with 3 components (30 observations in each cluster) in dimension $p = 500$.

In this experiment, at least, the gap statistic seems unimodal (as a function of s). If it were the case, we could use a golden section search, which would be much faster than an exhaustive grid search.

¹In our experiments, we choose $B = 25$ as in the code that comes with (Witten and Tibshirani, 2010).

4 Numerical experiments

We performed a number of numerical experiments, both on simulated data and on real (microarray) data to compare our method with other proposals. Throughout this section, we assume that the number of clusters is given, and we use the gap statistic of Tibshirani et al. (2001) to choose the tuning parameter s in our algorithm.

4.1 A comparison of SAS Clustering with Sparse K-means and IF-PCA-HCT

We compare our Algorithm 1 with IF-PCA-HCT (Jin and Wang, 2014) and Sparse K-means (Witten and Tibshirani, 2010) in the setting of Section 3.2. We note that IF-PCA-HCT was specifically designed for that model and that Sparse K-means was shown to numerically outperform a number of other approaches, including standard K-means, COSA (Friedman and Meulman, 2004), model-based clustering (Raftery and Dean, 2006), the penalized log-likelihood approach of (Pan and Shen, 2007) and the classical PCA approach. We use the gap statistic to tune the parameters of SAS Clustering and Sparse K-means. (SAS_gs uses a grid search while SAS_gss uses a golden section search.) IF-PCA-HCT is tuning-free — it employs the higher criticism to automatically choose the number of features.

In Table 1, we report the performance for these three methods in terms of Rand index (Rand, 1971) for various combinations of μ and p . Each situation was replicated 50 times. As can be seen from the table, SAS Clustering outperforms IF-PCA-HCT, and performs at least as well as Sparse K-means and sometimes much better (for example when $p = 500$ and $\mu = 0.7$). We examine a dataset from this situation in depth, and plot the weights resulted from Sparse K-means on this dataset, see Figure 3. As seen in this figure, and also as mentioned in (Witten and Tibshirani, 2010), Sparse K-means generally results in more features with non-zero weights than the truth. These extraneous features, even with small weights, may negatively impact the clustering result. In this specific example, the Rand index from Sparse K-means is 0.763 while our approach gives a Rand index of 0.956. Let $S_* \subset [p]$ denote the true feature set and \hat{S} the feature set that our method return. In this example, $|S_* \Delta \hat{S}| = 12$.

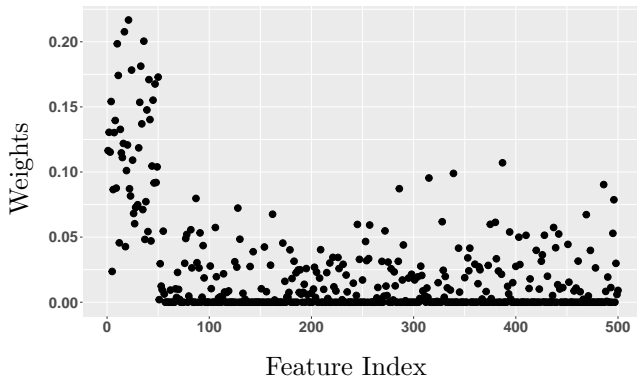


Figure 3: A typical example of the weights that Sparse K-means returns.

4.2 A more difficult situation (same covariance)

In Section 4.1, the three groups had identity covariance matrix, assumed to be known. In this section, we continue comparing our approach with Sparse K-means and IF-PCA-HCT under a

μ	methods	p = 100	p = 200	p = 500	p = 1000
0.6	SAS_gs	0.907 (0.048)	0.875 (0.066)	0.827 (0.076)	0.674 (0.096)
	SAS_gss	0.900 (0.054)	0.860 (0.066)	0.781 (0.008)	0.701(0.050)
	Sparse K	0.886 (0.068)	0.807 (0.064)	0.744 (0.046)	0.704 (0.043)
	IF-PCA	0.664(0.042)	0.645(0.051)	0.605 (0.045)	0.593(0.038)
0.7	SAS_gs	0.953 (0.030)	0.965 (0.028)	0.960 (0.032)	0.855 (0.102)
	SAS_gss	0.953 (0.031)	0.961 (0.031)	0.921 (0.088)	0.789 (0.104)
	Sparse K	0.942 (0.045)	0.915 (0.071)	0.802 (0.087)	0.790 (0.087)
	IF-PCA	0.681(0.036)	0.653(0.044)	0.629(0.057)	0.614(0.055)
0.8	SAS_gs	0.986 (0.020)	0.985 (0.022)	0.987 (0.016)	0.966 (0.052)
	SAS_gss	0.984 (0.020)	0.983 (0.019)	0.987 (0.0178)	0.892 (0.122)
	Sparse K	0.985 (0.020)	0.975 (0.029)	0.961 (0.07)	0.948 (0.074)
	IF-PCA	0.691(0.043)	0.675(0.056)	0.639(0.068)	0.623(0.059)
0.9	SAS_gs	0.997 (0.008)	0.997 (0.008)	0.997 (0.007)	0.995 (0.010)
	SAS_gss	0.996 (0.010)	0.996 (0.009)	0.997 (0.009)	0.969 (0.076)
	Sparse K	0.996 (0.010)	0.992 (0.013)	0.992(0.016)	0.993 (0.013)
	IF-PCA	0.700(0.031)	0.682(0.051)	0.654(0.057)	0.627(0.065)
1.0	SAS_gs	0.999 (0.005)	1.000 (0.003)	1.000 (0.003)	0.999 (0.004)
	SAS_gss	0.998 (0.007)	1.000 (0.003)	1.000 (0.004)	0.998 (0.006)
	Sparse K	0.998 (0.007)	0.999 (0.005)	0.996 (0.010)	0.996 (0.009)
	IF-PCA	0.717(0.034)	0.710(0.039)	0.659(0.063)	0.639(0.060)

Table 1: Comparison results for the simulations in Section 4.1. The reported values are the mean (and standard error) of the Rand indexes over 50 simulations.

Method	SAS_gs	SAS_gss	Sparse K-means	IF-PCA
Rand index	0.915 (0.0592)	0.907 (0.053)	0.819 (0.076)	0.607 (0.046)
$ S_* \triangle \hat{S} $	12.3 (4.6)	14.0 (9.7)	290.0 (113.2)	117.8 (55.6)

Table 2: Comparison of SAS Clustering with Sparse K-means and IF-PCA in the setting of Section 4.2. Reported at the Rand index and symmetric difference, averaged over 50 repeats. The standard deviations are in parentheses.

more difficult situation, where each of the 3 clusters have 30 points sampled from different p -variate normal distributions ($p = 500$), with different mean vectors

$$\boldsymbol{\mu}_1 = [1.02, 1.04, \dots, 2, \underbrace{0, \dots, 0}_{450 \text{ zeros}}], \quad \boldsymbol{\mu}_2 = [2.02, 2.04, \dots, 3, \underbrace{0, \dots, 0}_{450 \text{ zeros}}], \quad \boldsymbol{\mu}_3 = [3.02, 3.04, \dots, 4, \underbrace{0, \dots, 0}_{450 \text{ zeros}}],$$

and same diagonal covariance matrix $\boldsymbol{\Sigma}$ across groups, a random diagonal matrix with eigenvalues in $[1, 5]$. We used 50 repeats. The results are reported in Table 2. We see there that, in this setting, our method is clearly superior to Sparse K-means and IF-PCA-HCT. We also report the symmetric difference $|S_* \triangle \hat{S}|$ between the estimated feature set \hat{S} and the true feature set S_* . Our algorithm is clearly more accurate in terms of feature selection.

4.3 A more difficult situation (different covariances)

In both Section 4.1 and Section 4.2, the three groups have the same covariance matrix. In this section, we continue comparing our approach with Sparse K-means and IF-PCA-HCT under an even more difficult situation, where the mean vectors are the same as in Section 4.2, but now the covariances are different: $\boldsymbol{\Sigma}_1$, $\boldsymbol{\Sigma}_2$ and $\boldsymbol{\Sigma}_3$ are random diagonal matrices with eigenvalues in $[1, 2]$, $[2, 3]$ and $[3, 4]$, respectively. We used 50 repeats in this simulation. The results, reported

Method	SAS_gs	SAS_gss	Sparse K-means	IF-PCA
Rand index	0.920 (0.054)	0.858 (0.098)	0.710 (0.022)	0.668 (0.041)
$ S_* \triangle \hat{S} $	8.7 (3.8)	13.0 (7.9)	297.2 (75.6)	118.6 (56.8)

Table 3: Comparison of SAS Clustering with Sparse K-means and IF-PCA in the setting of Section 4.3. Reported at the Rand index and symmetric difference, averaged over 50 repeats. The standard deviations are in parentheses.

in Table 3, are consistent with the results of Section 4.2: our method clearly outperforms Sparse K-means and IF-PCA-HCT, both in terms of clustering and feature selection.

Notice that the 3 clusters are well separated in the first 50 features as can be seen from the construction of the data, but when 450 noise features are present in the datasets, the task of clustering becomes difficult. See Figure 4(b) as an example where we project a representative dataset onto the first two principal components of the whole data matrix. However, if we are able to successfully select out the first 50 features and apply classical clustering algorithms, then we are able to achieve better results. See Figure 4(a), where we project the same dataset onto the first two principal components of the data submatrix consisting of the first 50 columns (features). To illustrate the comparisons, we also plot in Figure 4 the clustering results by these three methods.

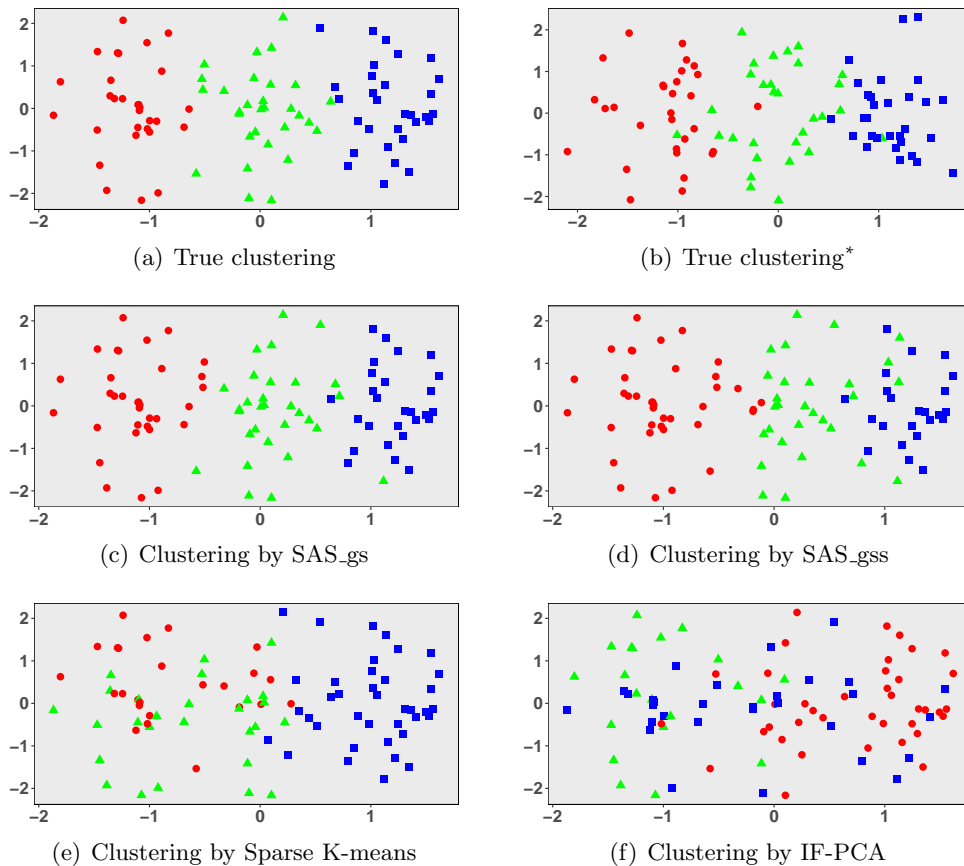


Figure 4: Projection of a dataset from Section 4.3 onto the first two principal components of the data submatrix, where only the first 50 columns are kept. *Different from the other 5 subfigures, here the data points are projected onto the first two principal components of the whole data matrix.

q	methods	$p = 30$	$p = 60$	$p = 100$	$p = 200$
0.6	SAS_gs	0.878 (0.060)	0.872 (0.042)	0.864 (0.057)	0.863 (0.053)
	Sparse K-medoids	0.694 (0.045)	0.663 (0.054)	0.654 (0.049)	0.639 (0.044)
0.7	SAS_gs	0.954 (0.023)	0.960 (0.026)	0.942 (0.026)	0.948 (0.033)
	Sparse K-medoids	0.807 (0.126)	0.763 (0.077)	0.716 (0.060)	0.686 (0.062)
0.8	SAS_gs	0.989 (0.011)	0.984 (0.019)	0.983 (0.019)	0.978 (0.021)
	Sparse K-medoids	0.946 (0.090)	0.889 (0.099)	0.846 (0.100)	0.787 (0.093)
0.9	SAS_gs	0.998 (0.005)	0.999 (0.003)	0.997 (0.007)	0.997 (0.006)
	Sparse K-medoids	0.997 (0.006)	0.994 (0.036)	0.983 (0.044)	0.966 (0.065)

Table 4: Comparison results for Section 4.4. The reported values are the mean (and standard error) of the Rand indexes over 50 simulations.

4.4 Clustering non-euclidean data

In the previous simulations, all the datasets were Euclidean. In this section, we apply our algorithm on categorical data (with Hamming distance) and compare its performance with Sparse K-medoids². In this example, we generate 3 clusters with 30 data points each from three different distributions on the Hamming space of dimension p . Each distribution is the tensor product of Bernoulli distributions with success probabilities $q_a \in [0, 1]$ for $a \in [p]$. For the first distribution, $q_a = q$ for $1 \leq a \leq 5$ and $q_a = 0.1$ otherwise. For the second distribution, $q_a = q$ for $6 \leq a \leq 10$ and $q_a = 0.1$ otherwise. For the third distribution, $q_a = q$ for $11 \leq a \leq 15$ and $q_a = 0.1$ otherwise. See Table 4, where we compare these two methods in terms of Rand index for various combination of q and p . Each situation was replicated 50 times. As can be seen from the table, SAS Clustering significantly outperforms Sparse K-medoids in most situations. We examined why, and it turns out that Sparse K-medoids works well if the tuning parameter s in equation (15) is given, but it happens that the gap statistic often fails to give a good estimate of s in this categorical setting. We are not sure why.

4.5 Applications to gene microarray data

We compare our approach with others on real data from genetics. Specifically, we consider the same microarray datasets used by Jin and Wang (2014) to evaluate their IF-PCA method. The comparison results, this time in terms of the classification error, are reported in Table 5, where some numbers are taken from (Jin and Wang, 2014). We quickly mention that SpectralGem (Lee et al., 2010) is PCA-type method and K-means++ (Arthur and Vassilvitskii, 2007) is Lloyd’s algorithm for K-means but with a more careful initialization than purely random.

In these datasets, our method is overall comparable to Sparse K-means and IF-PCA. It is interesting to note that SAS_gss outperforms SAS_gs on a couple of datasets. However, we caution the reader against drawing hard conclusions based on these numbers, as some of the datasets are quite small. For example, the Brain dataset has $\kappa = 5$ groups and a total sample size of $n = 42$, and is very high-dimensional with $p = 5, 597$.

5 Conclusion

We presented here a simple method for feature selection in the context of sparse clustering. The method is arguably more natural and simpler to implement than COSA or Sparse K-means. At

²We modified the function of Sparse K-means in the R package ‘sparcl’, essentially replacing K-means with K-medoids, so that it can be used to cluster categorical data.

Data set	κ	n	p	K-means	K-means++	Hier	SpecGem	IF-PCA	Sparse K	SAS _{gs}	SAS _{gss}
Brain	5	42	5597	.286	.472	.524	.143	.262	.190	.310	.310
Breast	2	276	22215	.442	.430	.500	.438	.406	.449	.485	.445
Colon	2	62	2000	.443	.460	.387	.484	.403	.306	.129	.403
Lung	2	181	12533	.116	.196	.177	.122	.033	.122	.099	.099
Lung(2)	2	203	12600	.436	.439	.301	.434	.217	.315	.315	.315
Leukemia	2	72	3571	.278	.257	.278	.292	.069	.028	.028	.028
Lymphoma	3	62	4026	.387	.317	.468	.226	.065	.016	.016	.016
Prostate	2	102	6033	.422	.432	.480	.422	.382	.373	.431	.431
SRBCT	4	63	2308	.556	.524	.540	.508	.444	.317	.460	.365
SuCancer	2	174	7909	.477	.459	.448	.489	.333	.477	.483	.483

Table 5: Comparison of SAS Clustering with other clustering methods on 10 gene microarray datasets. (In **bold** is the best performance.)

the same time, it performs comparably or better than these methods, both on simulated and on real data.

At the moment, our method does not come with any guarantees, other than that of achieving a local minimum if the iteration is stopped when no improvement is possible. Just like other iterative methods based on alternating optimization, such as Lloyd’s algorithm for K-means, proving a convergence to a good local optimum (perhaps even a global optimum) seems beyond reach at the moment. COSA and Sparse K-means present similar challenges and have not been analyzed theoretically. IF-PCA has some theoretical guarantees developed in the context of a Gaussian mixture model (Jin and Wang, 2014) — see also Jin et al. (2015). More theory for sparse clustering is developed in (Azizyan et al., 2013; Chan and Hall, 2010; Verzelen and Arias-Castro, 2014).

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