Spectral Self-supervised Feature Selection

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Abstract

Choosing a meaningful subset of features from high-dimensional observations in unsupervised settings can greatly enhance the accuracy of downstream analysis, such as clustering or dimensionality reduction, and provide valuable insights into the sources of heterogeneity in a given dataset. In this paper, we propose a self-supervised graph-based approach for unsupervised feature selection. Our method's core involves computing robust pseudo-labels by applying simple processing steps to the graph Laplacian's eigenvectors. The subset of eigenvectors used for computing pseudo-labels is chosen based on a model stability criterion. We then measure the importance of each feature by training a surrogate model to predict the pseudo-labels from the observations. Our approach is shown to be robust to challenging scenarios, such as the presence of outliers and complex substructures. We demonstrate the effectiveness of our method through experiments on real-world datasets, showing its robustness across multiple domains, particularly its effectiveness on biological datasets.

1 Introduction

Improvements in sampling technology enable scientists across many disciplines to acquire numerous variables from biological or physical systems. One of the critical challenges in real-world scientific data is the presence of noisy, information-poor, or nuisance features. While such features could be mildly harmful to supervised learning, they could dramatically affect the outcome of downstream analysis tasks (e.g., clustering or manifold learning) in the unsupervised setting (Mahdavi et al., 2019). There is thus a growing need for unsupervised feature selection schemes that enhance latent signals of interest by removing nuisance variables and thus advance reliable data-driven scientific discovery.

Unsupervised Feature Selection (UFS) methods are designed to identify a set of informative features that can improve the outcome of downstream analysis tasks such as clustering and manifold learning. With the lack of labels, however, selecting features becomes a challenge since the downstream task cannot be used to drive the selection of features. As an alternative, most UFS methods use a label-free criterion that correlates with the downstream task. For instance, many UFS schemes rely on a reconstruction prior (Li et al., 2017) and seek a subset of features that can be used to reconstruct the entire set of features as accurately as possible. Several works use Autoencoders (AE) to learn a reduced representation of the data while applying a sparsification penalty to force the AE to remove redundant features. This idea was implemented with several types of sparsity-inducing regularizers, including $\ell_{2,1}$ based (Chandra and Sharma, 2015; Han et al., 2018), relaxed ℓ_0 (Balın et al., 2019; Shaham et al., 2022; Svirsky and Lindenbaum) and more.

One of the most commonly used criteria for UFS is feature smoothness. According to this hypothesis, the structure of interest, such as clusters or a manifold, can be captured using the graph Laplacian matrix (Ng et al., 2001). The smoothness of features is measured using the Laplacian Score (LS) (He et al., 2005), which is based on the Rayleigh quotient of the Laplacian. A feature that is smooth with respect to the graph is considered to be associated with the primary underlying data structures. There are many other UFS methods that use a graph to select informative features Li et al. (2018); Roffo et al. (2017); Zhu et al. (2017; 2020); Xie et al. (2023). (Li et al., 2012) derived Nonnegative Discriminative Feature Selection (NDFS) , which performs feature selection and spectral clustering simultaneously. Its extension Li and Tang (2015) adds a loss term to prevent the joint selection of correlated features.

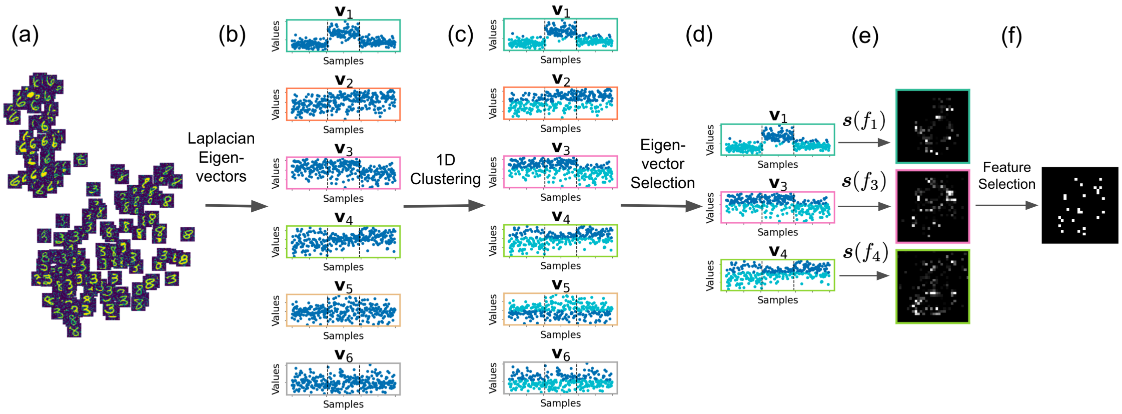


Figure 1: Illustration of SSFS. In (a) we show a tSNE scatter plot of noisy MNIST digits (3, 6, 8). (b) Presents the six leading eigenvectors computed based on the graph Laplacian of the data. Samples are ordered according to the identity of the digit. (c) We then use the k-medoids algorithm to define pseudo-labels $\boldsymbol{y}_i^*$. These are presented as colors overlayed on the eigenvectors. (d) We select the three eigenvectors whose pseud-labels are the most "stable" with respect to several prediction models (see Section 3.2). (e) For each data feature we estimate its importance score for each of the selected eigenvectors (see Section 3.3). (f) We aggregate the feature scores across eigenvectors.

Embedded unsupervised feature selection schemes aim to cluster the data while simultaneously removing irrelevant features. Examples include Wang et al. (2015), which performs the selection directly on the clustering matrix, and Zhu and Yang (2018), which learns feature weights while maximizing the distance between clusters. In recent years, several works have derived self-supervised learning methods for feature selection. The key idea is to design a supervised type learning task with pseudo-labels that do not require human annotation. A seminal work based on this paradigm is Multi-Cluster Feature Selection (MCFS) (Cai et al., 2010). MCFS uses the eigenvectors of the graph Laplacian as pseudo-labels and learns the informative features by optimizing over an ℓ_1 regularized least squares problem. More recently, Lee et al. (2021) used self-supervision with correlated random gates to enhance the performance of feature selection.

In this work, we present a spectral self-supervised scheme for feature selection. The key idea is to selectively and discriminatively use the eigenvectors of the graph Laplacian. We implement this process through a multi-stage approach. Firstly, we generate robust discrete pseudo-labels from the eigenvectors and filter them based on a stability measure. Next, we fit flexible surrogate classification models on the selected eigenvectors and query the models for feature scores. Using these components, we can identify informative features that are effective for clustering on real-world datasets.

2 Preliminaries

2.1 Laplacian score and representation-based feature selection

Generating a graph-based representation for a group of high-dimensional observations has become a common practice for unsupervised learning tasks. In manifold learning, methods such as ISOMAPS (Tenenbaum et al., 2000), LLE (Roweis and Saul, 2000), Laplacian eigenmaps (Belkin and Niyogi, 2003), and diffusion maps (Coifman and Lafon, 2006) compute a low-dimensional representation that is associated with the manifold's latent structure. In spectral clustering, a set of points is partitioned by applying the k-means algorithm to the leading Laplacian eigenvectors (Ng et al., 2001).

In graph methods, each node v_i corresponds to one of the observations $\boldsymbol{x}_i \in \mathbb{R}^p$. The weight W_{ij} between two nodes v_i, v_j is computed based on some kernel function $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$. For example, the popular Gaussian kernel is equal to,

$$K(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp\left(- \frac{\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{2\sigma^2} \right).$$

Where the parameter σ determines the bandwidth of the kernel function. Let $\boldsymbol{D}$ be a diagonal matrix with the degree of each node in the diagonal, such that $D_{ii} = \sum_j W_{ij}$. The unnormalized graph Laplacian matrix is equal to $\boldsymbol{L} = \boldsymbol{D} - \boldsymbol{W}$. For any vector $\boldsymbol{v} \in \mathbb{R}^n$ we have the following equality (Von Luxburg, 2007),

$$\boldsymbol{v}^T \boldsymbol{L} \boldsymbol{v} = \frac{1}{2} \sum_{i,j} \left(v_i - v_j\right)^2 W_{i,j}. \tag{1}$$

The quadratic form in equation 1 gives rise to a notion of graph *smoothness.* (Ricaud et al., 2019; Shuman et al., 2013). A vector is smooth with respect to a graph if it has similar values on pairs of nodes connected with an edge with a significant weight. This notion underlies the Laplacian score suggested as a measure for unsupervised feature selection (He et al., 2005). Let $\boldsymbol{f}_m \in \mathbb{R}^n$ denote the values of the m-th feature for all observations. The Laplacian score s_m is equal to,

$$s_m = \boldsymbol{f}_m^T \boldsymbol{L} \boldsymbol{f}_m = \frac{1}{2} \sum_{i,j} \left(f_{m,i} - f_{m,j}\right)^2 W_{ij}. \tag{2}$$

A low score indicates that a feature is smooth with respect to the computed graph and thus strongly associated with the latent structure of the high-dimensional data $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n$. The notion of the Laplacian score has been the basis of several other feature selection methods as well (Lindenbaum et al., 2021; Shaham et al., 2022; Zhu et al., 2012).

Let $\boldsymbol{v}_i, \lambda_i$ denote the i-th smallest eigenvector and eigenvalue of the Laplacian $\boldsymbol{L}$. A slightly different interpretation of equation 2 is that the score for each feature is equal to a weighted sum of its correlation with the eigenvectors, such that

$$s_m = \sum_{i=1}^{n} \lambda_i (\boldsymbol{f}_m^T \boldsymbol{v}_i)^2.$$

A potential drawback of the Laplacian score is its dependence on many eigenvectors. This may reduce its stability in measuring a feature's importance to the data's main structures. To overcome this limitation, Zhao and Liu (2007) derived an alternative score based only on a feature's correlation to the leading Laplacian eigenvectors. A related, more sophisticated approach is Multi-Cluster Feature Selection (MCFS) (Cai et al., 2010), which computes the solutions to the generalized eigenvector problem $\boldsymbol{L}\boldsymbol{v} = \lambda \boldsymbol{D}\boldsymbol{v}$. The leading eigenvectors are then used as pseudo-labels for a regression task with l_1 regularization. Specifically, MCFS applies Least Angle Regression (LARS) (Efron et al., 2004) to obtain, for each leading eigenvector $\boldsymbol{v}_i$, a sparse vector of coefficients $\boldsymbol{\beta}^i \in \mathbb{R}^p$. A feature score is computed by maximizing the absolute values of its corresponding coefficient, $s_j = \max_i |\beta^i_j|$. The output of MCFS is the set of features with the highest score. In the next section, we derive Spectral Self-supervised Feature Selection (SSFS), which improves upon the MCFS algorithm in several critical aspects.

3 Spectral Self-supervised Feature Selection

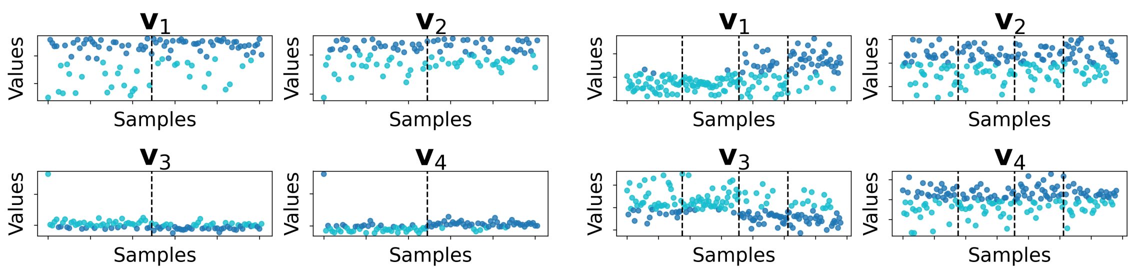
3.1 Rationale

As its title suggests, MCFS aims to uncover features that separate clusters in the data. Let us consider an ideal case where the observations are partitioned into k well-separated clusters, denoted $A_1, \dots, A_k$, such that the weight matrix $W_{ij} = 0$ if $\boldsymbol{x}_i, \boldsymbol{x}_j$ are in separate clusters. Let $\boldsymbol{e}^i$ denote an indicator vector for cluster i such that

$$e^i_j = \begin{cases} 1/\sqrt{|A_i|} & j \in A_i \\ 0 & \text{otherwise,} \end{cases}$$

where $|A_i|$ denotes the size of cluster A_i. In this scenario, the zero eigenvalue of the graph Laplacian has multiplicity k, and the corresponding eigenvectors are equal, up to a rotation matrix, to a matrix $E \in \mathbb{R}^{n \times d}$ whose columns are equal to $\boldsymbol{e}^1, \dots, \boldsymbol{e}^k$. In such a case, the k leading eigenvectors are indeed suitable for use as pseudo-labels for the feature selection task. Assuming that the clusters are amenable to a linear separation, the MCFS algorithm should provide highly informative features in terms of cluster separation.

However, cluster separation is often imperfect in many applications, which can make using leading eigenvectors for regression suboptimal. Here are some common scenarios: 1) High-dimensional datasets may contain



(a) Prostate-GE eigenvectors. (b) TOX-171 eigenvectors.

Figure 2: The first four Laplacian eigenvectors of two real datasets. Samples are sorted according to the real class label and colored by the outcome of a one-dimensional k-medoids per eigenvector. The vertical bar indicates the separation between the classes. In Prostate-GE, $\boldsymbol{v}_4$ is the most informative to the class labels, and an outlier can be seen on the upper left in the third and fourth eigenvectors. In TOX-171, $\boldsymbol{v}_3$ is more informative to the class labels than $\boldsymbol{v}_2$.

substructures in top eigenvectors, while the main structure of interest will appear later in spectrum. For illustration, consider the MNIST dataset visualized via t-SNE in Figure 1(a). The data contains images of $3, 6$ and 8. Panel (b) shows the elements of the six leading eigenvectors of the graph Laplacian matrix, sorted by their corresponding digits. The leading eigenvector shows a clear gap between images of digit 6 and the rest of the data. However, there is no clear separation between digits 3 and 8. Indeed, the next eigenvector is not associated with such a separation. Applying feature selection with this eigenvector may produce spurious features irrelevant to separating the two digits. This scenario is prevalent in the real datasets used in the experimental section. For example, Figure 2a shows four eigenvectors of a graph computed from observations containing the genetic expression data from prostate cancer patients and controls (Singh et al., 2002). The leading two eigenvectors, however, are not associated with the patient-control separation.

2) The leading eigenvectors may be affected by outliers. For example, an eigenvector may indicate a small group of outliers separated from the rest of the data. This phenomenon can also be seen in the third and fourth vectors of the Prostate-GE example in Figure 2a. While the fourth eigenvector separates the categories, it is corrupted by outliers and, hence, unsuitable for use as pseudo-labels in a classical regression task, as it might highlight features associated with the outliers.

3) The relation between important features and the separation of clusters may be highly non-linear. In such cases, applying linear regression models to obtain feature scores may be too restrictive.

Motivated by the above scenarios, we derive Spectral Self-supervised Feature Selection (SSFS). We explain our approach in detail in the following two sections.

3.2 Eigenvector processing and selection

Generating binary labels. Given the Laplacian eigenvectors $\boldsymbol{V} = (\boldsymbol{v}_1, ..., \boldsymbol{v}_d)$, our goal is to generate pseudo-labels that are highly informative to the cluster separation in the data. To that end, for each eigenvector $\boldsymbol{v}_i$, we compute a binary label vector $\boldsymbol{y}_i^*$ (pseudo-labels) by applying a one-dimensional k-medoids algorithm (Kaufman and Rousseeuw, 1990) to the elements of $\boldsymbol{v}_i$. In contrast to k-means, in k-medoids, the cluster centers are set to one of the input points, which makes the algorithm robust to outliers. In Figure 2, the eigenvectors are colored according to the output of the k-medoids. After binarization, the fourth eigenvector of the Prostate-GE dataset is highly indicative of the category. The feature selection is thus based on a classification rather than a regression task, which is more aligned with selecting features for clustering. In Section 5.2 we show the impact of the binarization step on multiple real-world datasets.

Eigenvector selection. Selecting k eigenvectors according to their eigenvalues may be unstable in cases where the eigenvalues exhibit a small spectral gap. We derive a robust criterion for selecting informative eigenvectors that is based on the stability of a model learned for each vector. Formally, we consider a surrogate model $h : \mathbb{R}^p \to \mathbb{R}$, and a feature score function $\boldsymbol{s}(h) \in \mathbb{R}^p$, where p denotes the number of features. The feature scores are non-negative and their sum is normalized to one. For example, h can be the logistic regression model $h(\boldsymbol{x}) = \sigma(\boldsymbol{\beta}^T \boldsymbol{x})$. In that case, a natural score function is the absolute value of the coefficient vector $\boldsymbol{\beta}$. For each eigenvector $\boldsymbol{v}_i$, we train a model h_i on B (non-mutually exclusive) subsets of the input data $\boldsymbol{X}$ and the pseudo-labels $\boldsymbol{y}_i^*$. We then estimate the variance of the feature score function, for every feature $m \in \{1, ..., p\}$:

$$\widehat{\text{Var}}(s_m(h_i)) = \frac{1}{B-1} \sum_{b=1}^{B} (s_m(h_{i,b}) - \bar{s}_m(h_i))^2.$$

This procedure is similar (though not identical) to the Delete-d Jackknife method for variance estimation (Shao and Wu, 1989). We keep, as pseudo-labels, the k binarized eigenvectors with the lowest sum of variance, $\hat{\mathcal{S}}_i = \sum_{m=1}^{p} \widehat{\text{Var}}(s_m(h_i))$. We denote the set of selected eigenvectors by I. A pseudo-code for the pseudo-labels generation and eigenvector selection appears in Algorithm 1.

3.3 Feature selection

For the feature selection step, we train k models, denoted $\{f_i \mid i \in I\}$, to predict the selected binary pseudo-labels based on the original data. Similarly to the eigenvector selection step, each model is associated with a feature score function $\boldsymbol{s}(f_i)$. The features are then scored according to the following maximum criterion,

$$\text{score}(m) = \max_{i \in I} s_m(f_i).$$

Finally, the features are ranked by their scores, and the top-ranked features are selected for the subsequent analysis. The choice of model for this step can differ from that used in the eigenvector selection step, allowing for flexibility in the modeling approach (see Section 3.4 for details). Pseudo-code for SSFS appears in Algorithm 2.

3.4 Choice of Surrogate Models

Our algorithm is compatible with any supervised model capable of providing feature importance scores. We combine the structural information from the graph Laplacian with the capabilities of various supervised models for unsupervised feature selection. Empirical evidence supports the use of more complex models such as Gradient-Boosted Decision Trees for various complex, real-world datasets (McElfresh et al., 2023; Chen and Guestrin, 2016). These models are capable of capturing complex nonlinear relationships, which we leverage by training them on pseudo-labels derived from the Laplacian's eigenvectors. For example, for eigenvector selection, one can use a simple logistic regression model for fast training on the resampling procedure and a more complex gradient boosting model such as XGBoost (Chen and Guestrin, 2016) for the feature selection step.

4 The importance of a proper selection of eigenvectors: analysis of the product manifold model

As described in Section 3.1, the principle of selecting the leading Laplacian eigenvectors as pseudo-labels is inspired by the case of highly separable clusters, where observations in different clusters have very low connectivity between them. In many cases, the separation between meaningful states (i.e., biological or medical conditions) may not be that clear. To illustrate this point, consider the MNIST example in Figure 1. The separation between digit 6 and the rest of the data is clear and appears in the leading Laplacian eigenvector. In contrast, digits 8 and 3 are not clearly separated. Figure 3a shows a scatter plot of these digits, where each image is located according to its coordinates in the third and fourth eigenvectors. Even when considering the most relevant eigenvectors, there is no clear separation between the digits. Instead, the transition between 3 and 8 is smooth and depends on the properties of the digits.

To provide some insight into the importance of eigenvector selection, we analyze a *product of manifold* model. Our analysis is based on results from two research topics: (i) the convergence, under the manifold assumption, of the Laplacian eigenvectors to the eigenfunctions of the Laplace Beltrami operator associated with the manifold, and (ii) the properties of manifold products. We next provide a brief background on these two topics.

Algorithm 1 Pseudo-code for Eigenvector Selection and Pseudo-labels Generation

Input: Dataset $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ (with n samples and p features), number of eigenvectors to select k, number of eigenvectors to compute d, surrogate models $H = \{h_i \mid i \in [d]\}$, feature scoring function $\boldsymbol{s} : \mathcal{F} \to \mathbb{R}^p$, number of resamples B

Initialize an empty list for the pseudo-labels $\mathcal{Y}^*$ and an empty list for the sums of features variance $\hat{\mathcal{S}}$
Compute the significant d eigenvectors of the Laplacian of $\boldsymbol{X}$: $\boldsymbol{V} = (\boldsymbol{v}_1, ..., \boldsymbol{v}_d)$
for $i = 1$ to d **do**
  Binarize the eigenvector $\boldsymbol{v}_i$ using k-medoids to obtain $\boldsymbol{y}_i^*$, and append to $\mathcal{Y}^*$
  for $b = 1$ to B **do**
    Subsample $((\boldsymbol{X})_b, (\boldsymbol{y}_i^*)_b)$ from $(\boldsymbol{X}, \boldsymbol{y}_i^*)$
    Fit the model $h_{i,b}$ to $((\boldsymbol{X})_b, (\boldsymbol{y}_i^*)_b)$
  end for
  for $m = 1$ to p **do**
    Estimate the variance of the m-th feature score:

$$\widehat{\mathrm{Var}}(s_m(h_i)) = \frac{1}{B-1} \sum_{b=1}^{B} (s_m(h_{i,b}) - \bar{s}_m(h_i))^2$$

  end for
  $\hat{\mathcal{S}}_i = \sum_{m=1}^{p} \widehat{\mathrm{Var}}(s_m(h_i))$
  $\hat{\mathcal{S}} \leftarrow \hat{\mathcal{S}} \cup \{\hat{\mathcal{S}}_i\}$
end for
Select the indices of the k smallest elements in $\hat{\mathcal{S}}$ and store in I
return $\mathcal{Y}^*$, I

Algorithm 2 Pseudo-code for Spectral Self-supervised Feature Selection (SSFS)

Input: Dataset $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ (with n samples and p features) number of eigenvectors to select k, number of eigenvectors to compute d, surrogate eigenvector selection models $H = \{h_i \mid i \in [d]\}$, surrogate feature selection models $F = \{f_i \mid i \in [d]\}$, feature scoring function $\boldsymbol{s} : \mathcal{F} \to \mathbb{R}^p$, number of resamples B, number of features to select ℓ.

Apply Algorithm 1 to obtain the pseudo-labels and the selected eigenvectors:
$\mathcal{Y}^*$, $I =$ **EigenvectorSelection**$(\boldsymbol{X}, k, d, H, \boldsymbol{s}, B)$
for i in I **do**
  Fit the model f_i on $(\boldsymbol{X}, \boldsymbol{y}_i^*)$
  Calculate the feature scores $\boldsymbol{s}(f_i)$
  Normalize the feature scores such that their sum is one
end for
for $m = 1$ to p **do**
  Compute the final score for the m-th feature:

$$\mathrm{score}(m) = \max_{i \in I} s_m(f_i)$$

end for
return a list of ℓ features with the highest score.

4.1 Convergence of the Laplacian eigenvectors

In many applications, the high dimensional observations are assumed to reside close to some manifold $\mathcal{M}$ with low intrinsic dimensionality, which we denote by d. Many papers in recent decades have analyzed the relation between the Laplacian eigenvectors and the manifold structure Von Luxburg et al. (2008); Singer and Wu (2017); García Trillos et al. (2020); Wormell and Reich (2021); Dunson et al. (2021); Calder and Trillos (2022). More formally, let $\boldsymbol{v}_k$ denote the k-th eigenvector of the graph Laplacian, and let g_k denote the k-th eigenfunction of the Laplace-Beltrami (LB) operator. We usually assume that g_k is normalized such that

$$\int_{\mathcal{M}} g_k(\boldsymbol{x})^2 \mu(\boldsymbol{x}) dV(\boldsymbol{x}) = 1,$$

where μ is the distribution function over $\mathcal{M}$. Under several assumptions and proper normalization of g_k, we have

$$\boldsymbol{v}_k \xrightarrow[n\to\infty]{} g_k(X).$$

where $g_k(X)$ is a vector of size n containing samples of the function g_k at the n rows of the data matrix X.

Let us provide a simple example. Consider n points sampled uniformly at random over an interval $[0, 1]$. The LB operator over an interval is the second derivative whose eigenfunctions are the harmonic functions $g_k(x) = \cos(k\pi x)$. Figure 3 shows the three Laplacian eigenvectors computed with $n = 10^2, 10^3$ and $3 \cdot 10^3$ points. As $n \to \infty$, the difference between $g_k(X)$ and v_k is decreases to 0.

Here, we use a convergence result from Cheng and Wu (2022), derived under the following assumptions: (i) The n observations were generated according to a uniform distribution over the manifold, such that $\mu(\boldsymbol{x})$ equals to a constant μ. (ii) Let λ_k denote the eigenvalue associated with the eigenfunction g_k. To ensure the stability of the eigenvectors, we assume a spectral gap between the smallest K eigenvalues bounded away from 0 such that,

$$\min_{i=1}^{K-1} (\lambda_{i+1} - \lambda_i) > \gamma > 0.$$

(iii) The graph weights are computed by a Gaussian kernel $\exp(-\|x_i - x_j\|^2/\epsilon_n)$, with a bandwidth $\epsilon_n \xrightarrow[n\to\infty]{} 0^+$ that satisfies $\epsilon_n^{d/2+2} > C_k \frac{\log n}{n}$ for a constant C_K.

Theorem 1 (Theorem 5.4 of Cheng and Wu (2022)) *For $n \to \infty$ and under assumptions (i)-(iii), with probability larger than $1-4K^2n^{-10}-(2K+6)n^{-9}$, the k-th eigenvector $\boldsymbol{v}_k$ of the unnormalized Laplacian satisfies*

$$\left\| \boldsymbol{v}_k - \alpha \boldsymbol{g}_k(\boldsymbol{X}) \right\|_2 = \mathcal{O}(\epsilon_n) + \mathcal{O}\left(\sqrt{\frac{\log n}{n \epsilon_n^{d/2+1}}} \right), \qquad k \le K, \tag{3}$$

where $\|\boldsymbol{v}_k\| = 1$ and $|\alpha| = o(1)$.

4.2 The product of manifold model

In a product of two manifolds, denoted $\mathcal{M} = \mathcal{M}_1 \times \mathcal{M}_2$, every point $\boldsymbol{x} \in \mathcal{M}$ is associated with a pair of points $\boldsymbol{x}_1, \boldsymbol{x}_2$ where $\boldsymbol{x}_1 \in \mathcal{M}_1$ and $\boldsymbol{x}_2 \in \mathcal{M}_2$. We denote by $\pi_1(\boldsymbol{x}), \pi_2(\boldsymbol{x})$ the canonical projections of a point in $\mathcal{M}$ to its corresponding points $\boldsymbol{x}_1, \boldsymbol{x}_2$ in $\mathcal{M}_1, \mathcal{M}_2$, respectively. For example, a $2D$ rectangle is a product of two $1D$ manifolds, where $\pi_1(\boldsymbol{x})$ and $\pi_2(\boldsymbol{x})$ select, respectively, the first and second coordinates.

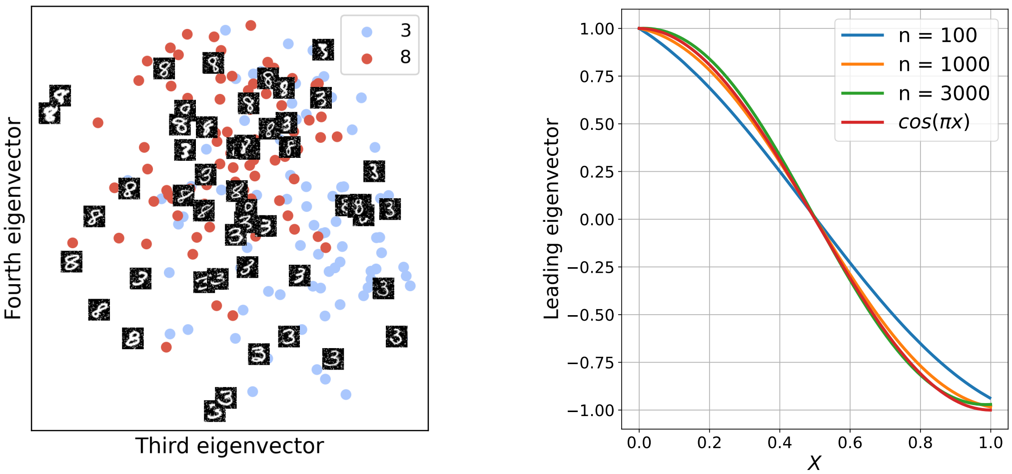
We denote by $g_i^{(1)}(\boldsymbol{x}), g_i^{(2)}(\boldsymbol{x})$ the i-th eigenfunction of the LB operator of $\mathcal{M}_1, \mathcal{M}_2$, respectively, evaluated at a point $\boldsymbol{x}$, and by $\lambda_i^{(1)}, \lambda_i^{(2)}$ the corresponding eigenvalues. In a manifold product $\mathcal{M}_1 \times \mathcal{M}_2$, the eigenfunctions are equal to the pointwise product of the eigenfunctions of the LB operator of $\mathcal{M}_1, \mathcal{M}_2$, and the corresponding eigenvalues are equal to the sum of eigenvalues, such that

$$g_{l,k}(\boldsymbol{x}) = g_l^{(1)}(\pi_1(\boldsymbol{x})) \cdot g_k^{(2)}(\pi_2(\boldsymbol{x})) \qquad \lambda_{l,k} = \lambda_l^{(1)} + \lambda_k^{(2)}. \tag{4}$$

For simplicity, we denote by $\boldsymbol{v}_{l,k}$ the (l, k)-th eigenvector of the Laplacian matrix, as ordered by $\lambda_{l,k}$. An example of a product of 2 manifolds is illustrated in Figure 4b. The figure shows the leading eight eigenvectors of the graph Laplacian. The eigenvectors are indexed by the vector $\boldsymbol{b} = [l, k]$. The full details of this example will be provided in the next section.

4.3 Considerations for eigenvector selection in a product-of-manifold model

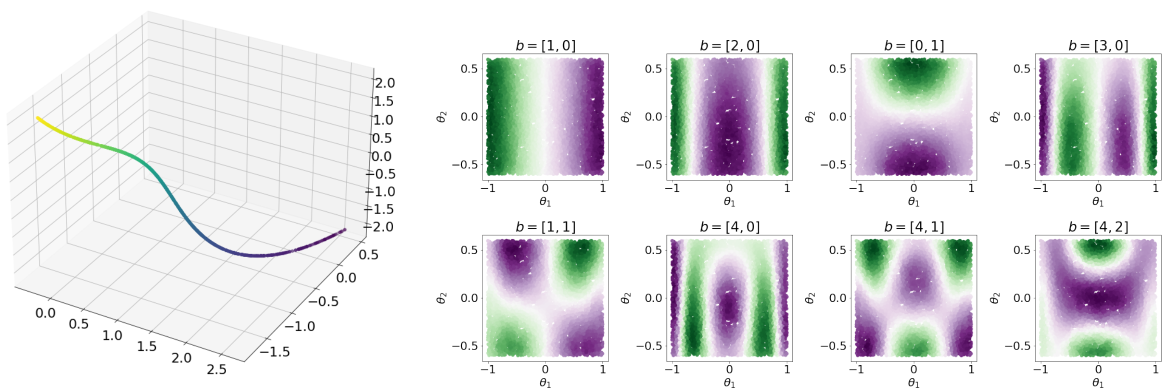
We analyze a setting where the p features can be partitioned into H sets according to their dependencies on a set of latent and independent random variables $\theta_1, \ldots, \theta_H$ with some bounded support. A feature $\boldsymbol{f}_m$



(a) Noisy MNIST: digits 3 and 8

(b) Convergence of eigenvectors for graph on an interval

Figure 3: Panel (a) shows a scatter plot of the noisy MNIST dataset, containing digits 3 and 8, where each image is located according to its coordinates in the third and fourth eigenvectors. Panel (b) shows the leading eigenvector of a graph computed over n points on a $1D$ interval and the leading eigenfunction $\cos(\pi x)$.



(a) Simulated data

(b) Eigenvectors of the simulated data

Figure 4: Panel (a) illustrates three features of a simulated dataset. Each feature is equal to a different polynomial of the same random latent variable θ_1. Each point in the 3D scatter plot is located according to the values of the three features and colored by the value of θ_1. Panel (b) shows the eigenvectors of the graph Laplacian matrix. Each point is located according to the value of (θ_1, θ_2) and colored by the value of its corresponding element in the eight leading eigenvectors. The eigenvectors are indexed by the vector b, whose elements b_i determine the eigenvector order in the submanifold $\mathcal{M}^{(i)}$.

that depends on θ_h consists of samples from a smooth transformation $\theta_h \xrightarrow{F_m} \boldsymbol{f}_m$. We denote by $X^{(h)}$ the submatrix that contains the features associated with θ_h. The smoothness of the transformations implies that the rows of $X^{(h)}$ constitute random samples from a manifold of intrinsic dimension 1.

Figure 4a shows a $3D$ scatter plot, where the axis are three such features with values generated by three polynomials of θ_1. The figure is an illustration of a manifold with a single intrinsic dimension embedded in a $3D$ space. The independence of the latent variables θ_h implies that the observations $\boldsymbol{x}_i \in \mathbb{R}^p$ are samples from a product of H manifolds, each of dimensionality 1 Zhang et al. (2021); He et al. (2023). The canonical projection $\pi^{(h)}(\boldsymbol{x})$ selects the features associated with the latent variable θ_h. According to the eigenfunctions properties in equation 4, the eigenfunctions are equal to the product of H eigenfunctions of the submanifolds $\mathcal{M}^{(h)}$, and can thus be indexed by a vector of size H, which we denote by $\boldsymbol{b} \in \mathbb{N}^H$.

$$g_{\boldsymbol{b}}(\boldsymbol{x}) = \prod_{h=1}^{H} g^{(h)}_{\boldsymbol{b}_h}\big(\pi^{(h)}(\boldsymbol{x})\big) \qquad \lambda_{\boldsymbol{b}} = \sum_{h=1}^{H} \lambda^{(h)}_{\boldsymbol{b}_h}.$$

Let $\boldsymbol{e}^{(h)}$ denote an index vector with elements $\boldsymbol{e}^{(h)}_j = 1$ if $j = h$ and 0 otherwise. The first eigenfunctions $g^{(h)}_0$ are equal to a constant for all submanifolds $\mathcal{M}^{(h)}$. Thus, The eigenfunctions $g_{\boldsymbol{e}^{(h)}}$ are equal to

$$g_{\boldsymbol{e}^{(h)}}(\boldsymbol{x}) = g^{(h)}_1\big(\pi^{(h)}(\boldsymbol{x})\big) \prod_{j \neq h}^{H} g^{(j)}_0\big(\pi^{(j)}(\boldsymbol{x})\big) = C g^{(h)}_1\big(\pi^{(h)}(\boldsymbol{x})\big), \tag{5}$$

where C is some constant. Importantly, the functions $g^{(h)}_1$ and thus $g_{\boldsymbol{e}^{(h)}}$, depend only on the parameter $\theta^{(h)}$. We define by $\mathcal{E}$ the family of vectors in $\mathbb{N}^H$ that include the indicator vectors $e^{(h)}$ or their integer products (e.g. $2e^{(h)}, 3e^{(h)}$ etc.). A similar derivation as in equation 5 shows that for every index vector $\boldsymbol{b} \in \mathcal{E}$, the eigenfunction $g_{\boldsymbol{b}}$ depends on only one of the latent variable in $\theta_1, \ldots, \theta_h$.

On the relevance of features for choosing eigenvectors as pseudo-labels. Our goal is to select a set of features that contains at least one (or more) features from each of the H partitions. Such a choice would ensure that the set contains information about all the H latent variables. Clearly, this imposes a requirement on the set of pseudo-label vectors: we would like at least one vector of pseudo-labels that is correlated with each latent variable.

It is instructive to consider the asymptotic case where $n \to \infty$ and hence according to Theorem 1 and the properties of manifold products, the eigenvectors $\boldsymbol{v}_b$ converge to $g_{\boldsymbol{b}}(\boldsymbol{X})$. A proper choice of eigenvectors for pseudo-labels would be the set $\{\boldsymbol{v}_{\boldsymbol{e}^{(h)}}\}_{h=1}^{H}$, as each of these vectors converges to the samples $g^{(h)}_1(\boldsymbol{X})$, and is thus associated with a different latent variable. However, there is no guarantee that these eigenvectors have the smallest eigenvalues.

Consider for example the case for the data illustrated in Figure 4a. Panel (c) shows the leading eight eigenvectors of the graph Laplacian. The leading two eigenvectors are functions of θ_1 and by choosing them we completely disregard θ_2 with an obvious impact on the feature selection accuracy. A better choice for pseudo-labels would be the first and third eigenvectors, indexed by $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$. Therefore, we need an improved criterion for selecting eigenvectors to serve as pseudolabels for the feature selection process. The following theorem, proven in Appendix A.1, implies that the feature vectors $\boldsymbol{f}_i$ are relevant for developing such a criterion.

Theorem 2 *We assume that the samples are generated according to our specified latent variable model and that assumptions (i)-(iii) are satisfied. Let $\boldsymbol{f}_i \in \mathbb{R}^n$ be a normalized, zero mean feature vector associated with parameter θ_h. Then,*

$$\boldsymbol{f}_i^T \boldsymbol{v}_b = \mathcal{O}(\epsilon_n) + \mathcal{O}\left(\sqrt{\frac{\log n}{n\epsilon_n^{d/2+1}}}\right) \qquad \forall \boldsymbol{b} \notin \mathcal{E}.$$

The theorem is proved via the following two steps. The details of the proof are provided in the appendix.

Step 1: We show that the inner product $\boldsymbol{f}_i^T g_{\boldsymbol{b}}(\boldsymbol{X})$ can be written as the inner product of two random vectors with independent elements. Thus, $\left|\boldsymbol{f}_i^T g_{\boldsymbol{b}}(\boldsymbol{X})\right|$ is of order $\mathcal{O}\Big(1/\sqrt{n}\Big)$ by standard concentration inequalities.

Step 2: Combine the convergence of $\boldsymbol{v}_{\boldsymbol{b}}$ to $g_{\boldsymbol{b}}(X)$ with the concentration result of step 1.

Theorem 2 implies that one can use the inner products to avoid selecting less informative eigenvectors that depend on more than one variable. Further guarantees, such as selection of a single vector from each variable, require additional assumptions on the feature values, which we do not make here.

In Algorithm 1 we compute the normalized measure of stability for the feature scores $\{s_m(h_i)\}_{m=1}^{p}$ obtained by the model h_i to predict the labels computed from the i-th eigenvector. When the model h_i is linear (or generalized linear), the score is strongly related to the simple inner product of Theorem 2. In that case, Theorem 2 indicates that the inner product between an uniformative eigenvectors and all features is close to zero. Thus, we expect the variance (after normalization) to be similar to the variance of random positive noise. The advantage of the stability measure over the simple linear product as an eigenvector selection criterion is that it allows for more flexibility in the choice of model.

5 Experiments

5.1 Evaluation on real world datasets

Data and experiment description. We applied SSFS to eight real-world datasets from various domains. Table 4 in Appendix C.1 gives the number of features, samples, and classes in each dataset. All datasets are available online [1].

We compare the performance of our approach to the following alternatives: (i) standard Laplacian score (LS) (He et al., 2005), (ii) Multi-Cluster Feature Selection (MCFS) (Cai et al., 2010), (iii) Nonnegative Discriminative Feature Selection (NDFS), (Li et al., 2012), (iv) Unsupervised Discriminative Feature Selection (UDFS) (Yang et al., 2011), (v) Laplacian Score-regularized Concrete Autoencoder (LS-CAE) (Shaham et al., 2022), (vi) Unsupervised Feature Selection Based on Iterative Similarity Graph Factorization and Clustering by Modularity (KNMFS) (Oliveira et al., 2022) and (vii) a naive baseline, where random selection is applied with a different seed for each number of selected features.

For evaluation, we adopt a criterion that is similar to, but not identical to, the one used in prior studies (Li et al., 2012; Wang et al., 2015). We select the top 2, 5, 10, 20, 30, 40, 50, 100, 150, 200, 250, and 300 features as scored by each method. Then, we apply k-means 20 times on the selected features and report the average clustering accuracy (along with the standard deviation), computed by (Cai et al., 2011):

$$\mathrm{ACC} = \max_{\pi} \frac{1}{N} \sum_{i=1}^{N} \delta(\pi(c_i), l_i),$$

where c_i and l_i are the assigned cluster and true label of the i-th data point, respectively, $\delta(x, y)$ is the delta function which equals one if $x = y$ and zero otherwise, and π represents a permutation of the cluster labels, optimized via the Kuhn-Munkres algorithm (Munkres, 1957).

Unlike the evaluation approach taken by Wang et al. (2015); Li et al. (2012), which entailed a grid search over hyper-parameters to report the optimum results for each method, our analysis employed the default hyper-parameters as specified by the respective implementations, including SSFS. This approach aims for a fair comparison to avoid favoring methods that are more sensitive to hyper-parameter adjustments. In addition, it acknowledges the practical constraints in unsupervised settings where hyper-parameter tuning is typically infeasible. Such differences in the approach to hyper-parameter selection could account for discrepancies between the results reported in previous studies and those in our study. See Appendix C for additional details.

Table 1 shows, for each method, the highest average accuracy and the number of features for which it was achieved similarly to (Li et al., 2012; Wang et al., 2015). Figure 5 presents a comparative analysis of clustering accuracy across various datasets and methods, considering the full spectrum of selected features. This comparison aims to account for the inherent variance in each method, addressing a limitation where the criterion of the maximum accuracy over the number of selected features might inadvertently favor methods exhibiting higher variance.

[1] `https://jundongl.github.io/scikit-feature/datasets.html`

Table 1: Average clustering accuracy on benchmark datasets along with the standard deviation. The number of selected features yielding the best clustering performance is shown in parentheses, the best result for each dataset highlighted in bold.

Dataset	Random	LS	MCFS	NDFS	UDFS	KNMFS	LS-CAE	SSFS
COIL20	65.1±2.1(250)	61.9±2.4(300)	67.4±3.3(300)	63.4±2.6(200)	61.9±3.5(300)	**68.1±2.0(300)**	64.2±3.1(30)	67.1±2.8(300)
GISETTE	70.2±0.1(150)	70.0±0.0(250)	70.7±0.0(5)	58.3±1.9(100)	69.1±0.1(50)	54.9±0.0(40)	**70.8±0.0(200)**	69.7±0.0(150)
Yale	47.8±3.5(250)	43.9±3.2(300)	44.4±2.9(300)	43.5±2.5(250)	43.8±2.3(50)	47.2±4.3(300)	46.2±1.6(10)	**50.3±2.3(100)**
TOX-171	44.2±1.8(250)	51.3±1.0(5)	44.5±0.5(5)	47.3±0.1(150)	40.2±3.8(250)	48.1±3.5(20)	50.1±5.3(200)	**59.4±2.5(100)**
ALLAML	73.2±1.7(300)	72.2±0.0(200)	75.0±0.0(150)	**76.6±0.7(2)**	66.4±1.3(50)	59.9±9.2(150)	63.9±0.0(2)	75.4±3.2(100)
Prostate-GE	63.0±0.7(30)	58.8±0.0(2)	61.8±0.0(100)	58.8±0.0(2)	63.6±0.3(50)	62.7±0.0(50)	63.7±0.0(40)	**75.9±0.5(10)**
ORL	58.9±1.8(300)	51.6±1.7(300)	57.0±2.8(300)	59.1±2.5(300)	57.3±2.4(300)	**63.2±2.0(150)**	61.0±2.0(300)	61.0±2.2(200)
ISOLET	59.5±1.8(300)	48.9±2.0(300)	50.7±1.5(300)	**63.1±2.4(200)**	44.6±1.7(300)	52.7±2.3(300)	63.0±2.6(300)	59.9±1.4(100)
Mean rank	4.12	5.88	4.62	4.94	6.44	4.38	3.31	**2.31**
Median rank	4.0	6.5	5.5	5.5	6.5	4.5	2.75	**2.25**

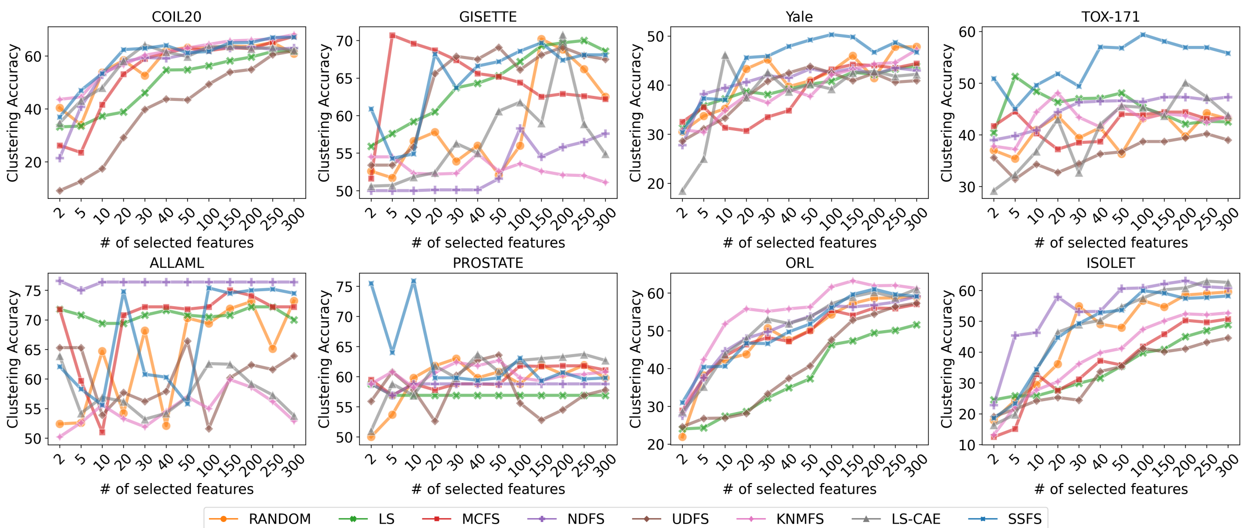


Figure 5: Clustering accuracy vs. the number of selected features on eight real-world datasets.

For SSFS, we use the following surrogate models: (i) The eigenvector selection model h_i is set to Logistic Regression with ℓ_2 regularization. We use scikit-learn's (Pedregosa et al., 2011) implementation with a default regularization value of $C = 1.0$. Feature scores are equal to the absolute value of the model's coefficients. (ii) The feature selection model f_i is set to XGBoost classifier with *Gain* feature importance. We use the popular implementation by DMLC (Chen and Guestrin, 2016).

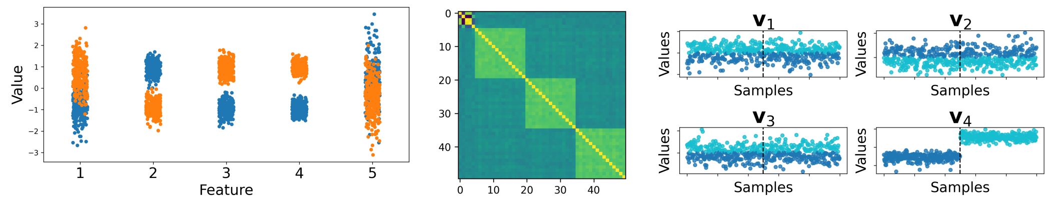
Note that we employ the default hyper-parameters for all surrogate models as provided in their widely used implementations. However, it's worth noting that one can undoubtedly leverage domain knowledge to select surrogate models and hyperparameters better suited to the specific domain. For each dataset, SSFS selects k from $d = 2k$ eigenvectors, where k is the number of distinct classes in the data.

Results. SSFS has been ranked as the best method in four out of eight datasets. It has shown a significant advantage over other competing methods, especially in the Yale, TOX-171, and Prostate-GE datasets. As discussed in Section 3.1, the Prostate-GE dataset has several outliers, and the fourth eigenvector plays a vital role in providing information about the class labels compared to the earlier eigenvectors. SSFS can effectively deal with such challenging scenarios, and this might explain its superior performance. Although our method is not ranked first in the other four datasets, it has produced results comparable to the leading method.

5.2 Ablation study

We demonstrate the importance of three SSFS components: (i) eigenvector selection, (ii) self-supervision with nonlinear surrogate models, and (iii) binarization of the Laplacian eigenvectors along with classifiers instead of regressors as surrogate models. The ablation study is performed on a synthetic dataset described in Section 5.2.1, and the eight real datasets used for evaluation in Section 5.1.

5.2.1 Synthetic data



(a) First 5 features (b) Covariance matrix (c) Eigenvectors

Figure 6: Visualizations of the synthetic data: Panel (a): scatter plot of the first five features corresponding to the Gaussian blobs, colored by the real label. Panel (b): the covariance matrix of the dataset. Panel (c): the top-4 eigenvectors, samples are sorted by the label and are partitioned by the vertical bar, colored according to the output of k-medoids.

Table 2: Ablation study: average clustering accuracy on benchmark datasets, the number of selected features is shown in parenthesis for the best clustering accuracy over the feature range.

Dataset	no selection	no XGBoost	no selection, regression	regression	SSFS
COIL20	65.0 (150)	62.1 (150)	**70.5 (100)**	69.0 (300)	67.1 (300)
GISETTE	**72.5 (10)**	64.9 (300)	64.6 (5)	64.6 (5)	69.7 (150)
Yale	48.6 (50)	42.7 (250)	49.8 (200)	47.4 (250)	**50.3 (100)**
TOX-171	50.9 (2)	45.6 (20)	45.0 (5)	45.5 (50)	**59.4 (100)**
ALLAML	**75.4 (100)**	66.7 (50)	71.1 (300)	71.1 (300)	**75.4 (100)**
Prostate-GE	59.8 (30)	69.6 (30)	61.8 (150)	61.8 (150)	**75.9 (10)**
ORL	60.0 (300)	56.8 (300)	58.5 (300)	58.5 (200)	**61.1 (200)**
ISOLET	57.0 (150)	57.1 (300)	**61.3 (300)**	58.7 (300)	59.9 (100)
Mean rank	2.94	4.0	3.0	3.5	**1.56**
Median rank	2.5	4.5	3.5	3.5	**1.25**

We generate a synthetic dataset as follows: the first five features are generated from two isotropic Gaussian blobs; these blobs define the clusters of interest. Additional 45 nuisance features are generated according to a multivariate Gaussian distribution, with zero mean and a block-structured covariance matrix $\mathbf{\Sigma}$, such that each block contains 15 features. The covariance elements $\mathbf{\Sigma}_{i,j}$ are equal to 0.5 if i, j are in the same block and to 0.01 otherwise. We generated a total of 500 samples; see Appendix B.1 for further details. In Figure 6a, you can see a scatter plot of the first five features, and in Figure 6b, you can see a visualization of the covariance matrix. Our goal is to identify the features that can distinguish between the two groups.

As Figure 6a demonstrates, the two clusters are linearly separated by three distinct features. Furthermore, examining Figure 6c reveals that while the fourth eigenvector distinctly separates the clusters, the higher-ranked eigenvectors do not exhibit this behavior. This pattern arises due to the correlated noise, significantly influencing the graph structure. The evaluation of this dataset is performed by calculating the true positive rate (TPR) with respect to the top-selected features and the discriminative features sampled from the two Gaussian blobs. The performance on the real-world datasets is measured similarly to Section 5.1.

5.2.2 Results

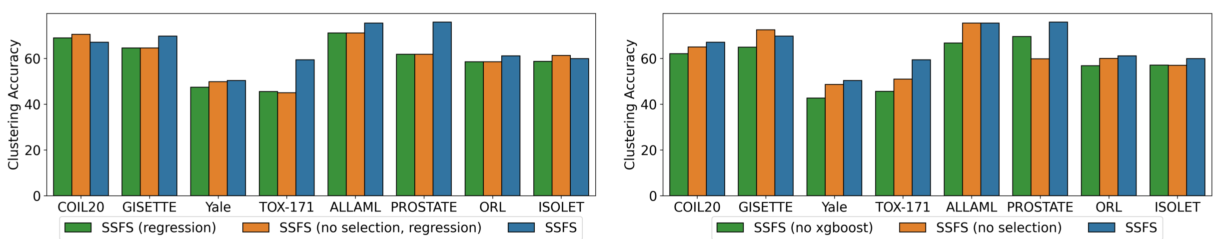
Eigenvector Selection. We compare to a variation of SSFS termed SSFS (no selection), where we don't filter the eigenvectors. We train the surrogate feature selector model on the leading k eigenvectors, with k set to the number of distinct classes in the data. Figure 7b, shows that our eigenvector selection scheme

Table 3: Synthetic data results: Top-3 selected features (sorted in descending order by rank), along with their TPR (relative to the first five features).

Method	Top-3 Features	TPR
SSFS	2, 9, 19	0.3
(no XGBoost)	4, 3, 2	1.0
(no selection)	43, 30, 49	0.0
(regression)	15, 17, 14	0.0
MCFS	47, 7, 43	0.0

provides an advantage in seven out of eight datasets. Similarly to Sec. 5.1, filtering the eigenvectors is especially advantageous on the Prostate-GE dataset, as our method successfully selects the most discriminative eigenvectors (see Figure 2a). On the synthetic dataset, the selection procedure provides a large advantage, as seen in Table 3. Figure 6c illustrates that the fourth eigenvector is the informative one with respect to the Gaussian blobs. Indeed, the fourth eigenvector and the third eigenvector are selected by the selection procedure. This eigenvector yields better features than MCFS and SSFS (no selection), which rely on the top two eigenvectors.

Classification and regression. We compare the following regression variants of SSFS , which use the original continuous eigenvectors as pseudo-labels (without binarization): (i) SSFS (regression): uses ridge regression for eigenvector selection and XGBoost regression for the feature selection as surrogate models. (ii) SSFS (no selection, regression): uses the top k eigenvectors without binarization and XGBoost regression. Figure 7a and Table 2 show that SSFS performs best on six of the eight real-world datasets. Interestingly, when using continuous regression as a surrogate model, the selection procedure does not seem to provide an advantage compared to no selection.



(a) Classification and regression

(b) Selection, and no XGBoost (logistic regression)

Figure 7: Ablation study results on the real-world datasets. The best clustering accuracy over the number of selected features is shown for each method.

Complex nonlinear models as surrogate models. We compare SSFS to a variant of our method denoted SSFS (no XGBoost), which employs a logistic regression instead of XGBoost as the surrogate feature selector model. Figure 7b shows that XGBoost provides an advantage compared to the linear model on real-world datasets. On the synthetic dataset, the linear variant provides better coverage for the top-3 features that separate the Gaussian blobs, compared to XGBoost (see Table 3 and Figure 6a). That is not surprising since, in this example, the cluster separation is linear in each informative feature. We note, however, that the top-ranked feature by SSFS with XGBoost is a discriminative feature for the clusters in the data (see Figure 6a); therefore, its selection can still be considered successful in the case of a single feature selection.

6 Discussion and future work

We proposed a simple procedure for filtering eigenvectors of the graph Laplacian and demonstrated that its application could have a significant impact on the outcome of the feature selection process. The selection is based on the stability of a classification model in predicting binary pseudo-labels. However, additional criteria, such as the accuracy of a specific model or the overlap of the chosen features for different eigenvectors, may provide information on the suitability of a specific vector for a feature selection task. We also illustrated the utility of expressive models, typically used for supervised learning, in unsupervised feature selection. Another direction for further research is using self-supervised approaches for *group feature selection* (GFS) for single modality (Sristi et al., 2022) or multi-modal data (Yang et al., 2023; Yoffe et al., 2024). In contrast to standard feature selection where the output is sparse, GFS aims to uncover groups of features with joint effects on the data. Learning models based on different eigenvectors may provide information about group effects with potential applications such as detecting brain networks in Neuroscience and gene pathways in genetics.

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A Product of manifold perspective.

A.1 Proof of Theorem 1.

As mentioned in the main text, the theorem is proven with the following two main steps:

Step 1: Prove that the inner product $\left|\boldsymbol{f}_i^T \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})\right|$ is of order $\mathcal{O}\Big(1/\sqrt{n}\Big)$ for all eigenfunctions $\boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})$ indexed by a vector $\boldsymbol{b} \notin \mathcal{E}$.

Step 2: Combine the result of step 1 with the convergence guarantees in Theorem 1 to bound the inner product $\boldsymbol{f}_i^T \boldsymbol{v}_{\boldsymbol{b}}$.

Step 1: According to our model, feature i is equal to a smooth transformation of a single latent variables. Assume w.l.o.g that the single variable is θ_1 such that $\boldsymbol{f}_i = F_i(\theta_1)$. By the product of manifold assumption, the eigenfunction $g_{\boldsymbol{b}}$ is equal to

$$\boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{x}) = \prod_{h=1}^{H} \boldsymbol{g}_{\boldsymbol{b}_h}(\pi^{(h)}(\boldsymbol{x})) = \boldsymbol{g}_{\boldsymbol{b}_1}(\pi^{(1)}(\boldsymbol{x})) \prod_{h=2}^{H} \boldsymbol{g}_{\boldsymbol{b}_h}(\pi^{(h)}(\boldsymbol{x})).$$

Let $\otimes$ denote the Hadamard product. We can write the inner product $\boldsymbol{f}_i^T \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})$ as,

$$\boldsymbol{f}_i^T \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X}) = \Big(\boldsymbol{f}_i \otimes g_{\boldsymbol{b}_1}(\pi^{(1)}(\boldsymbol{X}))\Big)^T \Big(\boldsymbol{g}_{\boldsymbol{b}_2}(\pi^{(2)}(\boldsymbol{X}))\otimes, \dots, \otimes \boldsymbol{g}_{\boldsymbol{b}_H}(\pi^{(H)}(\boldsymbol{X})). \tag{6}$$

The vectors $\boldsymbol{f}_i$ and $\boldsymbol{g}_{\boldsymbol{b}_1}(\pi^{(1)}(\boldsymbol{X}))$ both depend on θ_1 only. The vectors $\{\boldsymbol{g}_{\boldsymbol{b}_h}(\pi^{(h)}(\boldsymbol{X})\}_{h=2}^H$ depend, respectively, on $\theta_2, \dots, \theta_H$. We set

$$\boldsymbol{a}(\theta_1) = \boldsymbol{f}_i \otimes g_{\boldsymbol{b}_1}(\pi^{(1)}(\boldsymbol{X})) \qquad \boldsymbol{d}(\theta_2, \dots, \theta_H) = \boldsymbol{g}_{\boldsymbol{b}_2}(\pi^{(2)}(\boldsymbol{X}))\otimes, \dots, \otimes \boldsymbol{g}_{\boldsymbol{b}_H}(\pi^{(H)}(\boldsymbol{X})).$$

The elements of the random vectors $\boldsymbol{a}(\theta_1)$ and $\boldsymbol{d}(\theta_2, \dots, \theta_H)$ are statistically independent. In addition, we have that $\|\boldsymbol{f}_i\| = 1$ and

$$\|\boldsymbol{g}_h(\pi^{(h)}(\boldsymbol{X}))\| = 1 + o(1) \qquad \forall(h),$$

see for example (Cheng and Wu, 2022, Lemma 3.4). This implies that both $\boldsymbol{a}(\theta_1)$ and $\boldsymbol{d}(\theta_2, \dots, \theta_H)$ are bounded by $1 + o(1)$. The inner product between two independent random vectors with unit norm and iid elements is of order $\mathcal{O}(1/\sqrt{n})$, (see for example (Vershynin, 2020, Remark 3.2.5)). Thus,

$$|\boldsymbol{f}_i^T \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})| = |\boldsymbol{a}(\theta_1)^T \boldsymbol{d}(\theta_2, \dots, \theta_H)| = \mathcal{O}(1/\sqrt{n}).$$

Step 2: By the triangle inequality,

$$|\boldsymbol{f}_i^T \boldsymbol{v}_{\boldsymbol{b}}| = |\boldsymbol{f}_i^T(\boldsymbol{v}_{\boldsymbol{b}} - \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X}) + \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X}))| \le |\boldsymbol{f}_i^T(\boldsymbol{v}_{\boldsymbol{b}} - \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X}))| + |\boldsymbol{f}_i^T \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})|. \tag{7}$$

The first term on the right-hand side of equation 7 can be bounded by the Cauchy-Schwartz inequality and Theorem 1 via:

$$|\boldsymbol{f}_i^T(\boldsymbol{v}_{\boldsymbol{b}} - \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X}))| \le \|\boldsymbol{f}_i^T\| \|\boldsymbol{v}_{\boldsymbol{b}} - \boldsymbol{g}_{\boldsymbol{b}}(\boldsymbol{X})\| = \mathcal{O}(\epsilon_n) + \mathcal{O}\Bigg(\sqrt{\frac{\log n}{n\epsilon_n^{d/2+1}}}\Bigg). \tag{8}$$

The second term is bounded by step 1. Since the term in equation 8 dominates $\mathcal{O}(1/\sqrt{n})$ for any ϵ_n, this concludes the proof.

B Ablation study

B.1 Synthetic data generation

For the synthetic data, we generated 500 samples, where we used the `make_blobs` function from scikit-learn to generate the first five features, with arguments `cluster_std=1`, `centers=2`.

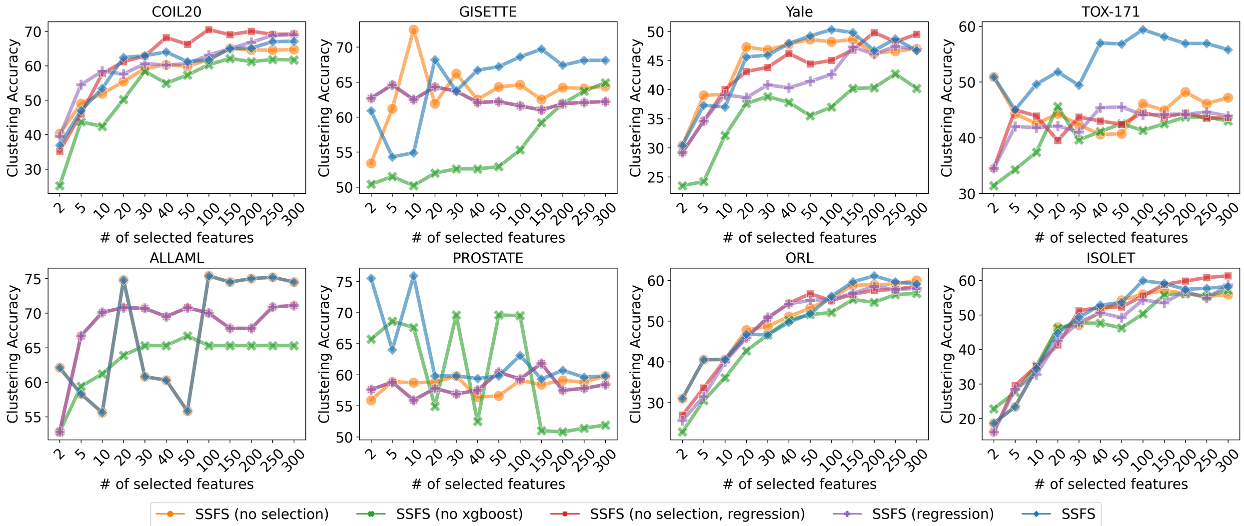

Figure 8: Ablation study: Clustering accuracy on real-world datasets

B.2 Detailed Experimental Results

In this section, we provide more detailed results of the ablation study. Figure 8 contains comparative analysis in terms of the performance for the whole selected feature range,

C Additional Experimental Details

C.1 Datasets

Table 4 provides information about the real-world datasets used in the experiments.

Table 4: Real-world datasets description.

Dataset	Samples	Dim	Classes	Domain
COIL20	1440	1024	20	Image
ORL	400	1024	40	Image
Yale	165	1024	15	Bio
ALLAML	72	7129	2	Bio
Prostate-GE	102	5966	2	Bio
TOX 171	171	5748	4	Bio
Isolet	1560	617	26	Speech
GISETTE	7000	5000	2	Image

For all datasets, the features are z-score normalized to have zero mean and unit variance.

C.2 Hyperparameters

For SSFS, we use the same hyperparameters, as follows:

- Number of eigenvectors to select k is set to the distinct number of classes in the specific dataset, they are selected from a total of $d = 2k$ eigenvectors.
- Size of each subsample is 95% of the original dataset.
- 500 resamples are performed in every dataset.

- For the affinity matrix, we used a Gaussian kernel with an adaptive scale $\sigma_i\sigma_j$ such that σ_i is the distance to the $k = 2$ neighbor of $\boldsymbol{x}_i$.

The Laplacian we used was the symmetric normalized Laplacian.

In the ablation study, for regression, we use scikit-learn ridge regression (for eigenvector selection) and DMLC XGBoost regressor (for the final feature scoring) with their default hyperparameters.

For all of the baseline methods, we used the default hyperparameters. So, for all methods, including SSFS, the hyperparameters are fixed for all datasets (excluding parameters that correspond to the number of features to select and the number of clusters).

For LS, MCFS, UDFS, and NDFS, we used an implementation from the scikit-feature library [2] and inputted the same similarity matrices as SSFS for the methods which accepted such an argument. We fixed a bug in MCFS implementation to choose by the max of the absolute value of the coefficients instead of the max of the coefficients (this improved MCFS performance). For LS-CAE, we used an implementation from [3]. For KNMFS, we used an implementation from [4].

[2]https://github.com/jundongl/scikit-feature
[3]https://github.com/jsvir/lscae
[4]https://github.com/marcosd3souza/KNMFS