A Novel Approach for Intrinsic Dimension Estimation via Ritz Values and Orthogonal Polynomials

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Abstract

The real-life data have a complex and non-linear structure due to their nature. These non-linearities and large number of features can usually cause problems such as the empty-space phenomenon and the well-known curse of dimensionality. Finding the nearly optimal representation of the dataset in a lower-dimensional space (i.e. dimensionality reduction) offers an applicable mechanism for improving the success of machine learning tasks. However, estimating the required data dimension for the nearly optimal representation (intrinsic dimension) can be very costly, particularly if one deals with big data. We propose a highly efficient and robust intrinsic dimension estimation approach that only relies on matrix-vector products for dimensionality reduction methods. An experimental study is also conducted to compare the performance of proposed method with state of the art approaches.

Keywords: Dimensionality Reduction, Intrinsic Dimension Estimation, Chebyshev Approximations, Machine Learning

1 Introduction

Dimensionality reduction approaches are crucial in various applications of machine learning tasks such as computer vision, robotics, natural language processing, medical diagnosis, recommendation systems or industrial IoT applications such as predictive maintenance which need to generate and process large amounts of data and variables. In general, dimensionality reduction improves the performance of machine learning tasks' by removing redundant features. In this regard, both linear and non-linear dimensionality reduction methods, specifically the manifold learning techniques are particularly efficient since they are based on the preservation of the geometric structure of the original feature space. In this manner, there are several approaches already available and studied extensively in the literature such as principal component analysis (PCA), Multidimensional scaling (MDS), Laplacian Eigenmaps (LE) and other. We refer the reader to (Lee and Verleysen, 2007) for a comprehensive survey of the available methods. However, it is well-known that these methods have two computational bottlenecks: i)construction of the variance (PCA), distance (MDS), or neighborhood (graph-embedding based techniques such as LE) matrices; ii)calculation of the solution of ordinary or generalized eigenvalue problems.

Due to these two bottlenecks, most of the dimensionality reduction methods are not scalable in terms of the problem size due to the rapid explosion of data at several domains and therefore they are not applicable for big data problems in a plain form (McQueen et al, 2016). Nevertheless, there are variety of approaches already available in the literature to speed-up the methods especially in high-performance computing platforms (Yano et al, 2021). Another way to improve the efficiency of these methods is to use a predetermined intrinsic dimension while solving the eigenvalue problem arising from the optimization problem that occurs during the dimensionality reduction. In the literature, one can find well-established, very efficient and accurate eigensolvers (Hernandez et al, 2005; Polizzi, 2009; Sameh and Wisniewski, 1982). Especially Krylov subspace based eigensolvers offer a fast convergence rate for finding the eigenpairs in a given interval. Intrinsic dimension estimators can exploit the advantages of Krylov subspace based methods, as proposed in this paper, to create an efficient approach for the determination of a nearly-optimal reduction order.

We propose a novel approach for estimating the intrinsic dimension of a given dataset. We employed several numerical techniques in the proposed method to avoid the expensive eigenvalue computations, which is the main bottleneck of most well-known intrinsic dimension estimation methods. In the proposed method, we applied several different algorithms in coherence, such as Conjugate Gradient and trace estimation. The main novelty of this approach is to construct the estimation of the intrinsic dimensionality problem only via matrix-vector products. In that way, the problem can easily be handled in large dimensions at high-performance computing systems since many existing state-of-the-art algorithms exist for the parallel matrix-vector multiplications.

The rest of the paper is organized as follows. In Section 2, we will briefly discuss the existing methods. In Section 3, we will present the mathematical tools we have employed to develop the proposed method and the details of the proposed method. We demonstrated the numerical results for a toy and artificially generated large data in Section 4. Finally, in Section 5, we present the conclusions.

2 Related Work

The existing intrinsic dimension (ID) estimators can be grouped into three categories: i) topological, ii) graph-based, and iii) projective methods (Campadelli et al, 2015). These methods have several advantages (such as high accurate estimation capability of topological estimators) discussed in this section. However, projective methods can be considered better in terms of computational complexity if an efficient eigensolver is implemented. In this paper, we propose an approach to improve its computational complexity by avoiding the eigendecomposition. Since our proposed method is related to projective methods, they will in detail as well. We will also briefly introduce the other techniques for comparison.

2.1 *Topological Estimators*

Topological estimators assume that the data has a shape of a lower-dimensional manifold $\mathcal{M} \in \mathcal{R}^d$ embedded in a higher dimensional space $\mathcal{R}^D$ through a locally smooth map $\phi : \mathcal{M} \to \mathcal{R}^D$ and accept the ID of the data as the topological dimension of the manifold.

Definition 1*(open cover)* Given a topological space $\mathcal{X}$ and a subset $\mathcal{Y} \subseteq \mathcal{X}$, a collection of open sets $\mathcal{U} = \cup_{i \in I} U_i$ is called an open cover of $\mathcal{Y}$ if $\mathcal{Y} \subseteq \mathcal{U}$ where I and U_i are an index set and an open set respectively.

Definition 2*(refinement of a cover)* A cover $\mathcal{U}' = \cup_{i \in I} U_i'$ is a refinement of a cover $\mathcal{U} = \cup_{i \in I} U_i$ if $\forall U_{\in \mathcal{U}'}' \exists U_{\in \mathcal{U}}$ such that $U' \subseteq U$.

Definition 3*(Topological Dimension as known as Lebesgue Covering Dimension)* The topological dimension of a topological space $\mathcal{X}$ is the smallest integer d if every finite covering $\mathcal{U}$ of $\mathcal{X}$ has a refinement $\mathcal{U}'$ such that no subset of $\mathcal{X}$ has more than $d+1$ intersecting open sets in $\mathcal{U}'$. If no minimal integer exists, $\mathcal{X}$ is said to have infinite topological dimension.

In (Li et al, 2009), a method for estimating the ID of the data is proposed by assuming that the data has the shape of a manifold in a lower dimension and the ID is accepted as the topological dimension of that manifold. However, as the authors pointed out, the proposed approach requires that the data set is well-sampled on a smooth manifold. Therefore, is not applicable for a noisy data set.

Since the topological dimension is practically inestimable, other alternatives have also been proposed. They can be categorized under two headings, *fractal*, and *nearest-neighbors-based* id estimators.

2.1.1 *Fractal Estimators*

In fractal ID estimators, it is assumed that $\mathcal{M}$ has somehow fractal structure, and ID is estimated by employing fractal dimension estimation. They are based on the idea that the volume of d dimensional set scales with its size r as r^d. So to estimate the fractal dimension, the number of neighborhoods in a radius r is counted, and its rate of growth based on r is computed. For d dimensional fractal, the rate of growth is r^d. Correlation Dimension (CD) Estimation (Grassberger and Procaccia, 1983) is a well-known example for *fractal-based* ID estimators.

Definition 4 *(Correlation Dimension)*
Let X_N be a finite sample set, $\|\cdot\|$ be the Euclidean norm and $I(\cdot)$ be the step function with the property $I(y) = 0$ if y<0, and $I(y) = 1$ otherwise. Then,

$$C(n, r) = \frac{2}{n(n-1)} \sum_{i=1}^{n} \sum_{j=i+1}^{n} I(r - \|x_i - x_j\|)$$

is defined as the correlation integral. It computes the probability of the distance between two points randomly selected from the set being less than or equal to r. And CD is given as

$$\lim_{r \to 0} \lim_{n \to \infty} \frac{\log C(n, r)}{\log r}.$$

In practical implementations, CD estimation finds an ID approximation by evaluating $C(n, r)$ with different r_i values and solving a linear least squares problem to the computed data points ($\log r_i$, $\log C(n, r_i)$). It should be noted that for a correct estimation, the number of data points must be very large (Valle and Oganov, 2010).

2.1.2 *Nearest-Neighbors-Based Estimators*

Nearest-Neighbors-Based ID Estimators approximate the ID by the distributions of data neighbors. One of the most cited example is Maximum Likelihood Estimator (MLE) which uses Poisson process approximation for the ID estimation and has $O(N^2 D)$ time complexity (Levina and Bickel, 2004). It estimates the local intrinsic dimension of x_i as

$$\hat{d}(x_i, k) = \left(\frac{1}{k} \sum_{j=1}^{k} \log \frac{T_{k+1}(x_i)}{T_j(x_i)} \right)^{-1}$$

where $T_j(x_i)$ is the distance between x_i and its jth nearest neighbor. To estimate global ID, the average of $\hat{d}(x_i, k)$ values for all data points should be considered as $\hat{d}(k) = \frac{1}{N}\sum_{i=1}^{N}\hat{d}(x_i, k)$.

A recent ID estimator based on MLE techniques is TLE (Amsaleg et al, 2019). Based on a new extreme-value theoretic analysis, the estimator employs MLE methods over all known pairwise distances among the sample participants. Also, an ID estimator recently proposed based on Methods of Moments(MOM) (Amsaleg et al, 2018).

Another proposed *Nearest-Neighbors-Based ID Estimator* is Manifold-Adaptive Dimension Estimation (MADA) (Farahmand et al, 2007) in which first the local ID's around data points are estimated by nearest neighbors techniques, and these are combined.

ESS ID estimator which estimates the ID based on the expected simplex skewness measure having $O(N^{d+1}D(d+1)^2)$ time complexity is another type of *Nearest-Neighbors-Based Estimators* (Johnsson et al, 2015).

A family of ID estimators using a similar approach is the Minimum Neighbor Distance—Maximum Likelihood (MiND$_{ML*}$) estimators which utilize a maximum likelihood method on the probability density function pertaining to the normalized nearest neighbor distances (Rozza et al, 2012). Let $p(x_i)$ be the ratio of the distance between x_i and its nearest neighbor and the distance between x_i and its $(k+1)^{th}$ nearest neighbor then $ll(d)$ can be defined as

$$ll(d) = \sum_{x_i \in X_N} \log g(x_i; \; k, d)$$

$$= N\log k + N\log d + (d-1)\sum_{x_i \in X_N}\log p(x_i) + (k-1)\sum_{x_i \in X_N}\log(1 - p^d(x_i)).$$

In MiND$_{MLi}$(integer variant of MiND$_{ML*}$), ID is estimated by $\hat{d} = \underset{d \in \{1..D\}}{\mathrm{argmax}}\, ll(d)$ with time complexity $O(N^2D^2)$ (Rozza et al, 2012).

For a real number ID approximation, they also propose MiND$_{MLk}$ which finds the maximum value of $ll(d)$ in $[1, D]$. It looks for the solution of $\frac{\partial ll}{\partial d} = 0$,

$$\frac{N}{d} + \sum_{x_i \in X_N}\left(\log p(x_i) - (k-1)\frac{p^d(x_i)\log p(x_i)}{1 - p^d(x_i)}\right) = 0$$

and

$$\hat{d} = \underset{0 < d \leq D}{\mathrm{argmax}}\, ll(d).$$

The time complexity of MiND$_{MLk}$ is $O(N^2D^2)$ (Rozza et al, 2012) and it should be noted that for $k = 1$ it is same as MLE.

Also in the same study, they propose MiND_{KL} estimator which also has $O(N^2D^2)$ time complexity and estimates ID as

$$\hat{d} = \underset{d\in\{1..D\}}{\text{argmin}} \left(\log\frac{N}{N-1} + \frac{1}{N}\sum_{i=1}^{N}\log\frac{\check{p}(\hat{r}_i)}{\hat{p}_d(\hat{r}_i)} \right)$$

where $\check{p}_d(\hat{r}_i)$ are the distances between $\hat{r}_i$ and its first neighbor in $\hat{r}$ and in $\check{r}_d$, respectively, in which $\hat{r} = \{\hat{r}_i\}_{i=1}^{N} = \{p(x_i)\}_{i=1}^{N}$, $\hat{p}(r) = \frac{N-1}{2p(r)}$ $p(r)$ is the distance between r and its nearest neighbor.

A more advanced ID estimator DANCo (Ceruti et al, 2014) has been proposed which is motivated by MiND_{KL} and has $O(N\log(N)D^2)$ time complexity. DANCo exploits angle and norm concentrations and estimates ID as

$$\hat{d} = \underset{d\in\{1..D\}}{\text{argmin}} \mathcal{KL}(g_{Data}, g_{Sphere}^d) + \mathcal{KL}(q_{Data}, q_{Sphere}^d)$$

where $\mathcal{KL}$ is Kullback–Leibler divergence operator, $g(r;\ k,d) = kdr^{d-1}(1-r^d)^{k-1}$, and $q(x;\ v,t)$ is the von Mises-Fisher distribution. Also in the same study, authors propose FastDANCo ID estimator which has $O(N\log(N)D)$ time complexity by performing some relaxations on DANCo (Ceruti et al, 2014).

A recently proposed ID estimator is TwoNN which computes the ID based on only two nearest neighbors of the data points (Facco et al, 2017). Let μ be the ratio of the distance between x_i and its second nearest neighbor and the distance between x_i and its nearest neighbor and $F(\mu) = (1 - \mu^{-d})1_{[1,+\infty]}(\mu)$, then ID can be estimated as

$$\hat{d} = \frac{\log(1-F(\mu))}{\log(\mu)}.$$

2.2 *Graph-Based Estimators*

Graph-based ID estimation approaches have some advantages, as they usually have lower computational complexity and due to the availability of theoretical tools in literature (Brito et al, 2013).

Examples of such estimators rely on different graph-theoretic structures such as, the ID estimators proposed in (Brito et al, 2013) and (Friedman and Rafsky, 1983) are based on k-sphere of influence graph and minimum spanning tree respectively.

In (Costa and Hero, 2006), the authors proposed an estimator based on nearest neighbors information. Hereinafter, it will be referred to as kNNG. In which $kNNG(X_N)$ is k-nn graph of X_N, $MST(X_N)$ is the minimum spanning tree of $kNNG(X_N)$, $\mathcal{L}(MST(X_N)) = \sum \|e_{i,j}\|^{\gamma}, \gamma \in (0,d)$, $\log(\mathcal{L}(MST(X_N)) = a\log(d)+b, a = \frac{d-\gamma}{d}$. To estimate d a set of cardinalities $\{n_k\}_{k=1}^{K}$ is chosen, and set of $(\log\mathcal{L}(MST(X_{n_k})), n_k)$ is computed. Then, the least squares method is performed on that set to find $\hat{a} \approx$ a. Finally, ID is approximated as round$\{\gamma/(1-\hat{a})\}$.

2.3 *Projective Estimators*

Projective ID estimation methods search for the best subspace which has minimum projection error to project the data (Camastra and Staiano, 2016). Here it should be noted that, their initial design purpose was dimensionality reduction. However, with some modifications, they can also be used for ID estimation. Most of them can be categorized into two types of techniques, Multidimensional Scaling(MDS) and PCA (Campadelli et al, 2015).

MDS methods are projection techniques that have the objective of preserving the pairwise distances of the data (Cox and Cox, 2008). Some known examples are Bennett's algorithm (Bennett, 1969), Sammon's mapping (Sammon, 1969), Curvilinear Component Analysis (CCA) (Demartines and Herault, 1997), Local Linear Embedding (LLE) (Roweis and Saul, 2000).

Due to the its variance-oriented reduction mechanism, PCA (Jolliffe, 1986) can be considered as a very favorable technique for the ID estimation. It aims to re-express the data with new bases, a combination of original ones, in a way that re-expressed data has maximum variance and minimum covariance. To perform that re-expression, data matrix $X \in \mathcal{R}^{NxD}$ is multiplied with orthonormal *principal component matrix* $\mathcal{P}$ whose columns are named as principal components. And these principal components are the eigenvectors of the *covariance matrix* $\mathcal{C} = \frac{1}{N-1}X_C^T X_C$ where X_C is the centered version of X. Namely, $X_C = X - \text{mean}(X)$.

In PCA, associated eigenvalues of eigenvectors give some information about the importance of the eigenvector in the basis change process. Namely, the greater the eigenvalue, the more information of the data in the direction of the associated eigenvector. Therefore, eigenvalues of the *covariance matrix* are used to estimate ID using PCA. The main idea is to eliminate relatively less important eigenvectors and keep the dominant ones. To do that a threshold $0 < \theta < 1$ or $\alpha \gg 1$ is determined, and ID is approximated as either based on the ratio of total variance:

$$d = \underset{k}{\text{argmin}} \left\{ \frac{\sum_{i=1}^{k} \lambda_i}{\sum_{i=1}^{D} \lambda_i} \geq \theta \right\}$$

or either based on the ratio between consecutive variances:

$$d = \underset{k}{\text{argmin}} \left\{ \frac{\lambda_k}{\lambda_{k+1}} \geq \alpha \right\}$$

where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_D \geq 0$ are the eigenvalues of $\mathcal{C}$.

PCA works well for linear data; different approaches have been proposed to extend it to non-linear data. One of them is Local PCA (LPCA), which suggests that firstly data should be separated into sub-regions, later PCA should be applied to each region separately. Then, the ID of the data can be determined by combining estimated sub-region's IDs (Fukunaga and Olsen, 1971).

Based on the Local PCA idea, another PCA-based ID estimator has been proposed in (Fan et al, 2013), in which an approximate minimal set cover algorithm and PCA applied locally to each subset of the cover. Also, in the same study, they proposed a noise filtering approach for PCA.

Another proposed alternative for nonlinear extension is called Kernel PCA (KPCA) (Schölkopf et al, 1998). KPCA tries to adapt PCA to a non-linear form by using a kernel function in the construction of covariance matrix.

One of the recent ID estimators in literature is the Fisher Separability algorithm (FSH) (Albergante et al, 2019), which estimates the ID of the data based on separability properties. At the beginning of the algorithm, the data is projected into the linear subspace spanned by the first k principal components where k is determined by $k = max\{i : \lambda_1/\lambda_i < C\}$ with C being a constant.

3 Methodology

In PCA based methods, two essential steps are the construction of a covariance matrix and its eigen-decomposition. These two steps become more and more costly as the dimension of the data increases. Therefore, in our proposed method, we aim to estimate the ID of the data by avoiding these steps. Instead of computing the eigen-decomposition of a covariance matrix, we approximate the eigenvalue distribution of it without constructing it.

The proposed approach can be divided into three main building blocks: a) estimation of the trace of the covariance matrix, which is equal to the summation of its eigenvalues, b) construction of the eigenvalue search intervals, c) estimation of the number of eigenvalues in the intervals to approximate the distribution of eigenvalues and estimate ID.

3.1 Trace Estimation of Covariance Matrix

For a *symmetric positive semi-definite* matrix $\mathcal{A} \in \mathcal{R}^{nxn}$, and the vector z whose components are *Rademacher random variables*, equal to $+1$ or -1 with equal probability, the trace can computed as (Hutchinson, 1989)

$$tr(\mathcal{A}) = E[z^T \mathcal{A} z], \ z \sim^{iid} \{-1,1\}^n \tag{1}$$

where idd is the abbreviation for Independent and Identically Distributed.

Hence, the trace can be approximated by averaging over some random samples

$$tr(\mathcal{A}) \approx \frac{1}{n_v} \sum_{k=1}^{n_v} z_k^T \mathcal{A} z_k.$$

But we have the data matrix $X \in \mathcal{R}^{NxD}$ and its centered version X_C, and require the trace of $\mathcal{C} = \frac{1}{N-1} X_C^T X_C$.

$$tr(\mathcal{C}) \approx \frac{1}{n_v} \sum_{k=1}^{n_v} z_k^T \mathcal{C} z_k$$

$$tr(\mathcal{C}) \approx \frac{1}{n_v} \sum_{k=1}^{n_v} z_k^T \frac{X_C^T X_C}{N-1} z_k$$

$$tr(\mathcal{C}) \approx \frac{1}{N-1} \left(\frac{1}{n_v} \sum_{k=1}^{n_v} z_k^T X_C^T X_C z_k \right)$$

$$tr(\mathcal{C}) \approx \frac{1}{N-1} \left(\frac{1}{n_v} \sum_{k=1}^{n_v} (X_C z_k)^T X_C z_k \right)$$

$$tr(\mathcal{C}) \approx \frac{1}{N-1} \left(\frac{1}{n_v} \sum_{k=1}^{n_v} h_k^T h_k \right) \tag{2}$$

where $h_k = X_C z_k$.

Optimizing the number of random vectors would be crucial for the algorithm's efficiency. For that, a statistical formula $n_v(\epsilon, \delta) = \frac{2(2+\frac{8\sqrt{2}}{3}\epsilon)\log(\frac{2}{\delta})}{\epsilon^2}$ proposed in (Skorski, 2021), gives the number of random vectors that guarantees less than ϵ relative error with $1 - \delta$ probability where $0 < \delta < 1$. Fig.(1) represents the change of the number of random vectors with respect to the parameters ϵ and δ.
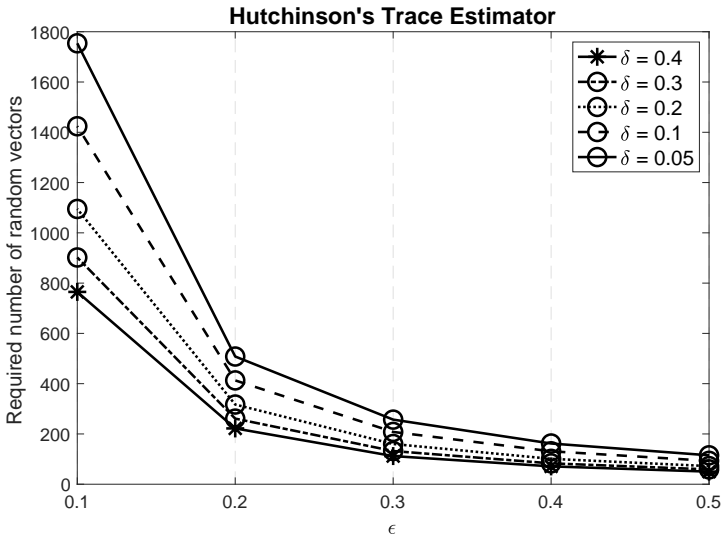

Fig. 1: Required random vector counts based on different ϵ and δ values where ϵ is the worst case relative error which is guaranteed with a probability of 1-δ

3.2 Detection of Eigenvalue Search Intervals

Although the trace estimation technique explained in the previous section can be used as an efficient tool for the estimation of the total variance of the

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Algorithm 1 Covariance Trace Estimator

    Inputs: X_C, ϵ, δ
    Output: τ
1:   $n_v \leftarrow \frac{2(2+\frac{8\sqrt{2}}{3}\epsilon)\log(\frac{2}{\delta})}{\epsilon^2}$
2:   $sum = 0$
3:   **for** k=1:n_v **do**
4:      z_k is constructed randomly using Eq. (1)
5:      $h_k = X_C z_k$
6:      $sum = sum + h_k^T h_k$
7:   **end for**
8:   $\tau = sum/(n_v(N-1))$

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data, the distribution of the eigenvalues of the covariance matrix should be also estimated efficiently. We employed a variant of Conjugate Gradient (CG) algorithm. Although the original CG algorithm is proposed by Hestenes and Steifel in 1952 (Hestenes and Stiefel, 1952), there are many recent studies in literature to improve its scalability and robustness for exascale computing platforms (Cools et al, 2018; Agullo et al, 2020; Greenbaum et al, 2021).

The Ritz values obtained from the CG algorithm are identical to the eigenvalues of the input matrix in exact arithmetic due to the similarity of the matrices (Scales, 1989). Therefore, we utilize the Ritz values that are obtained from Conjugate Gradient Least Square (CGLS) algorithm, which is an extension of CG algorithm for over-determined linear systems and solves $X_C^T X_C x = X_C^T b$ by performing the matrix-vector multiplication with the coefficient matrix, $X_C^T X_C$, implicitly. Hence, the Ritz values obtained from CGLS algorithm are same as the eigenvalues of $X_C^T X_C$ in exact arithmetic after D iterations.

Since we require the eigenvalues of the *covariance matrix*, $\mathcal{C} = \frac{X_C^T X_C}{N-1}$, we should run CGLS algorithm with X_C matrix, and divide the estimated eigenvalues by $N-1$. Here, the right hand side vector b is set to $b = X_C\mathbf{1}/\|X_C\mathbf{1}\|_2$ and $x_0 = \mathbf{0}$ where $\mathbf{1}$ and $\mathbf{0}$ are vectors of all ones and zeros, respectively. Note that if the target problem is arising from a regression problem, the output vector can be used as the right hand side vector and the approximate solution can also be used as an initial guess. Also notice that we only require the α and β values from the Alg.(2); therefore, we can skip the computations of x_is.

Our goal is neither to find all eigenvalues of the *covariance matrix* nor to solve the least squares problem; instead, we want to approximate a few Ritz values to construct our eigenvalue search intervals; therefore, we iterate the CGLS only a few times and obtain a few required Ritz values. At this point, it should be noted that in a few iterations, the Ritz values firstly converge to the extreme, maximal and minimal, eigenvalues (Demmel, 1997). We confirm and illustrate this by obtaining the Ritz values at first 10 iterations from the CGLS algorithm applied to the toy problem given in Section 4.1 as illustrated in Fig.(2).

Algorithm 2 Conjugate Gradient Least Squares

Input: X_C, b, x_0, $maxiter$
Output: x^*

1: $r_0 = b - X_C x_0$
2: $s_0 = X_C^T r_0$
3: $p_0 = s_0$
4: $\gamma_0 = \|s_0\|_2^2$
5: **for** i=0:$maxiter$ **do**
6:      $q_i = X_C p_i$
7:      $\alpha_i = \gamma_i / \|q_i\|_2^2$
8:      $x_{i+1} = x_i + \alpha_i p_i$
9:      $r_{i+1} = r_i - \alpha_i q_i$
10:      $s_{i+1} = X_C^T r_{i+1}$
11:      $\gamma_{i+1} = \|s_{i+1}\|_2^2$
12:      $\beta_i = \gamma_{i+1} / \gamma_i$
13:      $p_{i+1} = s_{i+1} + \beta_i p_i$
14: **end for**
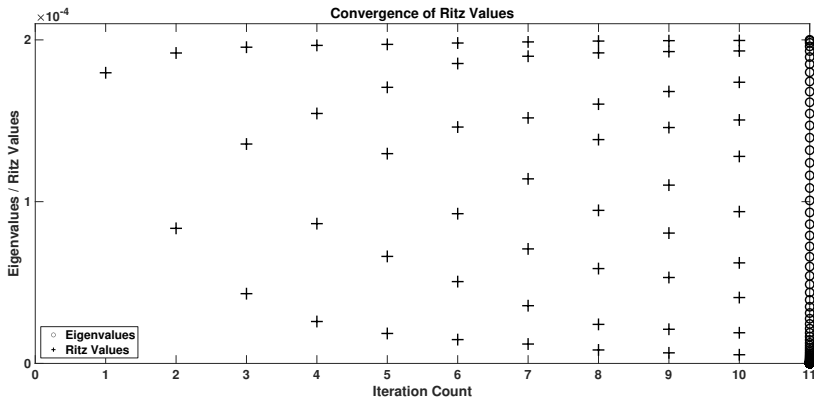15: $x^* = x_{maxiter}$

Fig. 2: The CGLS Algorithm is applied to the toy problem given in Section 4.1. The Eigenvalues / Ritz Values obtained after each iteration are given, and on the rightmost edge of the figure the exact eigenvalues of the covariance matrix are shown

3.3 Estimation of Eigenvalue Counts in an Intervals

Knowing the approximate number of the eigenvalues in a given interval can be very useful for load balancing, especially for large-scale eigenvalue calculations in parallel environments. It can also be beneficial to estimate the overall eigenvalue distribution of the covariance matrix. In this study, we will employ Chebyshev polynomial-based approaches for the approximate number of the eigenvalues in a specific interval determined by the few Ritz values of the

covariance matrix to estimate the intrinsic dimension without constructing and solving the corresponding eigenproblem. The eigenvalue count $\eta_{[a,b]}$ of the matrix $\mathcal{A}$ in an interval [a,b] is equal to the trace of projector $\mathcal{P}$, which is constructed by the summation of outer products of the associated eigenvectors of the eigenvalues in the interval.

$$\eta_{[a,b]} = \text{tr}(\mathcal{P}) \text{ where } \mathcal{P} = \sum_{\lambda_i \in [a,b]} u_i u_i^T.$$

However, the projector can not be directly constructed because eigenvectors are unknown. Instead, it can be approximated by using the first kind Chebyshev polynomials if the input matrix is Hermitian as (Di Napoli et al, 2016)

$$\mathcal{P} \approx \sum_{j=0}^{p} g_j^p \gamma_j T_i(\mathcal{A}).$$

Here, the well-known recursive relations between the first kind Chebyshev polynomials can be used to obtain the pth order Chebyshev polynomial such that $T_0(x) = 1$, $T_1(x) = x$ and $T_{i+1}(x) = 2xT(x)_i - T(x)_{i-1}$. Note that, although the input is a matrix here, the recursion will be still valid.

The Jackson coefficient for smoothing the approximation is defined as

$$g_j^p = \frac{sin(j+1)\alpha_p}{(p+2)sin\alpha_p} + (1 - \frac{j+1}{p+2})cos(j\alpha_p) \text{ where } \alpha_p = \frac{\pi}{p+2}. \tag{3}$$

The coefficients of the Chebyshev polynomials are defined as

$$\gamma_j = \begin{cases} \frac{1}{\pi}(arccos(a) - arccos(b)) & j = 0 \\ \frac{2}{\pi}(\frac{sin(jarccos(a)) - sin(jarccos(b))}{j}) & j > 0. \end{cases} \tag{4}$$

The above approximation is based on the assumption that all eigenvalues of $\mathcal{A}$ lie in the [-1,1] interval. To extend it to a generic spectrum $[\lambda_{min}, \lambda_{max}]$, the linear transformation in Eq.(5) can be used, however λ_{max} and λ_{min} are not known. Therefore, their estimations can be used. For the scheme to work accurately, the estimation for λ_{max} and λ_{min} must be greater than exact λ_{max} and smaller than exact λ_{min}, respectively (Di Napoli et al, 2016).

$$l(t) = \frac{t - (\lambda_{max} + \lambda_{min})/2}{(\lambda_{max} - \lambda_{min})/2} \tag{5}$$

Also, by applying the Hutchinson's Trace Estimator, the estimation can be done without constructing the approximated eigen-projector as (Di Napoli et al, 2016)

$$\eta_{[a,b]} \approx \frac{1}{n_v} \sum_{k=1}^{n_v} \sum_{j=0}^{p} z_k^T g_j^p \gamma_j T_i(l(\mathcal{A})) z_k.$$

Also, to avoid the matrix-matrix multiplications in the definition of the Chebyshev polynomials, a new vector $w_j = T_j(l(\mathcal{A}))z$ can be defined. That transforms the 3-term recurrence of the Chebyshev Polynomials (Di Napoli et al, 2016) to

$$w_{j+1} = 2l(\mathcal{A})w_j - w_{j-1}.$$

However, in the proposed method, we require the estimation for $\mathcal{C} = \frac{1}{N-1}X_C^T X_C$ matrix without constructing $\mathcal{C}$ explicitly since its computational and storage costs are expensive. Therefore, we should perform the action of matrix-matrix multiplications in the estimator implicitly to save computational time and storage. The linear transformation $l(t)$ should be applied to $\mathcal{C}$ which is also performed implicitly. If one consider the explicit form of the $\mathcal{C}$, the above recursion can be re-written as

$$w_{j+1} = 2\left(\frac{2X_C^T(X_C w_j) - \alpha(N-1)w_j}{\beta(N-1)}\right) - w_{j-1} \qquad (6)$$

where $\alpha = \lambda_{max} + \lambda_{min}$, $\beta = \lambda_{max} - \lambda_{min}$. Then, the number of eigenvalues of the covariance matrix can be estimated by

$$\eta_{[a,b]} \approx \frac{1}{n_v} \sum_{k=1}^{n_v} \sum_{j=0}^{p} z_k^T g_j^p \gamma_j w_j. \qquad (7)$$

Algorithm 3 Eigenvalue Count Estimator

Input: X_C, p, ϵ, δ, a, b, λ_{min}, λ_{max}
Output: $\eta_{[a,b]}$

1: $n_v \leftarrow \frac{2(2+\frac{8\sqrt{2}}{3}\epsilon)\log(\frac{2}{\delta})}{\epsilon^2}$
2: $\alpha \leftarrow \lambda_{max} + \lambda_{min}$
3: $\beta \leftarrow \lambda_{max} - \lambda_{min}$
4: $a \leftarrow \frac{2a-\alpha}{\beta}$
5: $b \leftarrow \frac{2b-\alpha}{\beta}$
6: $sum = 0$
7: **for** k=1:n_v **do**
8: $\quad$ z_k is constructed using Eq. (1)
9: $\quad$ **for** j=0:p **do**
10: $\quad\quad$ g_j^p is constructed using Eq. (3)
11: $\quad\quad$ γ_j is constructed using Eq. (4)
12: $\quad\quad$ w_j is constructed using Eq. (6)
13: $\quad\quad$ $sum = sum + z_k^T g_j^p \gamma_j w_j$
14: $\quad$ **end for**
15: **end for**
16: $\eta_{[a,b]} = sum/n_v$

Hence, the eigenvalue count can be approximated by Alg.(3), via two consecutive matrix-vector products, $X_C w_j$ and $X_C^T(X_C w_j)$ without constructing the covariance matrix explicitly.

The convergence rate of the proposed method is based on the gap between a, b, the eigenvalue distribution of the input matrix because if either a or b is near or included in an eigenvalue cluster the estimation may be overestimated or underestimated, and the estimations for λ_{max} and λ_{min}, and p is recommended to be at least 70 (Di Napoli et al, 2016). However, in our numerical experiments, a smaller p (20) produced acceptable results. It is because of the convergence of the Ritz values, and eigenvalue distribution of the covariance matrix of the data matrix. The biggest Ritz value fastly converges to the λ_{max}, which leads to better convergence for smaller p values, and gaps between middle Ritz values are bigger. Also, in the data covariance matrix, the biggest eigenvalues are much greater than the smallest eigenvalues, and generally smallest eigenvalues are clustered whereas the biggest are not and the proposed method does not care about the smallest eigenvalues.

3.4 Proposed Method

Algorithm 4 Proposed Method

    Input: X_C, p, n_k, ϵ, δ, t_v, a_t, f_t
    Output: d

1: τ is obtained using Alg. (1)
2: (μ_{n_k}, μ_1) is constructed using Alg. (2)
3: $n_v \leftarrow \frac{2(2 + \frac{8\sqrt{2}}{3}\epsilon)\log(\frac{2}{\delta})}{\epsilon^2}$
4: $\alpha \leftarrow 0$
5: $d \leftarrow 0$
6: **for** i=1:n_k **do**
7:     $\eta_{[\mu_{i+1}, \mu_i]}$ is obtained using Alg. (3)
8:     $\alpha_{[\mu_{i+1}, \mu_i]}$ is computed based on a_t
9:     $\alpha \leftarrow \alpha + \alpha_{[\mu_{i+1}, \mu_i]}$
10:    $d \leftarrow d + \eta_{[\mu_{i+1}, \mu_i]}$
11:    **if** $\alpha/\tau > t_v$ **then**
12:      break;
13:    **end if**
14: **end for**
15: d is finalized based on f_t

In the proposed method, first we estimate the trace of the covariance matrix τ via Alg.(1) and get a few Ritz values (μ_{n_k}, μ_1) where μ_1 is the largest via Alg.(2). Then, starting with the largest Ritz value interval, we estimate the number of eigenvalues $\eta_{[\mu_2, \mu_1]}$ in that interval via Alg.(3) (on line 7). At this point, we have the lower, upper bound, and estimated count of the eigenvalues.

Then, the question is how one can approximate the summation of eigenvalues in the interval $\alpha_{[\mu_2,\mu_1]}$. For that, we have three options indicated by the a_t parameter in the pseudocode (on line 8) which can either multiply the estimated eigenvalue count with the lower bound, the upper bound, or their mean. The numerical results have shown that the mean approximation for the eigenvalue summation is the most accurate one. Later, we check if the variance for that interval is bigger than the target variance t_v (on line 11), if not we proceed with the smaller interval and check for the cumulative variance. These iterations continue until we obtain a bigger approximated variance than t_v. Once we obtain a bigger approximated variance, we have three options to conclude the procedure, determined by t_f (on line 15). To finalize d, we can return the estimated ID; we can assume that eigenvalues are distributed linearly in the latest interval, and we can estimate the ID based on that assumption; or we can shorten our intervals and continue our method with them.

3.5 Practical Considerations

For the approximations of λ_{min} and λ_{max}, we use 0 and $c_1\mu_1$ respectively, where c_1 is a randomly chosen constant greater than 1. 0 is used as an approximation for the smallest eigenvalue because it is known that eigenvalues of the covariance matrix are larger than 0. Here, it should be remembered that the Alg.(3)'s convergence with respect to p is dependent on the approximations for λ_{min} and λ_{max}. Therefore, interpreting the smallest Ritz Value and finding an approximation for the smallest eigenvalue of the covariance matrix and better approximation for λ_{max} can improve the convergence performance of the proposed method.

At the first iteration of the algorithm, we run the Alg.(3) for the $\eta_{[\mu_1,c_2\mu_1]}$ interval where c_2 is a randomly chosen constant greater than 1 to approximate the number of eigenvalues of the covariance matrix which are larger than the largest Ritz value.

It is important that if the result of Alg.(3) (on line 7) of proposed method is 1, it indicates that only the lower bound exists in that interval; therefore, lower approximation should be used.

Since generally finding exactly 80% variance is not necessary, we defined a parameter acceptable range a_r. We do not perform finalization step if $t_v + a_r > \alpha/\tau > t_v - a_r$ (on line 11).

The proposed method suggested acceptable results for linear data; however, to improve its performance for nonlinear data, we performed several clustering approaches to the data such as well-known k-means and spectral clustering algorithms. Then, ID estimated for each cluster by applying the proposed approach and took the arithmetic mean of each cluster's estimated ID. Clustering algorithms create an additional computational cost, especially if spectral clustering (Ng et al, 2001; Pasadakis et al, 2022) is used. However, they can be parallelized (Manguoglu et al, 2010) and also one can easily recycle the computed neighborhood matrices for the non-linear data in the manifold learning application.

3.6 Cost Analysis

The proposed method only depends on the matrix-vector products; therefore, it has $O(NDn_k n_v p)$ time complexity. Moreover, since n_k, np, and p are weakly dependent on N and D and are also relatively small, the time complexity is $O(ND)$. Table (1) compares the time complexities of different ID estimators. The proposed method has the lowest time complexity.

Method	Time Complexity
Proposed Method	$O(ND)$
MLE	$O(N^2 D)$
MiND$_{\text{MLi}}$	$O(N^2 D^2)$
MiND$_{\text{MLk}}$	$O(N^2 D^2)$
MiND$_{\text{KL}}$	$O(N^2 D^2)$
DANCo	$O(N\log(N)D^2)$
FastDANCo	$O(N\log(N)D)$
ESS	$O(N^{d+1}D(d+1)^2)$

Table 1: Time complexities of different ID estimators

Moreover, the random vector multiplications for trace estimation in Alg.(1) and Alg.(3) are independent of each other hence they can be easily parallelized to speed up the running time of the proposed method. Also, in Alg.(3) the random vector multiplications can be computed incrementally, and after each increment the change of the result can be checked to stop the algorithm (Di Napoli et al, 2016). Therefore, there is a high probability that the algorithm can terminate in small number of iterations.

4 Numerical Experiments

To demonstrate the advantages and limits of the proposed approach, we used both artificially generated TF-IDF data and well-known synthetic benchmark data from the ID estimation literature. Numerical experiments are performed on an Intel Core i7 PC with 16GB memory using Matlab.

4.1 Synthetic Data

For the below experiments, a 5.000×500 matrix is created by the Scikit-Learn library make-low-rank function which creates a low-rank matrix with bell-shaped singular values (Pedregosa et al, 2011); in real life, this type of matrix can be seen in gray-level pictures of faces or TF-IDF vectors of text documents crawled from the web (Pedregosa et al, 2011). In our experiments, effective rank and tail strength of the matrix are 30 and 0,05, respectively. In the matrix, dimensions 20, 21, 22 and 23 corresponds to 78.16%, 80.29%, 82.24% and 84.03% variances respectively.

We target 80% variances in our test cases since it is a reasonable selection for the total variance in most of the cases. However, it is an adaptable parameter for the proposed approach. We defined the a_r as 2%, c_1 as 1.5, c_2 as 1.4, a_t

as mean, and f_t as linear. As shown in Fig.(3), number of the Chebyshev polynomials should be at least 20 for reasonable variance estimation. On the other hand, number of the Ritz intervals only causes some predictable fluctuations on the results.
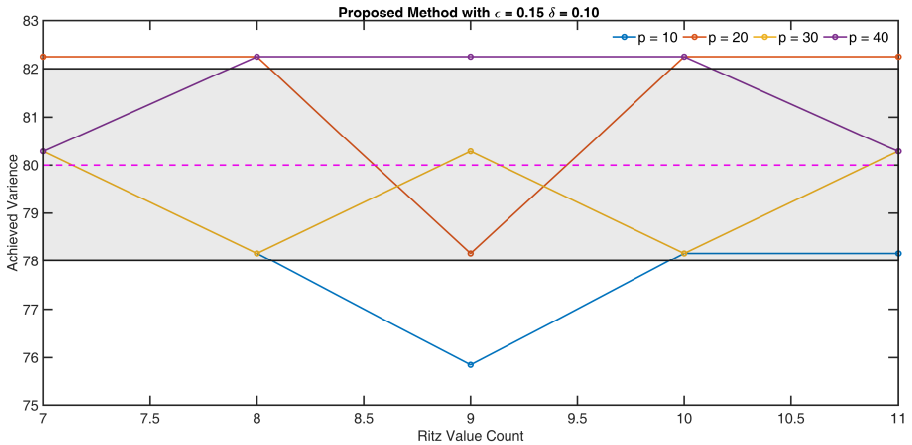

Fig. 3: Effect of the number of the Chebyshev polynomials (p) and the Ritz value counts on the total variance estimation where ϵ and δ are fixed (consequently the n_v is also fixed). An acceptable range of the variance is given as a shaded area in the figure

To measure the effect of the ϵ and δ parameters, we have used fixed values for the p and number of the Ritz intervals as 20 and 8 respectively by using the results shown in Fig.(4).

As expected, decreasing ϵ parameter for Hutchinson approximation makes the ID estimation more stable and more accurate. Although this improvement increase the overall computational time of the algorithm, this extra cost can easily be handled in high-performance computing systems due to the embarrassingly parallel nature of the Alg.(1) and Alg.(3). Note that, all calculations in Alg.(4) is only based on matrix-vector multiplications and can be easily realized in parallel environments.

Since the proposed method contains randomness, we tested each epsilon and delta configuration 10 times and Fig.(5) shows the statistical distribution of the individual tests via box-plots. Note that, in Fig.(5), instead of showing the estimated variance, we depicted the estimated ID. It can be concluded that as the n_v increase, the results get more stable with the cost of increasing the number of random vectors using the trace and projector estimation.
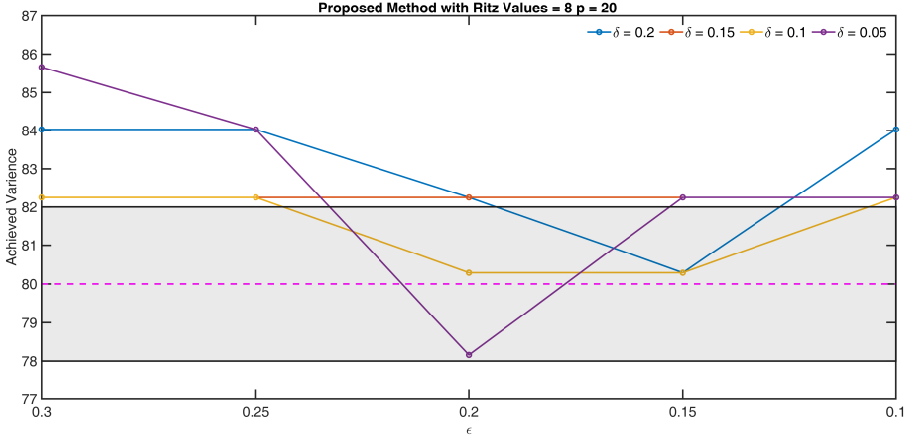
Fig. 4: Effect of the ϵ and δ (consequently the n_v) on the total variance estimation where p and Ritz values are fixed. An acceptable range of the variance is given as a shaded area in the figure

4.2 Benchmark Data

For the generation of the synthetic data sets we tested, the Scikit-Dimension library BenchmarkManifolds function (Bac et al, 2021), which creates 24 different data set based on (Hein and Audibert, 2005), was used. The parameters of the proposed method were 20, 8, 0.2, and 0.2 for p, n_k, ϵ, and δ respectively and cluster size for variants of the proposed method was 2. We also tested a wide variety of intrinsic dimension estimators to show the efficiency of our method. All these results are given in Table 7. The main observation from these results, the proposed method is giving competitive results concerning most approaches we have tested. The last row of the Table 7 gives the mean of the relative estimation errors, which is defined as the difference between the ID value of the dataset and the estimated one divided correspond. If these results are examined carefully, one can conclude that the proposed approach with k-means clustering has a lower estimation error than the other projection-based ID estimators. On the other hand, topological estimators mostly have better estimations. Nevertheless, as discussed in section 2, topological estimators predominantly suffer from high computational costs. Therefore, especially for the large datasets, the proposed approach can be used as a fast and reliable estimator. Note that all estimators were tested by using the functions in (Bac et al, 2021) with their default values, and no parameter optimizations were conducted. Notice that for $\mathcal{M}_{10d}$ dataset, the result of FSH method is "nan". As the authors pointed out, that is because of the implementation in (Bac et al, 2021). Hence, we excluded $\mathcal{M}_{10d}$ from the FSH method tests.

We have focused on the proposed approach in the second representation of the results. In Fig.(6.a), the proposed method and its variants are compared based on the relative dimension estimation errors. Although the general trend
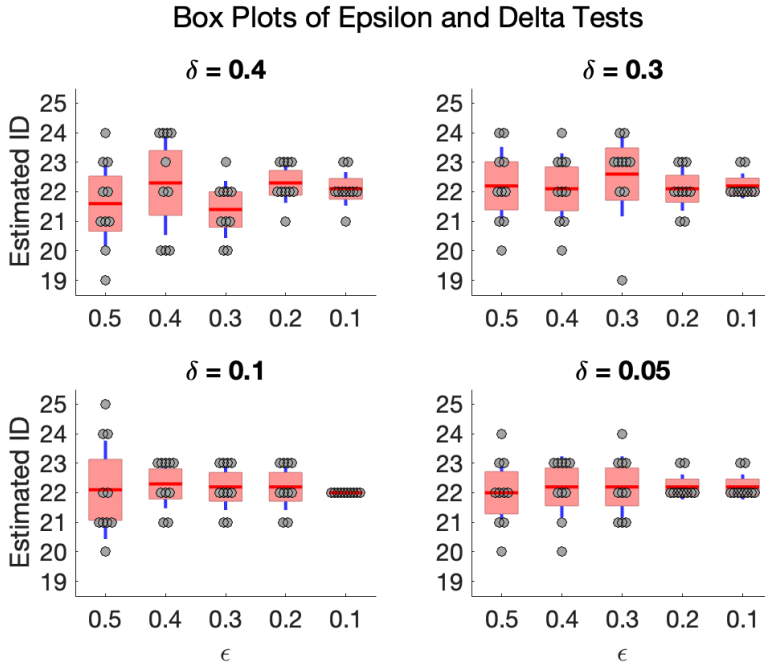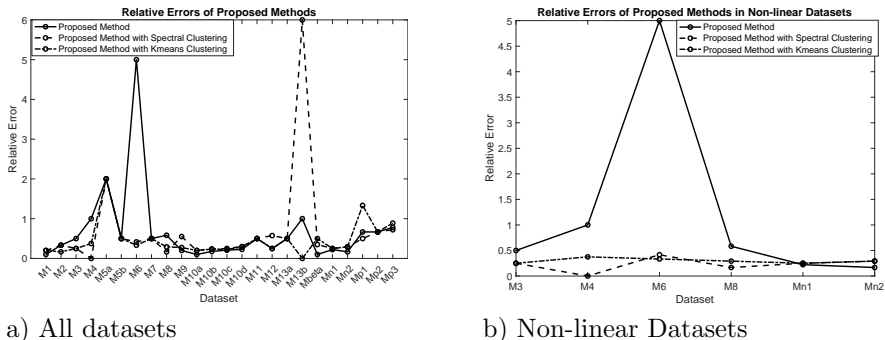
Fig. 5: Estimated ID has been obtained for every ϵ-δ pair 10 times and their statistical distributions are presented where gray disk, red line, light red box, and blue line correspond to the result of an individual run, the median, the interquartile range, and non-outlier range of the corresponding runs, respectively

of all variants is having an error of less than one for most of the problems in the datasets with all three variants in $\mathcal{M}_{5a}$ the error is large for all of them. This dataset contains three features and represents a 1-D Helix structure. Its highly non-linear structure and the low number of dimensions is the leading cause of this situation. Another two crucial peak points of the figures are $\mathcal{M}_6$ for the vanilla version of the proposed method and $\mathcal{M}_{13b}$ for the proposed method with spectral clustering. Again this worst case occurs due to the nature of the benchmark data. $\mathcal{M}_6$ is a highly non-linear manifold data; therefore, the vanilla version cannot capture the non-linear nature of the data. On the other hand, the expected intrinsic dimension of $\mathcal{M}_{13b}$ is only one, while its number of features is 13 with only 3 of them greater than 0. Therefore, Ritz values unpredictably converged, they suggested some unreal eigenvalues between 0 and the lowest eigenvalue of $\mathcal{M}_{13b}^T \mathcal{M}_{13b}$ which causes the greater suggestion of ID. It should be noted that this is related to the randomness of the proposed method because different tests on this dataset yielded different results, for instance, while Ritz value count 3, the PM_{spec} suggested the ID as 1.5 and 2. However, these are not reflected in the table to preserve the wholeness of the

testing parameters. Moreover, the removal of $\mathcal{M}_{13b}$ from the tests of PM_{spec} nearly reduces its mean relative error to 0.44 which is very competitive with other methods. Also, it can be seen that none of the proposed methods can even approximately capture the ID of the $\mathcal{M}_p$ family which is non-linearly embedded paraboloids. In Fig.(6.b), the clear advantage of clustering approaches for the highly non-linear datasets is depicted. Hence, it can be concluded that the estimation accuracy of the proposed method and variants are depended on the shape of a dataset.

a) All datasets   b) Non-linear Datasets

Fig. 6: Relative errors of the variants of the proposed methods for all and only non-linear datasets

5 Conclusion

Large-scale data analysis usually needs dimensionality reduction application to reduce computational time and improve the accuracy of the target machine learning applications. However, without an apriori knowledge of intrinsic dimension, it can be a costly operation. This study proposes a novel and computationally efficient intrinsic dimension estimation approach based on Ritz values and Chebyshev polynomials. The proposed method is a projective, but its main advantage is its ability to estimate the intrinsic dimension without constructing and solving the underlying eigenvalue problem. We have performed several tests on various problems ranging from linear to highly non-linear structures. The performance of the proposed approach is compared with other well-known estimators in the literature.

Furthermore, the dominant computational kernel of the method is based on only matrix-vector multiplication operations, and it is parallelizable inherently. Therefore it is a proper candidate for large-scale data analysis on parallel computing platforms.

6 Declarations

Author Contributions: All authors contributed to the study conception, methodology, and design. Algorithmic design, data curation and visualization were performed by Kadir Özçoban, Murat Manguoğlu and E. Fatih Yetkin. The first draft of the manuscript was written by Kadir Özçoban and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript, and consent for publication.

Data and Code Availability: We obtained the data from a publicly available repository/generator, as described in Section 4.2. The code is developed as a part of an ongoing project but can be shared upon request.

Dataset	ID	PM	PM_{Spec}	PM_{Kmeans}	PFO	PFN	PMG	PRT	PPR	PKS	PBS	CID	FSH	KNN	MADA	$Mind_{ML}$	MLE	MOM	TLE	TNN	DANCo	ESS
$\mathcal{M}_1$	**10.00**	9.00	8.00	8.00	11.00	7.00	1.00	1.00	10.94	5.00	1.00	8.91	11.02	11.00	9.62	9.10	9.53	8.60	10.10	9.28	11.00	10.18
$\mathcal{M}_2$	**3.00**	2.00	2.00	3.50	**3.00**	2.00	**3.00**	1.00	2.27	2.00	**3.00**	2.87	2.92	4.00	3.07	2.90	3.03	2.79	3.13	2.92	2.96	2.90
$\mathcal{M}_3$	**4.00**	2.00	3.00	5.00	5.00	2.00	2.00	1.00	2.75	2.00	3.00	3.58	3.34	1.00	4.14	3.77	4.03	3.77	4.21	3.79	4.67	4.02
$\mathcal{M}_4$	**4.00**	8.00	**4.00**	5.50	8.00	5.00	1.00	1.00	7.96	**4.00**	1.00	3.75	5.81	**4.00**	4.34	3.86	4.18	4.49	4.42	3.74	5.04	5.03
$\mathcal{M}_{5a}$	**1.00**	3.00	3.00	3.00	3.00	2.00	2.00	**1.00**	2.40	2.00	**1.00**	1.01	2.91	3.00	1.08	**1.00**	1.06	1.17	1.11	0.98	**1.00**	1.63
$\mathcal{M}_{5b}$	**2.00**	3.00	3.00	3.00	3.00	**2.00**	**2.00**	1.00	2.23	**2.00**	1.00	2.79	2.91	1.00	3.17	2.37	2.82	2.86	2.91	1.97	2.47	2.88
$\mathcal{M}_6$	**6.00**	36.00	8.50	8.00	12.00	9.00	12.00	1.00	11.95	12.00	1.00	**6.00**	8.43	2.00	7.34	6.25	6.91	7.16	7.12	5.87	8.76	8.52
$\mathcal{M}_7$	**2.00**	3.00	3.00	3.00	3.00	**2.00**	1.00	1.00	2.95	1.00	1.00	1.96	2.88	3.00	2.09	**2.00**	2.07	2.01	2.14	1.94	2.21	2.15
$\mathcal{M}_8$	**12.00**	19.00	10.00	15.50	24.00	17.00	24.00	2.00	23.77	24.00	1.00	11.33	17.95	5.00	14.43	10.00	14.24	13.21	13.83	13.80	11.99	19.50
$\mathcal{M}_9$	**20.00**	16.00	9.00	14.50	**20.00**	11.00	19.00	1.00	19.86	9.00	1.00	13.48	19.07	3.00	15.12	10.00	15.14	13.49	15.25	14.77	19.00	19.41
$\mathcal{M}_{10a}$	**10.00**	11.00	8.00	8.00	11.00	6.00	2.00	1.00	10.97	5.00	1.00	8.58	10.43	11.00	9.15	8.89	9.20	8.39	9.62	9.10	11.00	10.30
$\mathcal{M}_{10b}$	**17.00**	14.00	13.00	13.00	18.00	10.00	**17.00**	1.00	17.88	8.00	1.00	12.80	17.10	4.00	13.96	10.00	13.90	12.47	14.20	13.96	18.00	17.29
$\mathcal{M}_{10c}$	**24.00**	19.00	18.00	18.50	25.00	14.00	23.00	2.00	24.76	14.00	1.00	16.41	23.27	5.00	17.87	10.00	17.97	15.90	18.01	18.05	24.01	24.38
$\mathcal{M}_{10d}$	**70.00**	54.00	49.00	50.00	71.00	39.00	69.00	3.00	69.05	35.00	1.00	31.62	nan	71.00	36.65	10.00	37.17	31.47	34.71	39.85	71.00	69.95
$\mathcal{M}_{11}$	**2.00**	3.00	3.00	3.00	3.00	1.00	**2.00**	1.00	2.15	**2.00**	1.00	1.97	1.97	**2.00**	2.10	**2.00**	2.07	2.21	2.16	2.02	2.26	2.49
$\mathcal{M}_{12}$	**20.00**	15.00	8.50	15.00	**20.00**	11.00	11.00	1.00	19.82	11.00	1.00	12.74	20.30	6.00	16.04	10.00	16.22	13.98	15.47	17.04	12.05	19.79
$\mathcal{M}_{13a}$	**2.00**	3.00	3.00	3.00	3.00	1.00	1.00	1.00	1.86	**2.00**	**2.00**	1.94	2.88	1.00	2.08	**2.00**	2.06	1.93	2.13	1.96	2.23	2.05
$\mathcal{M}_{13b}$	**1.00**	2.00	7.00	**1.00**	2.00	**1.00**	3.00	**1.00**	2.03	2.00	3.00	4.01	1.97	**1.00**	3.78	1.20	1.75	1.83	1.84	**1.00**	**1.00**	1.95
$\mathcal{M}_{beta}$	**10.00**	9.00	6.50	5.00	**10.00**	7.00	20.00	1.00	10.62	**10.00**	11.00	3.47	5.27	40.00	6.64	6.31	6.63	5.78	6.21	6.54	8.02	5.92
$\mathcal{M}_{n1}$	**18.00**	14.00	13.50	13.50	27.00	13.00	36.00	1.00	18.82	**18.00**	19.00	12.58	17.00	11.00	14.31	10.00	14.26	12.71	14.29	14.24	21.00	18.39
$\mathcal{M}_{n2}$	**24.00**	20.00	17.00	17.00	36.00	18.00	48.00	1.00	25.08	**24.00**	25.00	15.42	23.30	16.00	17.87	10.00	17.85	15.63	17.49	18.26	31.00	24.85
$\mathcal{M}_{p1}$	**3.00**	1.00	1.50	7.00	1.00	1.00	11.00	1.00	1.24	1.00	2.00	2.14	0.90	1.00	3.07	2.90	3.04	2.73	3.13	2.99	3.20	2.85
$\mathcal{M}_{p2}$	**6.00**	2.00	2.00	2.00	1.00	21.00	20.00	1.00	1.06	1.00	2.00	2.63	0.89	21.00	5.14	5.08	5.19	4.22	5.34	5.48	7.01	4.89
$\mathcal{M}_{p3}$	**9.00**	2.00	15.50	1.00	1.00	1.00	29.00	1.00	1.03	1.00	2.00	2.92	0.89	30.00	6.55	6.52	6.64	4.76	6.70	7.23	8.94	6.12
$Mean_{error}$		0.68	0.68	0.46	0.50	0.49	0.82	0.73	0.39	0.49	0.62	0.36	0.39	0.77	0.29	0.23	0.18	0.25	0.20	0.12	0.13	0.20

Fig. 7: The relative errors for all datasets are obtained using different ID estimators. The mean of the relative errors for each estimator is given in the last row. The ID of the datasets is given in the first column. If an estimator obtains the exact ID, then the corresponding value is emphasized in bold.

References

Agullo E, Cools S, Yetkin EF, et al (2020) On soft errors in the conjugate gradient method: Sensitivity and robust numerical detection. SIAM Journal on Scientific Computing 42(6):C335–C358. https://doi.org/10.1137/18M122858X, URL https://doi.org/10.1137/18M122858X, https://arxiv.org/abs/https://doi.org/10.1137/18M122858X

Albergante L, Bac J, Zinovyev A (2019) Estimating the effective dimension of large biological datasets using fisher separability analysis. 2019 International Joint Conference on Neural Networks (IJCNN) https://doi.org/10.1109/ijcnn.2019.8852450

Amsaleg L, Chelly O, Furon T, et al (2018) Extreme-value-theoretic estimation of local intrinsic dimensionality. Data Mining and Knowledge Discovery 32(6):1768–1805. https://doi.org/10.1007/s10618-018-0578-6

Amsaleg L, Chelly O, Houle ME, et al (2019) Intrinsic dimensionality estimation within tight localities. Proceedings of the 2019 SIAM International Conference on Data Mining p 181–189. https://doi.org/10.1137/1.9781611975673.21

Bac J, Mirkes EM, Gorban AN, et al (2021) Scikit-dimension: A python package for intrinsic dimension estimation. Entropy 23(10):1368. https://doi.org/10.3390/e23101368

Bennett R (1969) The intrinsic dimensionality of signal collections. IEEE Transactions on Information Theory 15(5):517–525. https://doi.org/10.1109/tit.1969.1054365

Brito M, Quiroz A, Yukich J (2013) Intrinsic dimension identification via graph-theoretic methods. Journal of Multivariate Analysis 116:263–277. https://doi.org/10.1016/j.jmva.2012.12.007

Camastra F, Staiano A (2016) Intrinsic dimension estimation: Advances and open problems. Information Sciences 328:26–41. https://doi.org/10.1016/j.ins.2015.08.029

Campadelli P, Casiraghi E, Ceruti C, et al (2015) Intrinsic dimension estimation: Relevant techniques and a benchmark framework. Mathematical Problems in Engineering 2015:1–21. https://doi.org/10.1155/2015/759567

Ceruti C, Bassis S, Rozza A, et al (2014) Danco: An intrinsic dimensionality estimator exploiting angle and norm concentration. Pattern Recognition 47(8):2569–2581. https://doi.org/10.1016/j.patcog.2014.02.013

Cools S, Yetkin EF, Agullo E, et al (2018) Analyzing the effect of local rounding error propagation on the maximal attainable accuracy of the pipelined conjugate gradient method. SIAM Journal on Matrix Analysis and Applications 39(1):426–450. https://doi.org/10.1137/17M1117872, URL https://doi.org/10.1137/17M1117872, https://arxiv.org/abs/https://doi.org/10.1137/17M1117872

Costa JA, Hero AO (2006) Determining intrinsic dimension and entropy of high-dimensional shape spaces. Statistics and Analysis of Shapes p 231–252. https://doi.org/10.1007/0-8176-4481-4_9

Cox MA, Cox TF (2008) Multidimensional scaling. Handbook of Data Visualization p 315–347. https://doi.org/10.1007/978-3-540-33037-0_14

Demartines P, Herault J (1997) Curvilinear component analysis: A self-organizing neural network for nonlinear mapping of data sets. IEEE Transactions on Neural Networks 8(1):148–154. https://doi.org/10.1109/72.554199

Demmel JW (1997) 7. Iterative Methods for Eigenvalue Problems, Siam, p 361–387

Di Napoli E, Polizzi E, Saad Y (2016) Efficient estimation of eigenvalue counts in an interval. Numerical Linear Algebra with Applications 23(4):674–692. https://doi.org/10.1002/nla.2048

Facco E, d'Errico M, Rodriguez A, et al (2017) Estimating the intrinsic dimension of datasets by a minimal neighborhood information. Scientific Reports 7(1). https://doi.org/10.1038/s41598-017-11873-y

Fan M, Zhang X, Chen S, et al (2013) Dimension estimation of image manifolds by minimal cover approximation. Neurocomputing 105:19–29. https://doi.org/10.1016/j.neucom.2012.04.037

Farahmand Am, Szepesvári C, Audibert JY (2007) Manifold-adaptive dimension estimation. Proceedings of the 24th international conference on Machine learning - ICML '07 https://doi.org/10.1145/1273496.1273530

Friedman JH, Rafsky LC (1983) Graph-theoretic measures of multivariate association and prediction. The Annals of Statistics 11(2). https://doi.org/10.1214/aos/1176346148

Fukunaga K, Olsen D (1971) An algorithm for finding intrinsic dimensionality of data. IEEE Transactions on Computers C-20(2):176–183. https://doi.org/10.1109/t-c.1971.223208

Grassberger P, Procaccia I (1983) Measuring the strangeness of strange attractors. Physica D: Nonlinear Phenomena 9(1-2):189–208. https://doi.org/10.1016/0167-2789(83)90298-1

Greenbaum A, Liu H, Chen T (2021) On the convergence rate of variants of the conjugate gradient algorithm in finite precision arithmetic. SIAM Journal on Scientific Computing 43(5):S496–S515. https://doi.org/10.1137/20M1346249, URL https://doi.org/10.1137/20M1346249, https://arxiv.org/abs/https://doi.org/10.1137/20M1346249

Hein M, Audibert JY (2005) Intrinsic dimensionality estimation of submanifolds in rd. Proceedings of the 22nd international conference on Machine learning - ICML '05 https://doi.org/10.1145/1102351.1102388

Hernandez V, Roman JE, Vidal V (2005) SLEPc: A scalable and flexible toolkit for the solution of eigenvalue problems. ACM Trans Math Software 31(3):351–362

Hestenes M, Stiefel E (1952) Methods of conjugate gradients for solving linear systems. Journal of Research of the National Bureau of Standards 49(6):409. https://doi.org/10.6028/jres.049.044

Hutchinson M (1989) A stochastic estimator of the trace of the influence matrix for laplacian smoothing splines. Communications in Statistics - Simulation and Computation 18(3):1059–1076. https://doi.org/10.1080/03610918908812806

Johnsson K, Soneson C, Fontes M (2015) Low bias local intrinsic dimension estimation from expected simplex skewness. IEEE Transactions on Pattern Analysis and Machine Intelligence 37(1):196–202. https://doi.org/10.1109/tpami.2014.2343220

Jolliffe I (1986) Principal component analysis. Springer New York, NY

Lee JA, Verleysen YM (eds) (2007) Nonlinear Dimensionality Reduction. Springer New York, NY, https://doi.org/https://doi.org/10.1007/978-0-387-39351-3

Levina E, Bickel P (2004) Maximum Likelihood Estimation of Intrinsic Dimension, vol 17. MIT Press

Li CG, Guo J, Xiao B (2009) Intrinsic dimensionality estimation within neighborhood convex hull. International Journal of Pattern Recognition and Artificial Intelligence 23(01):31–44. https://doi.org/10.1142/s0218001409007016

Manguoglu M, Cox E, Saied F, et al (2010) Tracemin-fiedler: A parallel algorithm for computing the fiedler vector. In: International Conference on High

Performance Computing for Computational Science, Springer, pp 449–455

McQueen J, Meilă M, VanderPlas J, et al (2016) Megaman: Scalable manifold learning in python. Journal of Machine Learning Research 17(148):1–5. URL http://jmlr.org/papers/v17/16-109.html

Ng A, Jordan M, Weiss Y (2001) On spectral clustering: Analysis and an algorithm. Advances in neural information processing systems 14

Pasadakis D, Alappat CL, Schenk O, et al (2022) Multiway p-spectral graph cuts on grassmann manifolds. Machine Learning 111(2):791–829

Pedregosa F, Varoquaux G, Gramfort A, et al (2011) Scikit-learn: Machine learning in Python. Journal of Machine Learning Research 12:2825–2830

Polizzi E (2009) Density-matrix-based algorithm for solving eigenvalue problems. Phys Rev B 79:115,112. https://doi.org/10.1103/PhysRevB.79.115112, URL https://link.aps.org/doi/10.1103/PhysRevB.79.115112

Roweis ST, Saul LK (2000) Nonlinear dimensionality reduction by locally linear embedding. Science 290(5500):2323–2326. https://doi.org/10.1126/science.290.5500.2323

Rozza A, Lombardi G, Ceruti C, et al (2012) Novel high intrinsic dimensionality estimators. Machine Learning 89(1-2):37–65. https://doi.org/10.1007/s10994-012-5294-7

Sameh AH, Wisniewski JA (1982) A trace minimization algorithm for the generalized eigenvalue problem. SIAM Journal on Numerical Analysis 19(6):1243–1259

Sammon J (1969) A nonlinear mapping for data structure analysis. IEEE Transactions on Computers C-18(5):401–409. https://doi.org/10.1109/t-c.1969.222678

Scales JA (1989) On the use of conjugate gradient to calculate the eigenvalues and singular values of large, sparse matrices. Geophysical Journal International 97(1):179–183. https://doi.org/10.1111/j.1365-246x.1989.tb00494.x

Schölkopf B, Smola A, Müller KR (1998) Nonlinear component analysis as a kernel eigenvalue problem. Neural Computation 10(5):1299–1319. https://doi.org/10.1162/089976698300017467

Skorski M (2021) Modern analysis of hutchinson's trace estimator. 2021 55th Annual Conference on Information Sciences and Systems (CISS) https://doi.org/10.1109/ciss50987.2021.9400306

Valle M, Oganov AR (2010) Crystal fingerprint space – a novel paradigm for studying crystal-structure sets. Acta Crystallographica Section A Foundations of Crystallography 66(5):507–517. https://doi.org/10.1107/s0108767310026395

Yano T, Futamura Y, Imakura A, et al (2021) Efficient implementation of a dimensionality reduction method using a complex moment-based subspace. In: The International Conference on High Performance Computing in Asia-Pacific Region. Association for Computing Machinery, New York, NY, USA, HPC Asia 2021, p 83–89, https://doi.org/10.1145/3432261.3432267, URL https://doi.org/10.1145/3432261.3432267