Dimensionality Reduction with Evolutionary Shephard-Kruskal Embeddings

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Abstract: This paper introduces an evolutionary iterative approximation of Shephard-Kruskal based dimensionality reduction with linear runtime. The method, which we call evolutionary Shephard-Kruskal embedding (EvoSK), iteratively constructs a low-dimensional representation with Gaussian sampling in the environment of the latent positions of the closest embedded patterns. The approach explicitly optimizes the distance preservation in low-dimensional space, similar to the objective solved by multi-dimensional scaling. Experiments on a small benchmark data set show that EvoSK can perform better than its famous counterparts multi-dimensional scaling and isometric mapping and outperforms stochastic neighbor embeddings.

1 INTRODUCTION

Dimensionality reduction (DR) is the important problem class in machine learning that offers methods for reducing the data dimensionality to a reasonable degree, e.g., for preprocessing in classification or for data space visualization (Lee and Verleysen, 2007). Many DR methods compute a pointwise embedding of high-dimensional patterns based on different criteria. Prominent examples are principal component analysis (PCA) (Jolliffe, 1986), kernel PCA (Schölkopf et al., 1998), multi-dimensional scaling (MDS) (Borg and Groenen, 2005), isometric mapping (ISOMAP) (Tenenbaum et al., 2000), and t-distributed stochastic neighbor embedding (t-SNE) (van der Maaten and Hinton, 2008). With growing data set sizes, methods are required that scale well with the number of patterns.

In dimensionality reduction we seek for low-dimensional representations $\mathbf{z}_i \in \mathcal{R}^q$ for each high-dimensional pattern $\mathbf{x}_i \in \mathcal{R}^d$ with $i = 1, \ldots, N$ and $d < q$ without losing essential information. This information can be distances between patterns, or neighborhoods of patterns, which should be maintained in low-dimensional space. This paper presents an approach that iteratively constructs a low-dimensional representation with evolutionary Gaussian sampling for minimizing the Shepard-Kruskal measure in each step.

The paper is structured as follows. Section 2 gives an introduction to related work while introducing a short taxonomy of iterative evolutionary embedding methods. Section 3 introduces the novel EvoSK approach. It is experimentally evaluated in Section 4 and compared to MDS, ISOMAP, and t-SNE. Conclusions are drawn in Section 5 with an overview of prospective future work.

2 RELATED WORK

Many DR algorithms have been introduced that process data sets pattern by pattern. They are also known as incremental or streaming methods. But for the class of DR methods, only few variants have been introduced in the past, e.g., a variant of PCA that is able to process streaming data (Mitliagkas et al., 2013). MDS computes the embeddings based on a Cholesky or singular value decomposition resulting in eigenvalues, whose eigenvectors with the q-largest eigenvalues are the low-dimensional embeddings.

The line of research on methods that iteratively construct a solution with stochastic sampling has recently been established (Kramer, 2015a; Kramer, 2015b). It began as variant of unsupervised regression. Figure 1 shows a small taxonomy of this emerging field. All variants have in common that they iteratively construct an embedding based on randomly sampling in the environment using Gaussian sampling. The latent positions of the closest embedded patterns are the origin of this sampling pro-

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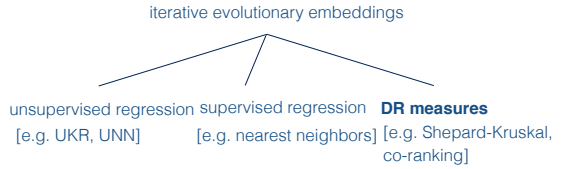


Figure 1: Taxonomy of iterative evolutionary embedding.

cess. Methods from the three branches differ in the selection criterion they employ. The left part of the taxonomy is based on the reconstruction error of unsupervised regression. Unsupervised regression maps patterns from the low-dimensional space to the high-dimensional space using a multi-label regression method (Meinicke et al., 2005). The optimization problem is to optimally reconstruct the high-dimensional patterns. Unsupervised nearest neighbors (Kramer, 2015b) employs nearest neighbor regression, while unsupervised kernel regression (UKR) is based on the Nadaraya-Watson estimator.

The middle part of the taxonomy is based on the optimization of embeddings using label information. Instead of the reconstruction error, it makes use of the regression error, i.e., the low-dimensional patterns are optimized to achieve the same regression error as their high-dimensional counterparts (Kramer, 2015a).

The right part of the taxonomy is new and the first approach in this line of research is introduced in this paper. We propose the employment of DR measures like the Shephard-Kruskal measure or the co-ranking matrix (Hastie et al., 2009).

3 SHEPHARD-KRUSKAL EMBEDDINGS

This section introduces the evolutionary Shephard-Kruskal embedding approach, which is called EvoSK in the following. Similar to the approaches that have been introduced for the iterative evolutionary embeddings of unsupervised regression, the mechanism is introduced inductively.

Let $\mathbf{X} = [\mathbf{x}]_{i=1}^{N}$ be the patterns that have to be embedded. The first pattern $\mathbf{x}_1$ is embedded at an arbitrary position in latent space, e.g., at the origin $\mathbf{z}_1 = \mathbf{0}$. At this time the current latent matrix is $\overline{\mathbf{Z}} = [\mathbf{z}_1]$ with a corresponding pattern matrix $\overline{\mathbf{X}} = [\mathbf{x}_1]$. Now, let $\mathbf{x}_1, \ldots, \mathbf{x}_{n-1}$ be the sequence of embedded patterns with corresponding latent positions $\mathbf{z}_1, \ldots, \mathbf{z}_{n-1}$. Pattern $\mathbf{x}_n$ with $n \leq N$ is embedded by first searching for the closest embedded pattern

$$\mathbf{x}^* = \arg \min_{\mathbf{x}=\mathbf{x}_{n-k},\ldots,\mathbf{x}_n} \|\mathbf{x}_n - \mathbf{x}\|^2 \tag{1}$$

among the last k embedded patterns $\overline{\mathbf{X}} = [\mathbf{x}_j]_{j=n-k}^{n-1}$. We call parameter k window size in the following. Based on its latent position $\mathbf{z}^*$, μ candidate positions $\mathbf{z}_1^*, \ldots, \mathbf{z}_\mu^*$ are sampled using the Gaussian distribution $\hat{\mathbf{z}}_l \sim \mathcal{N}(0, \sigma)$ with

$$\mathbf{z}_l^* = \mathbf{z}^* + \hat{\mathbf{z}}_l \tag{2}$$

for $l = 1, \ldots, \mu$. For preservation of distances between patterns in low-dimensional space the standard deviation $\sigma = \|\mathbf{x}_n - \mathbf{x}^*\|$ is used for the sampling process, i.e., large distances result in large σ, small distances in sample close to $\mathbf{z}^*$.

From the μ candidate latent positions, the one leading to the lowest Shepard-Kruskal error E_{sk} is selected. E_{sk} measures the maintenance of distances in the low dimensional space (Hastie et al., 2009). Let $\mathbf{D_X}$ be the distance matrix in data space and $\mathbf{D_Z}$ be the distance matrix in the low-dimensional space. Both contain the pairwise Euclidean distances and are considered as normalized. The Shepard-Kruskal measure is defined as the norm of the differences of the normalized distance matrixes

$$E_{sk} = \|\mathbf{D_X} - \mathbf{D_Z}\|_F^2. \tag{3}$$

A low Shepard-Kruskal measure is preferable. For example, if distances are completely preserved, the Shepard-Kruskal measure is zero.

Figure 1 shows the pseudocode of the EvoSK approach. The search for the closest pattern in Line 4 reduces to a constant runtime, if window size k does not depend on N, as the number of considered comparisons in high-dimensional space does not grow with the number of embedded patterns. Further, the inner loop of μ sampling steps obviously also require a constant time.

Algorithm 1: Pseudo-code of EvoSK.

Require: $\mathbf{X}$, μ
  $\overline{\mathbf{Z}} = [\mathbf{0}]$, $\overline{\mathbf{X}} = [\mathbf{x}_1]$
  for $n = 2$ **to** N **do**
    choose $\mathbf{x}_n$
    select closest pattern $\mathbf{x}^*$ among $\overline{\mathbf{X}} = [\mathbf{x}_j]_{j=n-k}^{n-1}$ with latent position $\mathbf{z}^*$
    for $l = 1$ **to** μ **do**
      $\mathbf{z}_l^* \sim \sigma \cdot \mathcal{N}(\mathbf{z}^*, 1)$ with $\sigma = \|\mathbf{x}_n - \mathbf{x}^*\|^2$
    end for
    choose $\mathbf{z}_n = \arg\min_{\mathbf{z}=\mathbf{z}_1^*,\ldots,\mathbf{z}_\mu^*} E([\overline{\mathbf{Z}}, \mathbf{z}])$
    $\overline{\mathbf{Z}} = [\overline{\mathbf{Z}}, \mathbf{z}_n]$, $\overline{\mathbf{X}} = [\overline{\mathbf{X}}, \mathbf{x}_n]$
  end for
  return $\mathbf{Z}$

For $k = n$ the approach has quadratic runtime of $O(N^2)$. If data structures are applicable like ball-trees

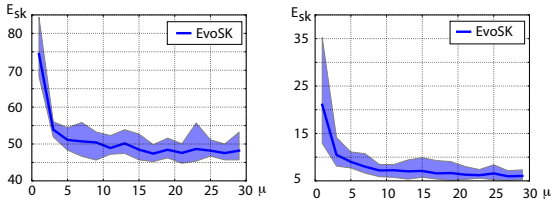
that allow a neighborhood search in $\log(N)$ the runtime reduces to $O(N \log N)$. For a constant window size of k the search can be performed in k or even $\log(k)$ steps offering a linear runtime of $O(N)$.

4 EXPERIMENTS

In this section, we analyze the DR pipeline evolution experimentally on a small set of benchmark problems. For this sake, we concentrate on an experimental comparison between EvoSK, MDS, ISOMAP, and t-SNE. The control methods and data sets (with exception of the *Wind* data set) are based on SCIKIT-LEARN (Pedregosa et al., 2011).

Table 1 shows the Shephard-Kruskal measure E_{sk} of EvoSK with best, mean, standard deviation, and worst values of 100 runs and a comparison to MDS, ISOMAP, and t-SNE. The experiments use a window size of $k = 50$ and all data sets use the first $N = 200$ patterns. The results show that EvoSK performs better in mean than MDS and ISOMAP on *Digits*, and on *Friedman*. On *Image*, only some runs, in particular the best one of EvoSK is better than the MDS and the ISOMAP result. However, on *Housing* and on the *Wind* data set, MDS and ISOMAP outperform EvoSK, while t-SNE is clearly outperformed by EvoSK on all data sets.

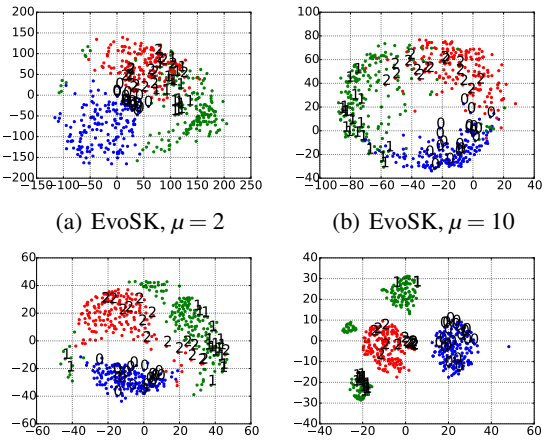
Our further experimental analysis has shown that the choice of k has no significant impact on the achieved Shephard-Kruskal measure as of 10% of N. Obviously the orientation to the last few embedded patterns is sufficient, as the sampling process is more important for the decision, at which position the patterns should be embedded.



(a) *Digits* (b) *Image*

Figure 2: Analysis of number μ of sampling steps in each iteration on the data sets *Digits* and *Image*.

An analysis of the search effort invested into the sampling process shows Figure 2. For the data sets *Digits* and *Image*, E_{sk} is shown depending on the number μ of sampling steps in each iteration. It turns out that E_{sk} is decreasing significantly with increasing μ. Few more sampling steps are beneficial and more lead to less improvements. The best and worst E_{sk} developments deviate from the mean only slightly on all data sets indicating that this dependency is significant.



(a) EvoSK, $\mu = 2$ (b) EvoSK, $\mu = 10$

(c) MDS (d) t-SNE

Figure 3: Visualization of embeddings of the *Digits* data set with EvoSK employing $\mu = 2, 10$ sampling steps in comparison to MDS and t-SNE.

In Figure 3 we visualize the embeddings of EvoSK. The plots show a comparison between the embeddings of EvoSK with the sampling sizes $\mu = 2, 10$ with MDS and t-SNE on the *Digits* data set with three classes and $N = 537$ patterns to a two-dimensional space. Colors and figures indicate the label assignment, i.e., the three digits the data contains. The plots show that EvoSK is clearly able to separate patterns from different classes with only few outliers. The observation that spending more effort into the search process is advantageous can also be confirmed by the visual inspection of the embeddings. For $\mu = 2$, i.e., only two alternatives in each step, the worst low-dimensional representation is computed with overlapping regions, while the embeddings with $\mu = 10$ have similar shapes like the MDS result. t-SNE computes low-dimensional representations with completely different shapes and three small areas for digit '1'.

EvoSK has numerous advantages in comparison to MDS and t-SNE. With only few and uncomplicated adaptations, it is applicable to large data sets. For embedding a novel pattern, the search for the closest embedded pattern lasts longer with growing data sets. The search can be accelerated with efficient data structures like ball-trees. A stochastic shortcut is to restrict the neighborhood search by sampling μ times from the embedded patterns and choosing the closest pattern $\mathbf{x}^*$ with counterpart $\mathbf{z}^*$.

Further, EvoSK can easily be employed to incomplete data sets. Let $\mathbf{x}_{-i}$ be a pattern that has to be embedded with missing value x_i. The best position for $\mathbf{y}$ can still be computed ignoring the dimensions, in which parts are missing, e.g., we define the error as

$$E_{sk,-i} = \|\mathbf{D}_{\mathbf{X},-i} - \mathbf{D}_{\mathbf{Z},-i}\|_F^2, \qquad (4)$$

Table 1: Experimental analysis of EvoSK and control methods on benchmark problem set mapping to a $q = 2$-dimensional space in terms of E_{sk}. The best results in each line are shown in bold numbers.

	EvoSK				control		
problem	best	mean	dev	worst	MDS	ISOMAP	t-SNE
Digits	**44.17**	45.25	0.89	46.52	48.50	46.91	100.01
Housing	0.27	0.63	0.26	1.01	**0.08**	0.36	33.52
Image	**4.09**	4.54	0.34	5.10	4.24	4.30	32.89
Friedman	**82.14**	83.45	1.63	86.66	92.07	91.65	140.52
Wind	22.32	26.52	3.23	30.17	16.11	**14.41**	84.98

where $\mathbf{D}_{\mathbf{X},-i}$ and $\mathbf{D}_{\mathbf{Z},-i}$ are the distance matrices with the i-th columns and rows missing.

5 CONCLUSIONS

The iterative evolutionary variant of MDS approximates a low-dimensional representation that minimizes the Shepard-Kruskal measure, i.e., optimizes the maintenance of distances of the high-dimensional space in its low-dimensional counterpart. This optimization objective is inspired by MDS. EvoSK is an approximation heuristic with random elements, in particular based on Gaussian sampling. The outcome of the DR result depends on the order the patterns are embedded. But the randomness is the key property to achieve a linear runtime.

In the line of research of iterative constructive embeddings, EvoSK is the first variant that considers only the last n embedded patterns resulting in linear runtime and turning out to be sufficient for minimization of the Shephard-Kruskal measure. Experimental results have shown that the introduced variants can compete with the related method MDS, ISOMAP, and with t-SNE.

The runtime of EvoSK is linear when employing a window size k. For a choice of $k = 50$, the embeddings turn out to show good characteristics. But the results show that EvoSK significantly depends on the effort μ invested into the sampling process.

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