On the Suitability of Connectivity-Extended Local Embedding for Drawing Multivariate Graphs

S. Fahnenschreiber¹, M. Laux¹ and T. von Landesberger¹

¹TU Darmstadt, Germany

Abstract

Multivariate networks are present in various domains such as biology, or social science. In such networks, the nodes often have several quantitative attributes, which determine similarity of nodes (e.g., person's characteristics in social networks). When interpreting these networks, often both node connectivity and node similarity need to be analyzed simultaneously. Such analysis can be supported by suitable layouts.

We present and evaluate a layout for graphs with multivariate numeric attributes, which combines graph structure and node similarity. It extends local dimension reduction techniques (esp. LLE, MEU, or ISOMAP) with graph connectivity information encoded in techniques' local neighborhood function. We evaluate these extensions and available layouts using two conflicting criteria: distance preservation and graph aesthetics. Although the results vary across data sets, the new approach is able to find a balance of these criteria.

Categories and Subject Descriptors (according to ACM CCS): Computer Graphics [I.3.3]: Viewing Algorithms—Computer Graphics [I.3.6]: Methodology and Techniques—Graphics data structures and data types

1. Introduction

Multivariate networks are data structures composed of nodes connected via edges, where nodes have associated multivariate attributes (i.e., multiple variables). Often these attributes are numeric. For example, in social networks, nodes are persons connected via their friendship relations. The persons often have multiple attributes (e.g., age, income, number of children, ...), which determine their similarity (e.g., persons with similar characteristics). In various analytical scenarios, both graph structure and node similarity needs to be considered simultaneously [MAH*12]. For example, social scientists may wish to examine whether friends are alike (i.e., "birds of a feather flock together").

The examination of networks is often supported by visualization using a suitable graph layout. A layout capable of jointly considering node connectivity and nodes with multivariate quantitative attributes would be advantageous for analysis of multivariate networks. It should provide suitable placement of nodes considering data characteristics and should support a multi-aspect data analysis [MAH*12].

By now, a wide variety of network layouts has been presented [DPS02, VLKS*11, HJ07, GFV12]. Broadly speaking,

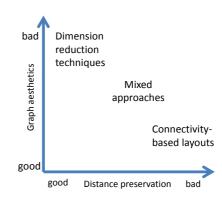


Figure 1: Layout types for drawing multivariate graphs.

three categories are relevant to our work: connectivity-based layouts, attribute-based layouts and mixed approaches (see Figure 1). Connectivity-based layouts (e.g., [KK89, FR91, GK01]) consider only graph structure. They provide pleasing drawings, however disregard node similarity. Dimension reduction-based methods place similar nodes close to each other (e.g., MDS [BP09, TPHL12]. However, they often lead to cluttered displays with long edges and many

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edge crossings. Mixed methods use both node attribute and node connectivity information. They often require categoric attributes (e.g., [SA06]). Some layouts use edge weights (e.g., [KK89]) or layout the graph in two steps initializing connectivity-based layouts by a preceding dimension reduction (e.g., [MAH*12]). To our knowledge, connectivity-extended local dimension reductions have not been used for layouts.

We present and evaluate a new mixed layout for drawing graphs with multivariate quantitative attributes. The proposed approach enhances local dimension reduction techniques with node connectivity information. Without loss of generality, our main idea assumes undirected unweighted graphs with multiple quantitative attributes as input.

We perform a comprehensive evaluation of various layout alternatives and compare them with traditional graph layouts (connectivity-based, attribute-based and mixed). We assess both graph aesthetics and similarity representation for several (smaller) real-world graphs from various application areas (e.g., social networks, biology, telecommunications). The results show that the enhanced techniques using a neighborhood function combining graph structure and node similarity provide reasonable results. They show a good compromise with respect to graph readability and dimension reduction quality. The results are comparable to the best mixed layouts (weighted Kamada Kawai [KK89]). However, the results vary with respect to the underlying graph structure.

The paper is structured as follows: Section 2 presents related work. Section 3 introduces definitions and Section 4 describes our approach. Section 5 presents the set-up and the evaluation results. Section 6 discusses aspects of our approach. Section 7 concludes and outlines future work.

2. Related Work

We review relevant graph layout categories: connectivity-based, dimension reduction-based and mixed layouts. A broad overview can be found in [VLKS*11, HJ07, GFV12].

2.1. Connectivity-based Approaches

These approaches use solely aesthetic criteria.

Force-based layouts form a basis of many graph layouts due to good aesthetic properties (e.g., Kamada-Kawai [KK89], Fruchtermann-Reingold [FR91]). They differ in the definition of the forces. Scalability can be improved, e.g., using a GPU implementation, heuristics or multi scale approaches [GHGH09,FLM95,GK01,KCH02,HJ05].

Several layouts are inspired by dimension reduction: The ISOM method [Mey98a] applies an inverted the Self-Organizing Map algorithm [Koh01]. High Dimensional Embedder (HDE) projects nodes from high-dimensional to two-dimensional space. For both, the layout quality may suffer for graphs with specific topologies.

2.2. Dimension Reduction-Based Layouts

Dimension reduction is widely used for visualization of multivariate data. Many approaches exist [HK06]. For graph layouts, MDS has been used for various graphs [Coh97, BP09, KB13, TPHL12] and PCA was proposed for drawing transition system graphs [PvW05]. Although is possible to layout graphs using other dimension reduction techniques, we are not aware of their usage. All dimension reductions focus on distance preservation and do not regard graph structure. This includes even DD-HDS [LVGF07], which performs dimension reduction with stress minimization using force-directed approach. It focuses on multivariate data without taking graph connectivity into account. Alternatively, GraphDice [BCD*10] uses interactive selection of two variables as layout coordinates. The positioning may not represent node distances well.

In sum, the layouts resulting from (global) dimension reduction represent node distances well, but often lead to cluttered displays with edge crossing problems. Moreover, to our knowledge, mainly "original" (global) dimension reduction techniques without connectivity information have been employed for graph drawing. Local embeddings with additional enhancements, as focused on in this paper, have not been studied well for graph layouts.

2.3. Mixed Approaches

Mixed approaches try to use both graph structure and graph attributes for node positioning.

Some connectivity-based layouts can be enhanced with node similarity information. For example, Kamada-Kawai and Fruchtermann-Reingold [KK89, FR91] layouts may include similarity information encoded as edge weights. Alternatively, the layouts can be initialized by node positions preserving node similarity (e.g. by using a preceding dimension reduction step) [MAH*12]. We evaluate them.

Several graph layouts use semantics of the graph nodes (i.e., categorical attributes). Nodes in the same category are placed in the same area and the layout of nodes within the area is optimized using standard layout algorithms (e.g., force-directed). The form and placement of these areas varies among layouts. For example, Semantic substrates [SA06] uses horizontal boxes and force-directed layout within them. Treenetviz and Space-Filling Force Directed layouts [GZ11, IMMS09] can be used for hierarchic structure of attribute categories. These methods are restricted to categoric node attributes.

Few methods try to directly enhance dimension reduction with graph connectivity. First, JauntyNets [JKZ13] places attributes as additional graph nodes on a circle. Original graph vertices are connected with forces among themselves and with attributes using additional forces. The idea is similar to RadViz [HGP99]. JauntyNets requires edge weights for graph positioning. Moreover, the final layout depends

strongly on the ordering of attributes on the circle. Second, GeoSOM [WT08] uses a modified self organizing map (SOM) with graph weights. The 3D 'earth'-formed SOM is drawn with a 2D cartographic projection. Graph edges at the projections's border are split, which leads to bad readability of graph connections. Moreover, SOM requires careful setting of several learning parameters.

3. Definitions

A graph (i.e., network) G = (V, E) is composed of a set of vertices (nodes) V and a set of edges (i.e., links) $E \subseteq [V^2]$ that connect pairs of adjacent vertices $e = (v_i, v_j)$ [Die05]. A path of length s in G is a sequence of connected nodes path $G(v_1, v_s) = v_1, v_2, \dots, v_s$ where $v_i \in V$ & $(v_i, v_{i+1}) \in E$.

In a multivariate graph, several attributes (i.e., variables) are associated with vertices: $v_i \rightarrow (a_{i1}, \dots, a_{il})$, where l is the dimensionality. Node similarity in attribute space $d^A(v_i, v_j)$ is defined as the Euclidean distance of their attribute vectors $d^A(v_i, v_j) = \sqrt{\sum_{k=1}^{l} \{(a_{ik} - a_{jk})^2\}}$.

4. Approach

In this paper, we present and evaluate a layout algorithm for graphs with multivariate numeric attributes. Our aim is to produce a layout which reveals both node similarities (data attribute structure) and graph connectivity. The node similarity is defined as the Euclidean distance of attributes (see Sec. 3). Without loss of generality, we assume undirected unweighted graphs with multiple numeric attributes.

The main idea of our approach is the enhancement of dimension reduction techniques with graph connectivity information. We decided to use dimension reduction techniques, which use local neighborhood, as they are better capable of finding structures in high dimensional space then global methods (e.g. MDS [CC10]). Moreover, they use local point neighborhood information for dimension reduction [Law11], which allows them to capture data topology in unstructured multivariate data (e.g., manifolds). We alter this function to capture additional graph structural information as needed in our case.

Our approach extends the neighborhood function so that it captures graph structure. We modify the neighborhood definitions N in the relevant parts of the algorithms. In this paper, we focus on three techniques: LLE [RS00], ISOMAP [TDSL00] and MEU [Law11]. Original implementations use as neighborhood n-nearest neighbors (nNN) in the attribute space N^A (see Fig. 2a). For graph layouts, we modify this function with graph-connectivity information. For example, we change the neighborhood N_i of vertex v_i in LLE layout (see Eq. 1). Other algorithms are changed analogously. Note, our approach could be applied also for other dimension reductions using local neighborhoods.

$$e(E) = \sum_{i=0}^{|V|} |v_i - \sum_{j=1}^{|N_i|} w_{ij} v_j|$$
 (1)

We developed and evaluated several neighborhood functions (see Fig. 2b-d).

- 1. Adjacency: Neighborhood $N^G(v_i)$ includes all nodes directly connected to the node v_i (see Fig. 2b).
- 2. *Graph Path*: Neighborhood $N^P(v_i)$ includes all nodes connected v_i via a path up to length 2 (see Fig. 2c).
- 3. Combination of attribute and graph neighborhood: This neighborhood set $N^C(v_i)$ contains the union of the set of n-nearest neighbors in the attribute space and the set of adjacent vertices to the vertex v_i (see Fig. 2d). This method combines the information on graph structure and attribute space structure, within local dimension reduction. We expect it to work best for our use case.

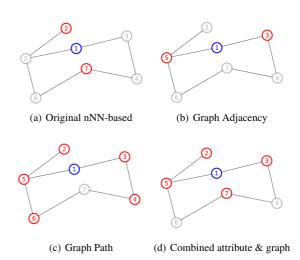


Figure 2: Different neighborhood heuristics. The red colored vertices are considered neighbors to the blue vertex. a) Original nNN neighborhood in attribute space (N^A , n=2) b) Adjacent vertices in the graph N^G . c) Graph path: Vertices within a path length of 2: N^{P_2} d) Combined: Union of attribute- and graph-based neighbors N^C

5. Evaluation

We evaluate our approach on a set of real world graphs with multivariate quantitative attributes. We assess the various neighborhood functions and sizes of our proposed layout and compare the results to selected state-of-the-art layouts. The evaluation relies on several quality criteria composed of graph aesthetics and dimension reduction measures.

5.1. Evaluation Datasets

We evaluate our approach using several real-world graphs with varying structure, attribute dimensionality and applica-

tion domain. We focused on real world graphs, as they represent real problems. The graphs are described below and their properties are shown in Table 1.

Name	#Nodes	#Edges	#Attributes	Avg. Deg.
Regulation	12	26	2500	4.25
Households	29	51	6	3.52
Documents	100	162	5	3.24
Phone Calls	400	916	5	4.58
Amazon	121	186	5	3.07
Patents	98	182	9	3.71

Table 1: Summary data statistics

Regulation: Graph of reactants with their regulating interactions. The attributes are the concentrations substances over time. Provided by Prof. Drossel at TU Darmstadt.

Households: Commonalities among family situations in neighboring geographic regions. European countries with common sea or land borders are connected by edges. The attributes are statistical indicators by OECD Family Database. Documents: Relationships between publications. Attributes are weights of the document's keywords. Source: PubMed. Phone Calls: Phone calls between persons. Attributes are daily phone call durations at 10 successive days. VAST Challenge 2008 data.

Amazon: Products and their co-purchasing. The attributes are numeric product characteristics. Source: SNAP.

Patents: Citations between US Patents. Attributes are patents characteristics. Source: SNAP.

In our evaluation, we concentrated on rather smaller graphs (with hundreds of nodes). This choice was motivated by the common graph exploration path, which often starts with a small subset of a graph being interactively expanded on demand [vHP09]. Moreover, smaller graphs can be visually examined in more detail then larger graphs.

5.2. Evaluation Layouts

We use all variants of the new proposed layout and compare them with a set of representative layouts from the relevant graph layout categories presented in Section 2.

- Connectivity-based layouts: We chose 2 types of layouts: force-directed Kamada-Kawai [KK89] and ISOM [Mey98b]. ISOM is based on inverted dim. reduction. We use JUNG [OMFS*05].
- Dimension reduction-based Layouts: We selected the
 most prominent dimension reduction layout: MDS
 [CC10] in the classical scaling version. Note we tested
 also MDS with stress reduction. It lead to very similar results. For the sake of space, we focus only on one version.
 We used MDSJ [Alg09] package as implementation.
- Mixed layouts We use enhanced force-based layouts with both edge weights representing the similarity and with MDS-based initialization. We chose Kamada-Kawai [KK89] layout extensions as representatives of enhanced

force-based layouts. We use a self-amended JUNG [OMFS*05] implementation.

New approach: We test extensions of three representative local embedding methods: ISOMAP [TDSL00], LLE [RS00] and MEU [Law11]. We use the original implementations provided in the MEU toolkit.

All local dimension reduction algorithms were run on all four neighborhood structures: original, adjacency, graph path and combined (see Section 4). For original and combined versions, we used 5 nearest neighbors: $5 \approx avg(deg) + 2$. This choice assures a balance of graphand attribute-based neighborhood. Section 5.5 analyzes the impact of this choice.

All layouts with random initial node placement were run 10 times in order to minimize the influence of randomization. Iterative approaches were run with 100 iterations. We present the mean of the calculated evaluation metrics.

5.3. Evaluation Criteria

We use two types of evaluation criteria: graph aesthetics and similarity representation. These criteria are derived from the need of a graph layout to facilitate the simultaneous examination of both graph structure and node similarity.

Graph aesthetics: We use the common graph aesthetic criteria used for evaluating graph layouts: number of edge crossings and even edge length [PCJ96, Pur02, BBD09].

Similarity Representation: We rely on common distance preservation (i.e., similarity representation) criteria [BP09, Coh97,SvLB00]. We look both on global and local similarity preservation. On a global level, we use Projection Precision Score (PP) [SvLB00]. On local level, we analyze how the distances between vertices in the original (attribute) space d^A are preserved in the projected (i.e., layout) space d^L . $\forall v_i, v_j \in V : d^L(v_i, v_j) \propto d^A(v_i, v_j)$.

5.4. Evaluation Results

We discuss results for the test graphs. First, we look at edge crossing and projection precisions on global graph level. Then, we analyze edge length distribution and node similarity preservation on local (i.e., vertex) level. Owing to space limitation, we discuss main results. Full set of results also for other quality criteria is in Annex.

5.4.1. Global Evaluation

We show the results for global criteria: the number of edge crossings (EC) [Pur02] and Projection Precision (PP) [SvLB00] criteria. For space efficiency, we plotted the results in a scatterplot (see Fig. 4). Each point is a result of one layout algorithm. Points are color coded according to layout type (see Fig. 3 bottom). This should ensure an easier comparability of results across scatterplots. Layouts close to the axis center (point 0,0) are better. Layouts in top left corner have good projection precision but high edge crossing. Layouts in bottom right corner have opposite propoerties.

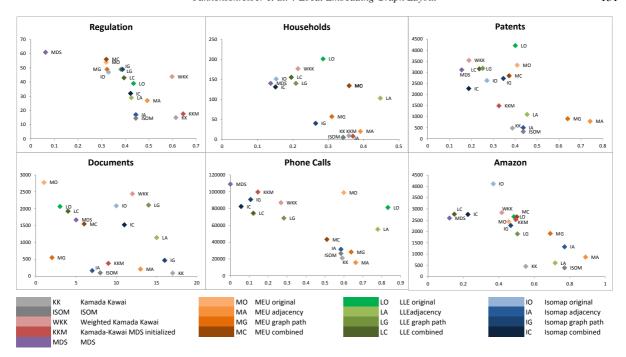


Figure 3: Number of Edge Crossings (Y axis) vs Projection Precision (X axis).

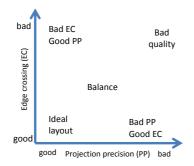


Figure 4: Evaluation chart explanation.

Figure 3 shows the results for all evaluated graphs. The results vary across the graphs. We assume that this variation is caused by a variability in both graph structure and node similarity distribution in the graph. Moreover, some layouts lead to strong overplotting of nodes (esp. original and adjacent dimension reduction layouts) which skews the criteria for the number of edge crossings. Nevertheless, several results can be observed across graphs.

As expected, MDS layout (violet, MDS) performs very well for projection precision, it has large edge crossing. On the other hand, layouts focusing on graph aesthetics: Kamada-Kawai (grey, KK) and ISOM (dark grey, ISOM) have good EC but bad PP scores. Mixed layouts show diverse results. Weighted Kamada-Kawai (pink, KKW) performs better then MDS-initiated Kamada-Kawai (red, KKM), however worse then most of our locally based lay-

outs. KKM has very similar results to original KK layout with bad PP and good EC. Our local layouts using adjacency (LA, MA, and IA) are mostly slightly better but comparable to MDS and KKM (see the points in right bottom corner). This can be explained by their strong focus on graph adjacency, disregarding node similarity. Layouts using graph path (LG, IG, and MG) vary in results across graphs. This may be a result of including more neighborhood vertices in the layout, but still without node similarity notion. It leads to worse results then original and combined layouts. Layouts using original local dimension reduction techniques (LO, IO, MO) perform well with regard to dimension reduction (PP), but have bad edge crossing results, often worse then the original MDS. Interestingly, the proposed layouts combining graph and similarity neighborhood (IC, LC, MC) have better results in EC then MDS with comparable PP quality for several graphs (e.g., phone calls, patents). For the documents graph, MG performs very well for both criteria. This indicates that the new layouts may be able to balance the two criteria comparably or better then other layouts.

5.4.2. Local Evaluation

On a local level, we evaluate the edge length (EL, i.e., distance of neighbors in the layout) and similarity representation (SR) for all vertex pairs.

We calculate and show the distances in attribute space (X-axis) and in layout space (Y-axis) for all neighbours (EL, local SR) (all SR) for all vertex pairs (see Fig. 6). Local SR and EL values are highlighted in red. The form of the red line

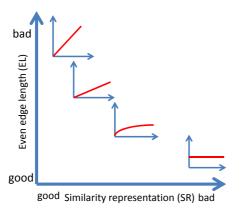


Figure 5: Exemplar results for edge length and similarity preservation criteria.

shows the quality of the result. Very good EL, but bad SP is visible as a "horizontal line" (see Fig. 5). Contrary, good SP, but bad EL, forms an increasing line. Thus, the two criteria are contradictory. A balance of these two criteria may be a bended line or a line with smaller slope.

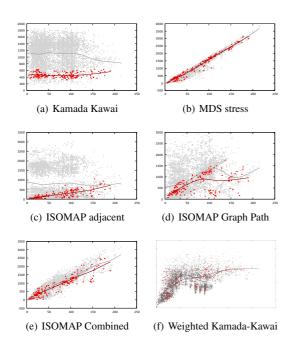


Figure 6: Quality of results for Amazon graph. X-axis: original distance, y-axis layout distance. Adjacent vertices (i.e., edge lengths) are red points, other vertex pairs are gray.

Due to space limitation, we show representative results for Amazon dataset focusing on ISOMAP-based layouts (see Figures 6 and 7). As expected Kamada-Kawai layout has best edge length distribution with horizontally positioned points, but does not preserve SR. MDS preserves distances well but has a large variability in edge lengths.

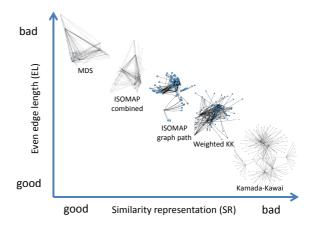


Figure 7: Result graph layouts arranged according to their quality criteria.

Mixed layouts and the new layouts have a distribution of EL and SR between the two extrema. Adjacency ISOMAP performs well for similar vertices, but underestimates distances for more distant vertices. It however leads to many extremely short edges (red points close to 0). Both ISOMAP graph path and weighted Kamada-Kawai show a variable behaviour both for edge lengths and global distances. ISOMAP combined preserves more distances then edge lengths, but is still better then MDS.

5.5. Influence of Neighborhood Size

We analyze how the choice of the neighborhood size influences the resulting layout. Only the combined version requires the setting of neighborhood size. Annex shows the drawings for all graphs, here we show representative results for the documents dataset.

Figure 8 shows that MEU layout strongly depends on the neighborhood size, while LLE and ISOMAP are more robust to size changes. This is explained by the construction of the combined neighborhood which unifies adjacency and n-nearest neighborhood so low size is often compensated by large adjacency neighborhood. We chose average degree + 2 as a rule of thumb, which corresponds to the level when MEU stabilizes.

6. Discussion

In this section, we discuss several aspects of our approach and its evaluation.

Graph type: Our approach and the evaluation focused on unweighted undirected graphs. Applying our algorithm to weighted graphs needs an extension of the neighborhood function. This could be done in the distance matrix employed internally by the algorithms.

Vertex attributes and node similarity: The presented version of our algorithm focused on numeric attributed nodes

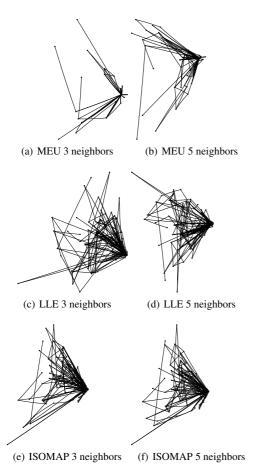


Figure 8: Results for combined MEU, LLE and ISOMAP for 3 and 5 neighbors (left and right).

measuring node similarity. Our approach is also usable for cases when only node similarities are available. They would be included directly in the distance matrix employed by the dimension reduction algorithms.

Runtime: The calculation complexity and runtime were not in the focus of our work. We used available implementations from various authors and in various languages (MATLAB, Java). Therefore, it is not possible to conduct a comparative runtime analysis. We also did not put any effort in parallelization nor in program optimization. For our datasets, the runtimes of up to a second allowed for interactive visualization. The implementations could be optimized in future.

Evaluated graphs: We used several real-world datasets for the evaluation. For a thorough evaluation, it would be advantageous to use many synthetic datasets with controlled characteristics combining various graph structures and various distributions of vertex values (i.e., their node similarity). These datasets are not available. Although the number of graphs is quite small, large graph variability already indicates the pros and cons of layouts. We employed graphs with hundreds of nodes, which was motivated by a common exploration principle: show details, expand on demand [vHP09].

7. Conclusions and Future Work

We presented and evaluated a layout for multivariate graphs. It extends local dimension reduction techniques with graph connectivity notion. An extensive evaluation of the new technique shows that the our layouts and weighted Kamada Kawai layouts are able to balance graph aesthetics and similarity preservation. Combined and graph path extensions are better then original and adjacency-extended local dimension reduction layouts. The results, however, depend on graph structure and distance distribution.

In the future, we would like to focus on optimization of our algorithm and its extension to other graph types such as trees or graphs with multivariate edge attributes. A user study evaluating the influence of the layouts on analytical tasks would be advantageous. It could also show which trade-off the users prefer: distance preservation vs. graph aesthetics.

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