How to Evaluate Dimensionality Reduction?
– Improving the Co-ranking Matrix

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Abstract

The growing number of dimensionality reduction (DR) methods available for data visualization has recently inspired the development of quality assessment measures, in order to evaluate the resulting low-dimensional representation independently from a methods’ inherent criteria. Several (existing) quality measures can be (re)formulated based on the so-called co-ranking matrix, which subsumes all rank errors (i.e., differences between the ranking of distances from every point to all others, comparing the low-dimensional representation to the original data). The measures are often based on the partitioning of the co-ranking matrix into 4 submatrices, divided at the K-th row and K-th column, calculating a weighted combination of the sums of each submatrix. Hence, the evaluation process typically involves plotting a graph over several (or even all possible) settings of the parameter K. Considering simple artificial examples, we argue that this parameter controls two notions at once, that need not necessarily be combined, and that the rectangular shape of submatrices is disadvantageous for an intuitive interpretation of the parameter. We debate that quality measures, as general and flexible evaluation tools, should have parameters with a direct and intuitive interpretation as to which specific error types are tolerated or penalized. Therefore, we propose to replace the parameter K with two distinct parameters to control these notions separately, and introduce a differently shaped weighting scheme on the co-ranking matrix. The two new parameters can then directly be interpreted, respectively, as a threshold up to which rank errors are tolerated, and a threshold up to which the rank-distances are significant for the quality evaluation. Moreover, we propose a color representation of local quality to visually support the evaluation process for a given mapping, where every point in the mapping is colored according to its local contribution to the overall quality value.
1 Introduction

The amount of electronic data available today is becoming larger and larger in virtually all application domains; at the same time, its complexity and dimensionality is increasing rapidly due to improved sensor technology and fine grained measurements as well as dedicated data formats. In consequence, humans can no longer directly deal with such collections by inspecting the text files. Rather, automated tools are required to support humans to extract the relevant information. One core technology is given by data visualization: relying on one of the most powerful senses of humans, it offers the possibility to visually inspect large amounts of data at once and to infer relevant information based on the astonishing cognitive capabilities of humans in visual grouping and similar.

Dimensionality reduction techniques constitute one important method in understanding high-dimensional data because they directly produce a low-dimensional visualization from high-dimensional vectorial data. Consequently, many dimensionality reduction techniques have been proposed in recent years. In the beginning, these methods were primarily linear, like principal component analysis (PCA), corresponding to low cost dimensionality reduction techniques with a well founded mathematical background. However, linear techniques cannot preserve relevant nonlinear structural elements of data. Therefore, recently, more and more nonlinear methods like Isomap \cite{1}, locally linear embedding (LLE) \cite{2}, and stochastic neighbor embedding (SNE) \cite{3} have become popular, see the overview \cite{4}, for example.

With more and more dimensionality reduction techniques being readily available, the user faces the problem which of the methods to choose for the current application. Usually, different techniques can lead to qualitatively very different results. This is due to several reasons: From a theoretical point of view, dimensionality reduction (DR) constitutes an ill-posed problem: Not all relations that exist in the data in the high-dimensional space can be faithfully represented in the low-dimensional space, and it is not clear, which relations should be preserved. This has resulted in different objective functions for the various DR techniques corresponding to qualitatively very different visualizations for a given data set. In addition, virtually all recent techniques have parameters to control the mapping. These parameters usually control (in some way) which relations should be preserved best. Hence, depending on the parameters of the method, even a single DR technique can lead to qualitatively very diverse results. In addition, many techniques do not lead to a unique solution, rather, multiple different outputs can be reached due to random aspects of the algorithm corresponding to different local optima of the objective. Thus, it is even possible that qualitatively different results can be obtained by a single method with a single set of model parameters.

It is usually not clear whether the different results obtained by one or several DR techniques correspond to different relevant structural aspects in the data which are possibly partially contradictory in low dimensions, or whether some of the methods and model parameters are less suited to preserve the relevant structural aspects in the given data set. Further, it can happen that suboptimal results are obtained simply because of numerical problems of a given technique such as (bad) local optima. At the same time, it is very hard for humans to judge the quality of a given mapping and the suitability of a specific technique and choice of parameters by visual inspection: the original data set is not accessible to the user due to its high dimensionality such that a human cannot compare a given visualization to ground truth easily. Therefore, there is a need to develop formal measures which judge the quality of a given mapping of data. Such formal measures should evaluate, in an automated and objective way, in how far structure of the original data corresponds to the structure observed in the low-dimensional representation.

Formal measures to evaluate the quality of a data visualization have several benefits: a formal measure directly indicates whether an observer can trust a given mapping or whether effects of the data visualization are caused by the choice of the method and parameters rather than structures in the data set. Further, a formal quality measure can help humans to choose a good method and a good set of parameters for a given data set. Often, it is not easy to
predict the effects of model parameters on the resulting mapping. Good quality measures can serve as a means to interactively optimize the parameters. Last not least, quality measures are generally important to automatically evaluate and compare DR techniques for research.

Several quality criteria to evaluate dimensionality reduction have been proposed in recent years, see [5] for an overview. As for dimensionality reduction itself, the problem to define formal evaluation criteria suffers from the ill-posedness of the task: it is not clear a priori which structural aspects of the data should be preserved in a given task. Most quality measures which have been proposed recently are based on neighborhood relations of the data. They measure in some way how far neighborhood relationships (e.g. ranks of data points) correspond to each other in the original space compared to the projection. Two recent quality measures offer a general approach and constitute frameworks that include earlier measures as special cases [5, 6]. Regarding this general framework, it becomes apparent that also the quality measure eventually depends on the needs of the user since the user can specify, depending on the task, which aspects of the data are particularly relevant. For example, when dealing with medical data, the user would prefer false positives over false negatives (whatever those may be in the case of dimensionality reduction). Also, data in which manifold structures are expected should be evaluated differently than clustered data.

Therefore, there is a need for intuitive and easily accessible quality measures which allow the user to determine the precise form of the measure based on the current application. That means, there is a need for quality measures with parameters which have an intuitive meaning and which can easily be set by the user. The co-ranking matrix [5] already goes into this direction by pointing out the relevance of the neighborhood rank which the user believes is important.

We will discuss that the global quality measure which has been derived based on this framework in the work [5] does not correspond to an intuitive interpretation by the user: on the one hand, it depends on absolute values of the ranks rather than the deviation of the ranks, i.e. the actual ‘errors’ made by a DR method. On the other hand, it relies on a single parameter only, the size of ranks taken into account, which controls both aspects: which errors are tolerated and which neighborhood relations are considered interesting for the mapping. We show in a simple example that this quality measure leads to unexpected values which do not correspond to an intuitive understanding.

As an alternative, based on the co-ranking framework, we propose a different family of quality criteria which are based on the values of the rank errors rather than the absolute values of the ranks. This family is parameterized by two parameters which control the size of errors which are tolerated on the one hand and the size of the neighborhood of points which should be mapped faithfully by the dimensionality reduction on the other hand. This way, the user can intuitively control the resulting quality measure. We also propose an intuitive way to link formal quality criteria to a given visualization and to actually visualize the quality of a mapping such that the user can immediately see which parts of the mapping are trustworthy and which are not.

2 Dimensionality Reduction and Quality Measures

Dimensionality reduction techniques are used for visualization by mapping a high-dimensional dataset $\Xi = \{\xi_1, \ldots, \xi_N\}$ to a low-dimensional dataset $X = \{x_1, \ldots, x_N\}$. By design and via parameters, DR methods specify which properties should be maintained by the mapping. Some techniques are based on global mappings such as linear techniques, which determine a matrix to reduce the dimensionality of the data set by a linear transformation, or topographic mapping such as the self-organizing map [7], which parameterize a mapping by a lattice of prototypes in the data space. Many modern nonlinear techniques are non-parametric: they map a given set of data points directly to their respective projections without specifying a functional form.
This way, the mapping has large flexibility and highly nonlinear effects can be obtained.

Non-parametric dimensionality reduction is often based on a cost function or objective, which evaluates in how far characteristics of the original data \( \xi \) are preserved by the projections \( x \). Appropriate projections are then determined minimizing this objective with respect to the parameters \( x \). For example, t-SNE maintains the neighborhood probabilities in both spaces, while LLE tries to place points in such a way that locally linear neighborhoods are maintained. See e.g. the article \([8]\) for a general formalization of popular non-parametric dimensionality reduction techniques in this way.

Let us look more closely at the LLE algorithm. First, one fixes a parameter \( K \), that specifies the number of neighbors used to reconstruct a point. For each point \( \xi_i \), find the \( K \) closest neighbors and find weights \( w_{ij} \) such that \( \xi_i \) is best represented by \( \sum_{j=1}^{N} w_{ij} \xi_j \), where at most \( K \) of the \( w_{ij} \)'s are allowed to be non-zero. Finally, low-dimensional mapped points \( x_i \) are chosen such that the differences between \( x_i \) and its neighbor-reconstruction \( \sum_{j=1}^{N} w_{ij} x_j \) are minimal.

A similar process description can be given for t-SNE \([3]\). First, using a fixed perplexity, the probabilities \( \pi_{ij} \) that point \( i \) in the high-dimensional space is neighbored to point \( j \) in the high-dimensional space are estimated. Similar probabilities \( p_{ij} \) for the low-dimensional space are estimated using a Student-t distribution. The positions in the low-dimensional space are optimized by minimizing the Kullback-Leibler divergence between these distributions, i.e., minimizing their dissimilarity.

In both cases, a quality criterion, depending on a parameter, is used to specify an optimal mapping. Thus, for non-parametric DR methods, there is often a close relationship of an objective function which in some way evaluates the quality of a mapping, and a DR algorithm which actually finds projections such that the quality is optimized. Of course, these criteria are partially chosen because they have a nice corresponding optimization method. For LLE, for example, a convex objective guarantees unique solutions. However, as demonstrated in the article \([6]\), a quality criterion itself can also be used to derive a DR model by means of a numeric optimization technique. Conversely, most existing non-parametric DR methods induce a quality measure by which a DR mapping can be evaluated. Naturally, these evaluation criteria are highly biased towards the corresponding DR technique. Further, they are usually not parameterized in an intuitive way and they also incorporate aspects which are important in order to obtain a numerically appealing optimization method rather than a valid evaluation criterion only.

Here we are interested in a criterion which evaluates the quality of DR mappings in a uniform and intuitive way, and which provides a parameterization that allows for an intuitive control by the user. Thereby, it is irrelevant whether the resulting objective also leads to a simple optimization scheme. First approaches in this direction have been proposed based on the co-ranking framework in the articles \([5,9]\).

### 3 The Co-ranking Framework

In the following, we introduce the co-ranking framework as proposed by Lee and Verleysen \([5]\) and we recall several established quality criteria based thereon. Let \( \delta_{ij} \) be the distance from \( \xi_i \) to \( \xi_j \) in the high-dimensional space. Analogously, \( d_{ij} \) is the distance from \( x_i \) to \( x_j \) in the low-dimensional space. From these distances we can compute the ranks of the neighbors for each point. The rank of \( \xi_j \) with respect to \( \xi_i \) in the high-dimensional space is given by

\[
\rho_{ij} = |\{ k \mid \delta_{ik} < \delta_{ij} \text{ or } (\delta_{ik} = \delta_{ij} \text{ and } 1 \leq k < j \leq N) \}|,
\]

where \( |A| \) is the cardinality of the set \( A \), resulting in the ranks \( \{1, \ldots, N-1\} \). Analogously, the rank of \( x_j \) with respect to \( x_i \) in the low-dimensional space is given by

\[
r_{ij} = |\{ k \mid d_{ik} < d_{ij} \text{ or } (d_{ik} = d_{ij} \text{ and } 1 \leq k < j \leq N) \}|.
\]
Many existing quality criteria measure in how far ranks of points are preserved after the reduction to a low-dimensional space. This way, local relationships are evaluated without referring to irrelevant issues such as e.g. scaling of the data.

To generalize such measures, the co-ranking matrix $Q$ \cite{10} is defined by

$$Q_{kl} = |\{(i,j) \mid \rho_{ij} = k \text{ and } r_{ij} = l\}|.$$ 

Errors of a DR mapping correspond to off-diagonal entries of this co-ranking matrix. A point $j$ that gets a lower rank with respect to a point $i$ in the low-dimensional space than in the high-dimensional space, i.e. $\rho_{ij} > r_{ij}$, is called an intrusion. Analogously, if $\xi_j$ has a higher rank in the low-dimensional space it is called an extrusion. As shown in Figure 1, intrusions and extrusions correspond to off-diagonal entries in the upper or lower triangle, respectively.

Usually, a DR mapping is not used to map all relationships of data faithfully. Rather, the preservation of local relationships is important. Hence, rank errors for large ranks are not as critical as rank errors of close points. For this reason, Lee and Verleysen distinguish two types of intrusions/extrusions, those within a $K$-neighborhood, which are benevolent, and those moving across this boundary, which are malign with respect to quality. A $K$-intrusion (resp. $K$-extrusion) is an intrusion for which $r_{ij} < K$ (resp. $\rho_{ij} < K$). Subsequently, mild $K$-intrusions are events for which $r_{ij} < \rho_{ij} \leq K$, while hard $K$-intrusions are defined by $r_{ij} \leq K < \rho_{ij}$. Mild $K$-extrusions and hard $K$-extrusions are defined accordingly.

Based on this setting, a simple quality measure can be defined: it counts the number of points that remain inside the $K$-neighborhood while projecting, i.e., all points which keep their rank, and all mild in- and extrusions:

$$Q_{NX}(K) = \frac{1}{KN} \sum_{k=1}^{K} \sum_{l=1}^{K} Q_{kl}. \quad (1)$$

The normalization ensures that the quality of a perfect mapping equals one.\footnote{Instead of expressing the quality, one could define a measure of error analogously, as $1 - Q_{NX}(K)$.}

The quality criterion is very similar to the local continuity meta-criterion (LCMC) that was proposed by Chen and Buja \cite{11}. In fact, it coincides up to a linear term that accounts for the
quality of a random mapping:

$$\text{LCMC}(K) = Q_{NX}(K) - \frac{K}{N-1}. \quad (2)$$

Note that the range of this quality measure depends on $K$, i.e. the size of the neighborhood which should be preserved by a DR mapping. Often, a graph of the quality values over all possible $K$ (or a sufficient selection thereof) is plotted. These measures have the disadvantage that they depend on $K$, and thus do not give a single decisive number that determines the quality of the mapping. Following the idea of locality-parameters in DR techniques (e.g., the number of neighbors in LLE and the perplexity in t-SNE) Lee and Verleysen make a similar local vs. global evaluation of the quality graph.

To estimate which values of $K$ should be considered local, the following splitting point was proposed in [5]:

$$K_{\text{max}} = \arg \max_{K} \text{LCMC}(K) = \arg \max_{K} \left( Q_{NX}(K) - \frac{K}{N-1} \right).$$

Subtracting the baseline ensures that there is a well-defined maximum that favors locality. Given the splitting point, a local and a global quality measure is obtained by averaging the respective parts of the quality graphs:

$$Q_{\text{local}} = \frac{1}{K_{\text{max}}} \sum_{K=1}^{K_{\text{max}}} Q_{NX}(K), \quad (3)$$

$$Q_{\text{global}} = \frac{1}{N-K_{\text{max}}} \sum_{K=K_{\text{max}}}^{N-1} Q_{NX}(K). \quad (4)$$

Both values range from 0 to 1. As local properties are more important, the authors advise to rank methods according to $Q_{\text{local}}$ and only to consider $Q_{\text{global}}$ in case of a tie.

4 A family of quality criteria based on rank errors

The co-ranking matrix as introduced in [5] offers a very elegant framework to formalize quality criteria based on rank errors. However, it has a severe drawback: The quality $Q_{NX}$ depends on the number of rank errors in a region of interest only, disregarding the size of rank errors.

Let us have a look at the evaluation measure $Q_{NX}$. A region of interest, i.e. a rank $K$ is fixed, following the idea that ranks which are very large (larger than $K$) are not meaningful in the data space and the projection space and thus, they can be disregarded. Hence, only errors within the region of interest are counted. The second role of $K$ is to define what is regarded an error: an error occurs if and only if the region of interest in the original space and the projection space does not coincide. Hence, the actual size of the rank error is not important. Rather, it is checked whether ranks $\leq K$ keep this property while projecting and vice versa. As an extreme case, points which change their rank from 1 to $K$ are not counted as errors, while points which change their rank only from $K$ to $K+1$ are.

This definition of $Q_{NX}(K)$ can lead to curious situations, which demonstrate the unintuitive character of the parameter $K$. Consider the pairwise swapping of points that is shown in Figure 2. The number of points can be chosen arbitrarily. Examining the structure quickly shows that the maximum rank error between these permutations is at most 4 (for example, when the base point moves left, and the other point moves right). Intuitively, if we consider

Note that the points are equidistant, and in case of a tie in distances, the point with the lower alphabetical letter gets assigned the lower rank.
rank error sizes up to 4 as acceptable, this mapping is perfect. This is, however, not the case when looking at $Q_{NX}(5)$: there are still errors. In fact, for every value of $K$ there will be some point that moves from, for example, rank $K$ to a slightly higher rank, and therefore be counted as an error. This is also confirmed by the graph in Figure 3(a) which displays the quality for a row of 20 points. It is hardly possible to detect an intuitive correlation of the size of $Q_{NX}(K)$ and the parameter $K$ based on the observation of the mapping, albeit its errors can be fully characterized by local pairwise swappings.

A look at the co-ranking matrix in Fig. 2 indicates the underlying structure in this case. Since the rank error is always smaller than 5, only 4 off-diagonals of the co-ranking matrix are non-vanishing. Note that the $i$th off-diagonal corresponds to rank errors of size $i$. The quality measure (1), however, only sums over rectangular parts of the co-ranking matrix. This observation also suggests how the quality (1) can be altered to lead to a more intuitive parameterization: rather than rectangular parts only, it should focus on a limited number of off-diagonals corresponding to the size of the rank deviation which is considered acceptable.

As already mentioned, $K$ has also a different role by singling out the region of interest based on the rationale that large ranks are not relevant anyway. For the original quality (1), this choice is controlled by the same parameter $K$: points up to rank $K$ only are considered relevant, at the same time leading to the consequence that errors within this range $K$ are fully accepted. It seems more intuitive to separating this control parameter: in addition to the size of the errors which are tolerated, a region of interest should be controlled independently.

Now, we will formalize this consideration by first reformulating the quality (1) such that the two different roles of $K$ become apparent, and then generalizing this formalization such that an explicit control of the region of interest and the tolerated rank error size becomes possible.

![Figure 2](image-url)  
**Figure 2:** On the left is an example mapping from a one-dimensional set of equidistant points to a slight reordering. Since the points are only pairwise swapped, the changes in rank-distances are rather small. For the same setup with 20 points, this is confirmed by the co-ranking matrix that is shown on the right, with entries depicted on a gray scale. White indicates a zero value, while black corresponds to the maximum value in the matrix.

### 4.1 Analysis of $Q_{NX}(K)$

As discussed in [5], formal evaluation measures judge in how far ranks of points are preserved. Hence, the evaluation measures are based on rank errors

$$E_{ij} = |\rho_{ij} - r_{ij}|$$

which measure the deviation of the rank of two points in the original space and the projection space, respectively. The parameter $K$ has two distinct functions: it limits the region of interest, i.e. the relevant ranks which are regarded when evaluating the quality; and it specifies what is regarded as an error, i.e. which rank deviations are tolerated.

Formally, the first role of $K$ can be captured by a rank significance function $w_s : R \times R \times N \to [0, 1]$ that determines, for any pair of points $i$ and $j$ the extent $w_s(\rho_{ij}, r_{ij}, K)$ to which their
Figure 3: The figure shows quality evaluations for the mapping presented in Figure 2, on the left with the established measure \( Q_{NX}(K) \), on the right with the proposed new measure \( Q'_{NX}(\kappa_s, \kappa_t) \). Both are evaluated for all possible parameter settings \( K \) and \((\kappa_s, \kappa_t)\) respectively. The particular position of \( K = 5 \) is highlighted on the graph in the left figure. \( Q_{NX}(K) \) with \( K \geq 5 \) does not yield values of 1 entirely, which seems rather unintuitive for the given mapping. As expected, the matrix for \( Q'_{NX}(\kappa_s, \kappa_t) \) does have ones, for all \( \kappa_s \geq 5 \).

The particular position of \( K = 5 \) is highlighted on the graph in the left figure. \( Q_{NX}(K) \) with \( K \geq 5 \) does not yield values of 1 entirely, which seems rather unintuitive for the given mapping. As expected, the matrix for \( Q'_{NX}(\kappa_s, \kappa_t) \) does have ones, for all \( \kappa_s \geq 5 \).

rank error should be taken into account. For the quality measure \( Q_{NX}(K) \), we have:

\[
w_s(\rho_{ij}, r_{ij}, K) = \begin{cases} 0 & \rho_{ij} > K \land r_{ij} > K \\ 1 & \text{otherwise.} \end{cases}
\]

To describe the second role of \( K \), we use a function \( w_t : \mathbb{R} \times \mathbb{R} \times \mathbb{N} \to [0, 1] \) that determines the weight of the rank error \( E_{ij} \) for points \( i \) and \( j \) based on their ranks \( \rho_{ij} \) and \( r_{ij} \). According to the definition of \( Q_{NX}(K) \), we have the following error tolerance function:

\[
w_t(\rho_{ij}, r_{ij}, K) = \begin{cases} 0 & (\rho_{ij} \leq K \land r_{ij} > K) \lor (\rho_{ij} > K \land r_{ij} \leq K) \\ 1 & \text{otherwise.} \end{cases}
\]

where we count the overlap of the \( K \) neighborhoods in the original space and the projection space, respectively. The quality is proportional to the number of points which are in the region of interest and which error is acceptable according to the error tolerance:

\[
Q_{NX}(K) = \frac{1}{KN} \sum_{i=1}^{N} \sum_{j=1}^{N} w_s(\rho_{ij}, r_{ij}, K) \cdot w_t(\rho_{ij}, r_{ij}, K).
\]

(5)

As discussed before, a problem of the error tolerance function \( w_t \) is that this function depends on the actual ranks and not on the rank error. Examining Figure 1 confirms this. A point with high-dimensional rank 1 and low-dimensional rank \( K \) is acceptable, although it has an absolute rank error of \( K - 1 \). On the other hand, a point that has high-dimensional rank \( K \) and low-dimensional rank \( K + 1 \) is not acceptable, although its rank error is only 1.

### 4.2 A quality measure based on rank errors

Because of this fact, we propose the following alternative error tolerance function

\[
w_t(\rho_{ij}, r_{ij}, \kappa_t) = \begin{cases} 0 & |\rho_{ij} - r_{ij}| > \kappa_t \\ 1 & \text{otherwise,} \end{cases}
\]

that depends on the rank error rather than the value of the ranks. The cut-off value \( \kappa_t \) determines which error sizes are accepted. We use the same rank significance function \( w_s \) as in (5),
Figure 4: New weighting scheme for the co-ranking matrix (right) as compared to the one proposed by Lee and Verleysen [5] (left): as before, the region of interest is limited to points which have a rank smaller than \( \kappa_s \) either in the original space or the projection space, i.e., the lower right corner is not considered. Within this region of interest, all pairs of points with a rank error smaller than a given tolerance \( \kappa_t \) are counted as correctly projected.

but substitute the parameter \( K \) by the the cut-off parameter \( \kappa_s \). Following equation (5), we then get a new quality measure:

\[
Q'_{NX}(\kappa_s, \kappa_t) = \frac{1}{\kappa_s N} \sum_{i=1}^{N} \sum_{j=1}^{N} w_s(\rho_{ij}, r_{ij}, \kappa_s) \cdot w_t(\rho_{ij}, r_{ij}, \kappa_t).
\]  

(6)

Because of the normalization, values are in the interval \([0, 1]\) with 1 corresponding to a perfect mapping. Figure 4 shows the region of the co-ranking matrix which is taken into account in this quality measure. One might also consider more complex or smooth functions for \( w_s \) and \( w_t \) than simple cut-offs with \( \kappa_s \) and \( \kappa_t \) respectively and corresponding normalization factors, to account for a smooth weighting of the neighborhood size and the size of the errors.

The new quality measure \( Q'_{NX}(\kappa_s, \kappa_t) \) now depends on two parameters instead of only one \( K \) which allow for an intuitive access: \( \kappa_t \) determines which size of the rank errors are tolerated, while \( \kappa_s \) singles out which ranks fall into the region of interest.

We can no longer plot only one graph to picture the quality of a mapping at different stages of \( K \). To get a rich impression of a mapping’s qualitative characteristics, one can instead display a 3D surface or colored matrix, where the position \((\kappa_s, \kappa_t)\) is assigned the value \( Q'_{NX}(\kappa_s, \kappa_t) \), see Figure 3(b) for an example. The matrix in Figure 3(b) shows all values of \( Q'_{NX}(\kappa_s, \kappa_t) \) for the example in Figure 2. It clearly shows that the maximum quality is reached for all \( \kappa_s > 4 \).

Similar to [5], it is possible to subtract the baseline given by a random mapping. Based on this ‘centered’ graph, a baseline can be determined up to which border local values in the matrix are interesting. Then, the given matrix can be connected to a single scalar by averaging over these numbers.

5 Local quality Assessment

The quality criteria introduced in the previous section average the contributions of all points. It can be useful to visually represent the quality (or analogously error) of a single point, in order to gain insight into local qualitative changes, especially when the deviation of the quality of the mapping in the single parts is very high. This principle has been used, for example, to visualize the topographic distortion of self-organizing maps, where one can display the distance
between neurons in the data space as a color in the topographic map, see [7]. Similarly, in the approach [12], the local topographic reliability of dimensionality reduction is displayed.

The quality measure as introduced above naturally gives rise to a local quality which, given a single point, displays the trustworthiness of the map in this area.

First, we examine what to count as visualization errors. To ease this, we assume that every rank change is counted as an error for now, i.e., $\kappa_t = 1$ and $\kappa_s = N - 1$. As a first attempt, one might choose the following point-wise error measure for point $i$:

$$Q'_i = \frac{1}{\kappa_s N} \sum_{j=1}^{N} \left( w_s(\rho_{ij}, r_{ij}, \kappa_s) \cdot w_t(\rho_{ij}, r_{ij}, \kappa_t) \right).$$

However, this is not optimal. Consider the simple example shown in Figure 5. Interchanging the elements a and c induces only rank changes for point b. Given the formula $Q'_i$, only point b would be indicated as erroneous, which does not really reflect our intuitive notion of error. Similarly, we can assume fixed positions for a and c, and move b towards c. Then the ranks for a and c change, while b's remain unchanged, and hence b gets no error. Therefore, we propose to use the symmetric quality:

$$Q'_i = \frac{1}{2\kappa_s N} \sum_{j=1}^{N} \left( w_s(\rho_{ij}, r_{ij}, \kappa_s) \cdot w_t(\rho_{ij}, r_{ij}, \kappa_t) + w_s(\rho_{ji}, r_{ji}, \kappa_s) \cdot w_t(\rho_{ji}, r_{ji}, \kappa_t) \right).$$

This choice assigns a reduced quality to all the three points in the example of Figure 5. Given this measurement, it is easy to color every point in a low-dimensional data visualization according to the local quality measured at the point.

We show an example where this simple coloring scheme clearly indicates which regions of a mapping can be considered trustworthy. In Figure 6(a) we show the popular 'swiss roll' benchmark data set, which consists of points in $\mathbb{R}^3$, uniformly sampled on a spiral-shaped two-dimensional manifold. The data is mapped by t-SNE using a high perplexity parameter which produces an 'unfolded' view of the manifold, with some local tearing and distortion, see Figure 6(b). The coloring clearly reveals the tears within the manifold as well as the larger rank errors that occur at the rightmost points caused by 'unrolling' and putting the inner end of the belt far away from its original neighbors on the next spiral loop level. In a real world scenario, where the original data is high-dimensional and its detailed structure is unknown to the user, the coloring of the mapped points may help to understand local characteristics of the mapping.

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Figure 6: The left figure shows a view of the swiss roll benchmark data set in its original three dimensions, the right-side picture shows a two-dimensional embedding of t-SNE, using a perplexity parameter of 50. Every data point is colored by its amount of contribution to the overall quality, see Equation (7), with $\kappa_s = 96$ and $\kappa_t = 70$. Altogether, the visualization by t-SNE seems to be appropriate for the given data, since the global manifold structure is largely maintained. This is confirmed by the quality-coloring. However, the coloring reveals local tearing of the manifold, as well as errors on the right border, caused by ‘unrolling’ the inner end of the spiral. The latter occurs when referring to the standard Euclidean distance in the original space. Taking geodesic distances, this effect vanishes and only the part where the manifold is teared would be highlighted. The overall quality evaluation is depicted in Figure 7.

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Figure 7: The figure shows quality evaluations for the mapping presented in Figure 6 on top with the established measure $Q_{NX}(K)$, on the bottom with the proposed new measure $Q'_{NX}(\kappa_s, \kappa_t)$. Both are evaluated for all possible parameter settings $K$ and $(\kappa_s, \kappa_t)$ respectively. We recommend to read the bottom matrix by first focusing on some error tolerance value $\kappa_t$, and then read one row of the matrix with all rank significance values $\kappa_s$. 