ON UNSUPERVISED NEAREST-NEIGHBOR REGRESSION AND ROBUST LOSS FUNCTIONS

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Abstract:

In many scientific disciplines structures in high-dimensional data have to be detected, e.g., in stellar spectra, in genome data, or in face recognition tasks. We present an approach to non-linear dimensionality reduction based on fitting nearest neighbor regression to the unsupervised regression framework for learning of low-dimensional manifolds. The problem of optimizing latent neighborhoods is difficult to solve, but the UNN formulation allows an efficient strategy of iteratively embedding latent points to fixed neighborhood topologies. The choice of an appropriate loss function is relevant, in particular for noisy, and high-dimensional data spaces. We extend unsupervised nearest neighbor (UNN) regression by the ε -insensitive loss, which allows to ignore residuals under a threshold defined by ε . In the experimental part of this paper we test the influence of ε on the final data space reconstruction error, and present a visualization of UNN embeddings on test data sets.

1 INTRODUCTION

sensitive loss. Conclusions are drawn in Section 5.

Dimensionality reduction and manifold learning have an important part to play in the understanding of data. In this work we extend the two constructive heuristics for dimensionality reduction called unsupervised K-nearest neighbor regression (Kramer, 2011) by robust loss functions. Meinicke proposed a general unsupervised regression framework for learning lowdimensional manifolds (Meinicke, 2000). The idea is to reverse the regression formulation such that lowdimensional data samples in latent space optimally reconstruct high-dimensional output data. We take this framework as basis for an iterative approach that fits KNN to this unsupervised setting in a combinatorial variant. The manifold problem we consider is a mapping $\mathbf{F}: \mathbf{y} \to \mathbf{x}$ corresponding to the dimensionality reduction for data points $\mathbf{y} \in \mathbf{Y} \subset \mathcal{R}^d$, and latent points $\mathbf{x} \in \mathbf{X} \subset \mathcal{R}^q$ with d > q. The problem is a hard optimization problem as the latent variables X are unknown

In Section 2 we will review related work in dimensionality reduction, unsupervised regression, and KNN regression. Section 3 presents the concept of UNN regression, and two iterative strategies that are based on fixed latent space topologies. In Section 4 we extend UNN to robust loss functions, i.e., the ε -in-

2 RELATED WORK

Dimensionality reduction is the problem of learning a mapping from high-dimensional data space to a space with lower dimensions, while losing as little information as possible. Many dimensionality reduction methods have been proposed in the past, a very famous one is principal component analysis (PCA), which assumes linearity of the manifold (Jolliffe, 1986; Pearson, 1901). An extension for learning non-linear manifolds is kernel PCA (Schölkopf et al., 1998) that projects the data into a Hilbert space. Further famous approaches for dimensionality reduction are Isomap by Tenenbaum *et al.* (Tenenbaum et al., 2000), locally linear embedding (LLE) by Roweis and Saul (Roweis and Saul, 2000), and principal curves by Hastie and Stuetzle (Hastie and Stuetzle, 1989).

2.1 Unsupervised Regression

The work on unsupervised regression for dimensionality reduction started with Meinicke (Meinicke, 2000), who introduced the corresponding algorithmic framework for the first time. In this line of

164 Kramer O.. ON UNSUPERVISED NEAREST-NEIGHBOR REGRESSION AND ROBUST LOSS FUNCTIONS. DOI: 10.5220/0003749301640170 In Proceedings of the 4th International Conference on Agents and Artificial Intelligence (ICAART-2012), pages 164-170 ISBN: 978-989-8425-95-9 Copyright © 2012 SCITEPRESS (Science and Technology Publications, Lda.) research early work concentrated on non-parametric kernel density regression, i.e., the counterpart of the Nadaraya-Watson estimator (Meinicke et al., 2005) denoted as unsupervised kernel regression (UKR).

Let $\mathbf{Y} = (\mathbf{y}_1, \dots, \mathbf{y}_N)$ with $\mathbf{y}_i \in \mathcal{R}^d$ be the matrix of high-dimensional patterns in data space. We seek for a low-dimensional representation, i.e., a matrix of latent points $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$, so that a regression function **f** applied to **X** *point-wise optimally reconstructs the patterns*, i.e., we search for an **X** that minimizes the reconstruction in data space. The optimization problem can be formalized as follows:

minimize
$$E(\mathbf{X}) = \frac{1}{N} \|\mathbf{Y} - \mathbf{f}(\mathbf{x}; \mathbf{X})\|^2$$
. (1)

 $E(\mathbf{X})$ is called data space reconstruction error (DSRE). Latent points **X** define the low-dimensional representation. The regression function applied to the latent points should optimally *reconstruct* the high-dimensional patterns. The regression model **f** induces its capacity, i.e., the kind of structure it is able to represent, to the mapping.

The unsupervised regression framework works as follows:

- Initialize latent variables $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$,
- minimize $E(\mathbf{X})$ w.r.t. DSRE employing an optimization / cross-validation scheme,
- evaluate embedding.

Many regression methods can fit into this framework. A typical example is unsupervised kernel regression, analyzed by Klanke and Ritter (Klanke and Ritter, 2007), but further methods can also be employed.

Klanke and Ritter (Klanke and Ritter, 2007) introduced an optimization scheme based on LLE, PCA, and leave-one-out cross-validation (LOO-CV) for UKR. Carreira-Perpiñán and Lu (Carreira-Perpiñán and Lu, 2010) argue that training of non-parametric unsupervised regression approaches is quite expensive, i.e., $O(N^3)$ in time, and $O(N^2)$ in memory. Parametric methods can accelerate learning, e.g., unsupervised regression based on radial basis function networks (RBFs) (Smola et al., 2001), Gaussian processes (Lawrence, 2005), and neural networks (Tan and Mavrovouniotis, 1995).

2.2 KNN Regression

In the following, we give a short introduction to Knearest neighbor regression that is basis of the UNN approach. KNN is a technique with long tradition. It was first mentioned by Fix and Hodges (Fix and Hodges, 1951) in the fifties in an unpublished US Air Force School of Aviation Medicine report as nonparametric classification technique. Cover and Hart (Cover and Hart, 1967) investigated the approach experimentally in the sixties. Interesting properties have been found, e.g., that for K = 1, and $N \rightarrow \infty$, KNN is bound by the Bayes error rate.

The problem in regression is to predict output values $\mathbf{y} \in \mathcal{R}^d$ of given input values $\mathbf{x} \in \mathcal{R}^q$ based on sets of N input-output examples $((\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_N, \mathbf{y}_N))$. The goal is to learn a function $\mathbf{f} : \mathbf{x} \to \mathbf{y}$ known as regression function. We assume that a data set consisting of observed pairs $(\mathbf{x}_i, \mathbf{y}_i) \in \mathbf{X} \times \mathbf{Y}$ is given. For a novel pattern \mathbf{x}' KNN regression computes the mean of the function values of its K-nearest neighbors:

$$\mathbf{f}_{knn}(\mathbf{x}') = \frac{1}{K} \sum_{i \in \mathcal{N}_{K}(\mathbf{x}')} \mathbf{y}_{i}$$
(2)

with set $\mathcal{N}_{K}(\mathbf{x}')$ containing the indices of the *K*-nearest neighbors of \mathbf{x}' . The idea of KNN is based on the assumption of locality in data space: In local neighborhoods of \mathbf{x} patterns are expected to have similar output values \mathbf{y} (or class labels) compared to $\mathbf{f}(\mathbf{x})$. Consequently, for an unknown \mathbf{x}' the label must be similar to the labels of the closest patterns, which is modeled by the average of the output value of the *K* nearest samples. KNN has been proven well in various applications, e.g., in the detection of quasars based on spectroscopic data (Gieseke et al., 2010).

3 UNSUPERVISED KNN REGRESSION

In this section we introduce the iterative strategy for UNN regression (Kramer, 2011) that is based on minimization of the data space reconstruction error (DSRE).

3.1 Concept

An UNN regression manifold is defined by variables $\mathbf{x} \in \mathbf{X} \subset \mathcal{R}^q$ with unsupervised formulation of an UNN regression manifold

$$\mathbf{f}_{UNN}(\mathbf{x};\mathbf{X}) = \frac{1}{K} \sum_{i \in \mathcal{N}_{K}(\mathbf{x},\mathbf{X})} \mathbf{y}_{i}.$$
 (3)

Matrix \mathbf{X} contains the latent points \mathbf{x} that define the manifold, i.e., the low-dimensional representation of data \mathbf{Y} . Parameter \mathbf{x} is the location where the function is evaluated. An optimal UNN regression manifold minimizes the DSRE

minimize
$$E(\mathbf{X}) = \frac{1}{N} \|\mathbf{Y} - \mathbf{f}_{UNN}(\mathbf{x}; \mathbf{X})\|_F^2$$
, (4)

with Frobenius norm

$$\|\mathbf{A}\|_{F}^{2} = \sqrt{\sum_{i=1}^{d} \sum_{j=1}^{N} |a_{ij}|^{2}}.$$
 (5)

In other words: an optimal UNN manifold consists of low-dimensional points X that minimize the reconstruction of the data points Y w.r.t. the KNN regression method. Regularization in UNN regression is not as important as regularization in other methods that fit into the unsupervised regression framework. For example, in UKR regularization means penalizing extension in latent space with $E_p(\mathbf{X}) = E(\mathbf{X}) + \lambda \|\mathbf{X}\|$, and weight λ (Klanke and Ritter, 2007). In KNN regression moving the low-dimensional data samples infinitely apart from each other does not have the same effect as long as we can still determine the Knearest neighbors. But for practical purposes (limitation of size of numbers) it might be reasonable to restrict continuous KNN latent spaces as well, e.g., to $\mathbf{x} \in [0,1]^q$. In the following section fixed latent space topologies are used that do not require further regularization.

3.2 Iterative Strategy 1

For KNN not the absolute positions of data samples in latent space are relevant, but the relative positions that define the *neighborhood relations*. This perspective reduces the problem to a combinatorial search for neighborhoods $\mathcal{N}_{K}(\mathbf{x}_{i}, \mathbf{X})$ with i = 1, ..., N that can be solved by testing all combinations of *K*-element subsets of *N* elements. The problem is still difficult to solve, in particular for high dimensions.

The idea of our first iterative strategy (UNN 1) is to iteratively assign the data samples to a position in an existing latent space topology that leads to the lowest DSRE. We assume fixed neighborhood topologies with equidistant positions in latent space, and therefore restrict the optimization problem of Equation (3) to a search in a subset of latent space.

As a simple variant we consider the linear case of the latent variables arranged equidistantly on a line $\mathbf{x} \in \mathcal{R}$. In this simplified case only the order of the elements is important. The first iterative strategy works as follows:

- 1. Choose one element $\mathbf{y} \in \mathbf{Y}$,
- 2. test all $\hat{N} + 1$ intermediate positions of the \hat{N} embedded elements $\hat{\mathbf{Y}}$ in latent space,
- 3. choose the latent position that minimizes $E(\mathbf{X})$, and embed \mathbf{y} ,
- remove y from Y, add y to Ŷ, and repeat from Step 1 until all elements have been embedded.



Figure 1: UNN 1: illustration of embedding of a lowdimensional point to a fixed latent space topology w.r.t. the DSRE testing all $\hat{N} + 1$ positions.

Figure 1 illustrates the $\hat{N} + 1$ possible embeddings of a data sample into an existing order of points in latent space (yellow/bright circles). The position of element \mathbf{x}_3 results in a lower DSRE with K = 2 than the position of \mathbf{x}_5 , as the mean of the two nearest neighbors of \mathbf{x}_3 is closer to \mathbf{y} than the mean of the two nearest neighbors of \mathbf{x}_5 .

Each DSRE evaluation takes *Kd* computations. It is easily possible to save the *K* nearest neighbors in latent space in a list, so that the search for indices $\mathcal{N}_{K}(\mathbf{x}, \mathbf{X})$ takes O(1) time. The embedding of *N* elements takes $(N+2) \cdot ((N+1)/2) \cdot Kd$ steps, i.e., $O(N^{2})$ time.

3.3 Iterative Strategy 2

The iterative approach introduced in the last section tests all intermediate positions of previously embedded latent points. We proposed a second iterative variant (UNN 2) that only tests the neighbored intermediate positions in latent space of the nearest embedded point $\mathbf{y}^* \in \hat{\mathbf{Y}}$ in data space (Kramer, 2011). The second iterative strategy works as follows:

- 1. Choose one element $\mathbf{y} \in \mathbf{Y}$,
- 2. look for the nearest $\mathbf{y}^* \in \hat{\mathbf{Y}}$ that has already been embedded (w.r.t. distance measure like Euclidean distance),
- choose the latent position next to x* that minimizes E(X) and embed y,
- 4. remove y from Y, add y to $\hat{\mathbf{Y}}$, and repeat from Step 1 until all elements have been embedded.

Figure 2 illustrates the embedding of a 2dimensional point **y** (yellow) left or right of the nearest point \mathbf{y}^* in data space. The position with the lowest DSRE is chosen. In comparison to UNN 1, \hat{N} distance comparisons in data space have to be computed, but only two positions have to be tested w.r.t. the data space reconstruction error. UNN 2 computes the



Figure 2: UNN 2: testing only the neighbored positions of the nearest point y^* in data space.

nearest embedded point \mathbf{y}^* for each data point taking $(N+1) \cdot (N/2) \cdot d$ steps. Only for the two neighbors the DSRE has to be computed, resulting in an overall number of $(N+1) \cdot N/2 \cdot d + N \cdot 2Kd$ steps. Hence, UNN 2 takes $O(N^2)$ time for the whole embedding.

3.4 Experiments

In the following, we present a short experimental evaluation of UNN regression on a 3-dimensional S data set (3D-S), and a test problem from the USPS digits data set (Hull, 1994). The 3D-S variant without a hole consists of 500 data points. Figure 3(a) shows the order of elements of the 3D-S data set at the beginning. The corresponding embedding with UNN 1 and K = 10 is shown in Figure 3(b). Similar colors correspond to neighbored points in latent space. Figure 4 shows the embedding of 100 data samples of 256dimensional (16 x 16 pixels) images of handwritten digits (2's). We embed a one-dimensional manifold, and show the high-dimensional data that is assigned to every 14th latent point. We can observe that neighbored digits are similar to each other, while digits that are dissimilar are further away from each other in latent space.



Figure 3: Results of UNN on 3D-S: (a) the unsorted S at the beginning, (b) the embedded S with UNN 1 and K = 10. Similar colors represent neighborhood relations in latent space.



Figure 4: UNN 2 embeddings of 100 digits (2's) from the USPS data set. The images are shown that are assigned to every 14th embedded latent point. Similar digits are neighbored in latent space.

4 ROBUST LOSS FUNCTIONS

Loss functions have an important part to play in machine learning, as they define the error and thus the design objective. In this section we introduce the ε insensitive loss for UNN regression.

4.1 ε-Insensitive Loss

In case of noisy data sets over-fitting effects may occur. The employment of the ε -insensitive loss allows to ignore errors beyond a level of ε , and avoids over-fitting to curvatures of the data that may only be caused by noise effects¹. With the design of a loss function, the emphasis of outliers can be controlled. First, the residuals are computed. In case of unsuper-

¹Of course, it is difficult to decide, and subject to the application domain, if the curvature of the data manifold is substantial or noise.

vised regression, the error is computed in two steps:

The distance function δ : R^q × R^d → R maps the difference between the prediction f(x) and the desired output value y to a value according to the distance w.r.t. a certain measure. We employ the Minkowski metric:

$$\delta(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^{N} |\mathbf{f}(\mathbf{x}_i) - \mathbf{y}_i)|\right)^{1/p}, \quad (6)$$

which corresponds to the Manhattan distance for p = 1, and to the Euclidean distance for p = 2.

The loss function L: R → R maps the residuals to the learning error. With the design of the loss function the influence of residuals can be controlled. In the best case the loss function is chosen according to the needs of the underlying data mining model. Often, low residuals are penalized less than high residuals (e.g. with a quadratic function). We will concentrate on the ε-insensitive loss in the following.

Let *r* be the residual, i.e., the distance δ in data space. L_1 and L_2 loss functions are often employed, see the Frobenius norm (Equation 5). The L_1 loss is defined as

$$L_1(r) = ||r||, (7)$$

and L_2 is defined as

$$L_2(r) = r^2. (8)$$

We will use the L_2 loss for measuring the final DSRE, but concentrate on the ε -insensitive loss L_{ε} during training of the UNN model. The L_{ε} is defined as:

$$L_{\varepsilon}(r) = \begin{cases} 0 & \text{if } |r| < \varepsilon \\ |r| - \varepsilon & \text{if } |r| \ge \varepsilon \end{cases}$$
(9)

 L_{ε} is not differentiable at $|r| = \varepsilon$.

4.2 Experiments

In the following, we concentrate on the influence of loss functions on the UNN embedding. For this sake, we employ two kinds of ways to evaluate the final embedding: We measure the final L_2 -based DSRE, visualize the results by colored embeddings, and show the latent order of the embedded objects. We concentrate on two data sets, i.e., a 3D-S data set with noise, and the USPS handwritten digits.

4.2.1 3D-S with Noise

In the first experiment, we concentrate on the 3D-*S* data set. Noise is modeled by multiplying each data point of the 3D-*S* with a random value drawn from

the Gaussian distribution: $\mathbf{y}' = \mathcal{N}(0, \boldsymbol{\sigma}) \cdot \mathbf{y}$. Table 1 shows the experimental results of UNN 1 and UNN 2 concentrating on the ε -insensitive loss for K = 5, and Minkowski metric with p = 2 on the 3D-S data set with hole $(3D-S_h)$. The left part shows the results for 3D-S without noise, the right part shows the results with noise ($\sigma = 5.0$). At first, we concentrate on the experiments without noise. We can observe that (1) the DSRE achieved by UNN 1 is minimal for the lowest ε , and (2), for UNN 2 low DSRE values are achieved with increasing ε (to a limit as of $\varepsilon = 3.0$), but the best DSRE of UNN 2 is worse than the best of UNN 1. Observation (1) can be explained as follows. Without noise for UNN 1 ignoring residuals is disadvantageous: all intermediate positions are tested, and a good local optimum can be reached. For observation (2) we can conclude that a way against local optima of UNN 2 is to ignore residuals.

For the experiments with noise of the magnitude $\sigma = 5.0$ we can observe a local DSRE minimum: for $\epsilon = 0.8$ in case of UNN 1, and $\epsilon = 3.0$ in case of UNN 2. For UNN 1 local optima caused by noise can be avoided by ignoring residuals, for UNN 2 this is already the case without noise. Furthermore, for UNN 2 we observe the optimum at the same level of ϵ .

Table 1: Influence of the ε -insensitive loss on final DSRE (L_2) of UNN for problem 3D- S_h with, and without noise

	$\sigma = 0.0$		$\sigma = 5.0$	
ε	UNN 1	UNN 2	UNN 1	UNN 2
0.2	47.432	77.440	79.137	85.609
0.4	48.192	77.440	79.302	85.609
0.6	51.807	76.338	78.719	85.609
0.8	50.958	76.338	77.238	84.422
1.0	64.074	76.427	79.486	84.258
2.0	96.026	68.371	119.642	82.054
3.0	138.491	50.642	163.752	80.511
4.0	139.168	50.642	168.898	82.144
5.0	139.168	50.642	169.024	83.209
10.0	139.168	50.642	169.024	83.209

Figures 5 (a) and (b) show embeddings of UNN 1 and UNN 2 without noise, and the settings $\varepsilon = 0.2$, and $\varepsilon = 3.0$, corresponding to the settings of Table 1 that are shown in bold. Similar colors correspond to neighbored embeddings in latent space. The visualization shows that for both embeddings neighbored points in data space have similar colors, i.e., they correspond to neighbored latent points. The UNN 1 embedding results in a lower DSRE. This can hardly be recognized from the visualization. Only the blue points of UNN 2 seem to be distributed on the upper and lower part of the 3D-*S*, which may represent a local optimum.

Figures 6 (a) and (b) show the visualization of the



Figure 5: Visualization of the best UNN 1 and UNN 2 embeddings (lowest DSRE, bold values in Table 1) of $3D-S_h$ without noise.

UNN embeddings on the noisy 3D-*S*. The structure of the 3-dimensional *S* is obviously disturbed. Nevertheless, neighbored parts in data space are assigned to similar colors. Again, the UNN 1 embedding seems to be slightly better than the UNN 2 embedding, blue points can again be observed at different parts of the structure, representing local optima.

4.2.2 USPS Digits

To demonstrate the effect of the ε -insensitive loss for data spaces with higher dimensions, we employ the USPS handwritten digits data set with d = 256 again by showing the DSRE, and presenting a visualization of the embeddings. Table 2 shows the final DSRE (w.r.t. the L_2 -loss) after training with the ε -insensitive loss with various parameterizations for ε . We used the setting K = 10, and p = 10.0 for the Minkowski metric. The results for digit 5 show that a minimal DSRE has been achieved for $\varepsilon = 3.0$ in case of UNN 1, and $\varepsilon = 5.0$ for UNN 2 (a minimum of R = 429.75561was found for $\varepsilon = 4.7$). Obviously, both methods can profit from the use of the ϵ -insensitive loss. For digit 7, and UNN 1 ignoring small residuals does not seem to improve the learning result, while for UNN 2 $\varepsilon = 4.0$ achieves the best embedding.

Figure 7 shows two UNN 2 embeddings of the handwritten digits data set for $\varepsilon = 2.0$, and $\varepsilon = 20.0$.

Figure 6: Visualization of the best UNN 1 and UNN 2 embeddings (lowest DSRE, bold values in Table 1) of 3D- S_h with noise $\sigma = 5.0$.

Table 2: Influence of ϵ -insensitive loss on final DSRE of UNN on the digits data set.

	digits 5's		digits 7's	
ε	UNN 1	UNN 2	UNN 1	UNN 2
0.0	423.8	440.2	225.4	222.8
1.0	423.8	440.2	225.4	222.8
2.0	423.8	440.2	225.6	222.8
3.0	423.5	440.2	238.1	221.0
4.0	441.3	440.2	262.1	218.2
5.0	488.7	432.3	264.8	221.4
6.0	496.9	434.2	265.6	220.8
10.0	494.6	434.3	268.4	220.8



Figure 7: Comparison of UNN 2 embeddings of 5's from the handwritten digits data set. The figures show every 14th embedding of the sorting w.r.t. 100 digits for $\varepsilon = 2.0$, and $\varepsilon = 20.0$.

For both settings similar digits are neighbored in latent space. But we can observe that for $\varepsilon = 20.0$ a

broader variety in the data set is covered. The loss function does not concentrate on fitting to noisy parts of the data, but has the capacity to concentrate on the important structures of the data.

5 CONCLUSIONS

Fast dimensionality reduction methods are required that are able to process huge data sets, and large dimensions. With UNN regression we have fitted well-known established regression technique into the unsupervised setting for dimensionality reduction. The two iterative UNN strategies are efficient methods to embed high-dimensional data into fixed onedimensional latent space. We have introduced two iterative local variants that turned out to be performant on test problems in first experimental analyses. UNN 1 achieves lower DSREs, but UNN 2 is slightly faster because of the multiplicative constants of UNN 1. We concentrated on the employment of the E-insensitive loss, and its influence on the DSRE. It Meinicke, P. (2000). Unsupervised Learning in a Generalcould be observed that both iterative UNN regression strategies could benefit from the ɛ-insensitive loss, in particular the iterative variant UNN 2 could be improved employing a loss with $\varepsilon > 0$. Obviously, local optima can be avoided. The experimental results have shown that this effect cannot only be observed for low-dimensional data with noise, but also for highdimensional, i.e., the digits data set.

Our future work will concentrate on the analysis of local optima of UNN embeddings, and on possible extensions to guarantee global optimal solutions. This work will include the analysis of stochastic global search variants. Furthermore, the UNN strategies will be extended to latent topologies with higher dimensionality. Another possible extension of UNN is a continuous backward mapping from latent to data space $\mathbf{f}: \mathbf{x} \to \mathbf{y}$ employing a distance-weighted variant of KNN. A backward mapping can be used for generating high-dimensional data based on sampling in latent space.

REFERENCES

- Carreira-Perpiñán, M. Á. and Lu, Z. (2010). Parametric dimensionality reduction by unsupervised regression. In Conference on Computer Vision and Pattern Recognition (CVPR), pages 1895-1902.
- Cover, T. and Hart, P. (1967). Nearest neighbor pattern classification. IEEE Transactions on Information Theory, 13:21-27.
- Fix, E. and Hodges, J. (1951). Discriminatory analysis, nonparametric discrimination: Consistency properties. 4.

- Gieseke, F., Polsterer, K. L., Thom, A., Zinn, P., Bomanns, D., Dettmar, R.-J., Kramer, O., and Vahrenhold, J. (2010). Detecting quasars in large-scale astronomical surveys. In International Conference on Machine Learning and Applications (ICMLA), pages 352–357.
- Hastie, Y. and Stuetzle, W. (1989). Principal curves. Journal of the American Statistical Association, 85(406):502-516.
- Hull, J. (1994). A database for handwritten text recognition research. IEEE Trans. on PAMI, 5(16):550-554.
- Jolliffe, I. (1986). Principal component analysis. Springer series in statistics. Springer, New York.
- Klanke, S. and Ritter, H. (2007). Variants of unsupervised kernel regression: General cost functions. Neurocomputing, 70(7-9):1289-1303.
- Kramer, O. (2011). Dimensionalty reduction by unsupervised nearest neighbor regression. In Proceedings of the 10th International Conference on Machine Learning and Applications (ICMLA). IEEE, to appear.
- Lawrence, N. D. (2005). Probabilistic non-linear principal component analysis with gaussian process latent variable models. Journal of Machine Learning Research, 6:1783-1816.
- ized Regression Framework. PhD thesis, University of Bielefeld.
- Meinicke, P., Klanke, S., Memisevic, R., and Ritter, H. (2005). Principal surfaces from unsupervised kernel regression. IEEE Trans. Pattern Anal. Mach. Intell., 27(9):1379-1391.
- Pearson, K. (1901). On lines and planes of closest fit to systems of points in space. Philosophical Magazine, 2(6):559-572.
- Roweis, S. T. and Saul, L. K. (2000). Nonlinear dimensionality reduction by locally linear embedding. Science, 290:2323-2326.
- Schölkopf, B., Smola, A., and Müller, K.-R. (1998). Nonlinear component analysis as a kernel eigenvalue problem. Neural Computation, 10(5):1299-1319.
- Smola, A. J., Mika, S., Schölkopf, B., and Williamson, R. C. (2001). Regularized principal manifolds. Journal of Machine Learning Research, 1:179–209.
- Tan, S. and Mavrovouniotis, M. (1995). Reducing data dimensionality through optimizing neural network inputs. AIChE Journal, 41(6):1471-1479.
- Tenenbaum, J. B., Silva, V. D., and Langford, J. C. (2000). A global geometric framework for nonlinear dimensionality reduction. Science, 290:2319-2323.