

Impact of Data Dimensionality Reduction on Neural Based Classification: Application to Industrial Defects

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Abstract. A major step for high-quality optical surfaces faults diagnosis concerns scratches and digs defects characterisation. This challenging operation is very important since it is directly linked with the produced optical component's quality. To complete optical devices diagnosis, a classification phase is mandatory since a number of correctable defects are usually present beside the potential "abiding" ones. Unfortunately relevant data extracted from raw image during defects detection phase are high dimensional. This can have harmful effect on behaviors of artificial neural networks which are suitable to perform such a challenging classification. Reducing data dimension to a smaller value can however decrease problems related to high dimensionality. In this paper we compare different techniques which permit dimensionality reduction and evaluate their possible impact on classification tasks performances.

1 Introduction

We are involved in fault diagnosis of optical devices in industrial environment. In fact, classification of detected faults is among chief phases for succeeding in such diagnosis. Aesthetic flaws, shaped during different manufacturing steps, could provoke harmful effects on optical devices' functional specificities, as well as on their optical performances by generating undesirable scatter light, which could seriously degrade the expected optical features. Taking into account the above-mentioned points, a reliable diagnosis of these defects in high-quality optical devices becomes a crucial task to ensure products' nominal specification and to enhance the production quality. Moreover, the diagnosis of these defects is strongly motivated by manufacturing process correction requirements in order to guarantee mass production (repetitive) quality with the aim of maintaining acceptable production yield.

Unfortunately, detecting and measuring such defects is still a challenging dilemma in production conditions and the few available automatic control solutions remain ineffective. That's why, in most of cases, the diagnosis is performed on the basis of a human expert based visual inspection of the whole production. However, this usual

solution suffers from several acute restrictions related to human operator's intrinsic limitations (reduced sensitivity for very small defects, detection exhaustiveness alteration due to attentiveness shrinkage, operator's tiredness and weariness due to repetitive nature of fault detection and fault diagnosis tasks).

To overcome these problems we have proposed a detection approach based on Nomarski's microscopy issued imaging [1] [2]. This method provides robust detection and reliable measurement of outward defects, making plausible a fully automatic inspection of optical products. However, the above-mentioned detection process should be completed by an automatic classification system in order to discriminate the "false" defects (correctable defects) from "abiding" (permanent) ones. In fact, because of industrial environment, a number of correctable defects (like dusts or cleaning marks) are usually present beside the potential "abiding" defects. That is why the association of a faults' classification system to the aforementioned detection module is a foremost supply to ensure a reliable diagnosis. In a precedent paper [3], we proposed a method to extract relevant data from raw Nomarski images. In the aim of effectively classify these descriptors, neural network based techniques seem appropriate because they have shown many attractive features in complex pattern recognition and classification tasks [4] [5]. But we are dealing with high dimensional data (13 and more components vectors), therefore behaviour of a number of these algorithms could be affected. To avoid this problem we are investigating different dimension reduction techniques for achieving better classification (in terms of performance and processing time).

This paper is organized as follows: in the next section, motivations for reducing data dimensionality and also SOM, CCA and CDA, three technique carrying out this task are introduced. These techniques have been tested using an experimental protocol presented in Section 3. The Section 4 deals with experiments results: first a comparison of data projection quality and an analysis of their possible impact on classification tasks are carried out. Secondly this impact is demonstrated on a classification task involving Multilayer Perceptron artificial neural network. Finally, the Section 5 will conclude this work and will give a number of perspectives.

2 Data Dimensionality Reduction Techniques

It can be found in literature, lot of examples using various dimension reduction techniques (linear or not) as a preliminary step before more refined processing, among which, Self Organizing Maps (SOM) [6;7], Curvilinear Component Analysis (CCA) [8;9] and Curvilinear Distance Analysis (CDA) [10].

2.1 The "curse of dimensionality"

Dealing with high-dimensional data indeed poses problems, known as "curse of dimensionality" [9]. First, sample number required to reach a predefined level of precision in approximation tasks, increases exponentially with dimension. Thus, intuitively, the sample number needed to properly learn problem becomes quickly much

too large to be collected by real systems, when dimension of data increases. Moreover surprising phenomena appear when working in high dimension [11] : for example, variance of distances between vectors remains fixed while its average increases with the space dimension, and Gaussian kernel local properties are also lost. These last points explain that behaviour of a number of artificial neural network algorithms could be affected while dealing with high-dimensional data. Fortunately, most real-world problem data are located in a manifold of dimension p much smaller than its raw dimension. Reducing data dimensionality to this smaller value can therefore decrease the problems related to high dimension.

2.2 Self-Organizing Maps (SOM)

Self-Organizing Map is a classical method originally proposed by Kohonen [12]. This algorithm projects multidimensional feature space into a low-dimensional presentation. Typically a SOM consists of a two dimensional grid of neurons. A vector of features is associated with each neuron. During the training phase, these vectors are tuned to represent the training data under constraint of neighbourhood conservation. Similar data are projected to the same or nearby neurons in the SOM, while different ones are mapped to neurons located further from each other, resulting in clustered data. Thus, SOM is an efficient tool for quantizing the data's space and projecting this space onto a low-dimensional space, while conserving its topology. SOM is often used in industrial engineering [13], [14] to characterize high-dimensional data or to carry out classification tasks. Unfortunately it suffers from major drawbacks: first the configuration of the topology is static and should be fixed a priori (what is efficient only for little values of projection subspace dimension), moreover the method defines only a discrete nonlinear subspace, and finally algorithm is computationally too expensive to be practically applied for projection space dimension higher than 3.

2.3 Curvilinear Component Analysis (CCA)

The goal of this technique proposed by Demartines [15] is to reproduce the topology of a n -dimension original space in a new p -dimension space (where $p < n$) without fixing any configuration of the topology. To do so, a criterion characterizing the differences between original and projected space topologies is processed:

$$E_{CCA} = \frac{1}{2} \sum_i \sum_{j \neq i} (d_{ij}^n - d_{ij}^p)^2 F(d_{ij}^p) \quad (1)$$

Where d_{ij}^n (respectively d_{ij}^p) is the Euclidean distance between vectors x_i and x_j of considered distribution in original space (resp. in projected space), and F is a decreasing function which favors local topology with respect to the global topology. This energy function is minimized by stochastic gradient descent [16]:

$$\forall i \neq j, \Delta x_i^p = \alpha(t) \frac{d_{ij}^n - d_{ij}^p}{d_{ij}^p} u(\lambda(t) - d_{ij}^p) (x_i^p - x_j^p), \quad (2)$$

Where $\alpha: \mathfrak{R}^+ \rightarrow [0,1]$ and $\lambda: \mathfrak{R}^+ \rightarrow \mathfrak{R}^+$ are two decreasing functions representing respectively a learning parameter and a neighborhood factor. CCA provides also a similar method to project, in continuous way, new points in the original space onto the projected space, using the knowledge of already projected vectors.

2.4 Curvilinear Distance Analysis (CDA)

Since CCA encounters difficulties with unfolding of very non-linear manifolds, an evolution called CDA has been proposed [17]. It involves curvilinear distances (in order to better approximate geodesic distances on the considered manifold) instead of Euclidean ones. Curvilinear distances are processed in two steps way. First is built a graph between vectors by considering k-NN, \mathcal{E} , or other neighbourhood, weighted by Euclidean distance between adjacent nodes. Then the curvilinear distance between two vectors is computed as the minimal distance between these vectors in the graph using Dijkstra's algorithm. Finally the original CCA algorithm is applied using processed curvilinear distances. This algorithm allows dealing with very non-linear manifolds and is much more robust against the choices of α and λ functions.

3 Experimental Validation Protocol

In order to obtain exploitable data for a classification scheme, we first needed to extract relevant information of raw Nomarski's microscopy issued images. We proposed to proceed in two steps [2]: first a detected items' images extraction phase and then an appropriated coding of the extracted images. The image associated to a given detected item is constructed considering a stripe of ten pixels around its pixels. Thus the obtained image gives an isolated (from other items) representation of the defect (e.g. depicts the defect in its immediate environment). Figure 1 gives four examples of detected items' images using the aforementioned technique. It shows different characteristic items which could be found on optical device in industrial environment.

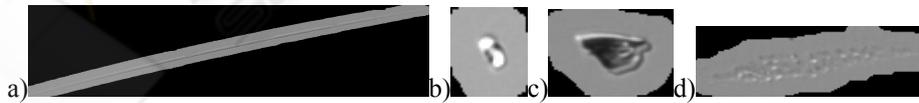


Fig. 1. Images of characteristic items: a) scratch; b) dig; c) dust; d) cleaning marks.

The information contained in such images is highly redundant. Furthermore, the generated images don't have necessarily the same dimension (typically this dimension can turn out to be thousand times as high). That is why these raw data (images) can-

not be directly processed and have to be appropriately encoded. This is done using a set of Fourier-Mellin transform issued invariants described bellow. The Fourier-Mellin transform of a function $f(r; \theta)$, in polar coordinates, is given by relation (1), with $q \in \mathbb{Z}$, $s = \sigma + ip \in \mathbb{C}$ (see[18]):

$$M_f(q; s) = \int_{r=0}^{\infty} \int_{\theta=0}^{2\pi} r^{s-1} \exp(-iq\theta) f(r; \theta) dr d\theta \quad (3)$$

In [19], are proposed a set of features invariant on geometric transformation:

$$I_f(q; s) = M_f(q; s) [M_f(0; \sigma)]^{-s} [M_f(1; \sigma)]^{-q} |M_f(1; \sigma)|^q \quad (4)$$

In order to validate the above-presented concepts and to provide an industrial prototype, an automatic control system has been realized. It involves an Olympus B52 microscope combined with a Corvus stage, which allows scanning an entire optical component. 50x magnification is used, that leads to microscopic 1.77mm x 1.33 mm fields and 1.28 μ m x 1.28 μ m sized pixels. These facilities were used to acquire a great number of defects images. These images were coded using Fourier-Mellin transform with $\sigma = 1$ and $(q, p) \in \{(q, p) / (q = 0; 0 \leq p \leq P) \cup (1 \leq q \leq Q; -P \leq p \leq P)\}$ where $P = 1$ and $Q = 2$ (see Equation 2). Such transform provides a set of 13 features for each item. Three experiments called A, B, C were carried out, using two optical devices. Table 1 shows the different parameters corresponding to these experiments. It's important to note that, in order to avoid false classes learning, items images depicting microscopic field boundaries or two (or more) different defects are discarded from used database. First, since database C is issued from a cleaned device, it's constituted with almost only "permanent" defect. And because database B came from the measurement of the same optical device but without cleaning phase, it's constituted with the same type of "permanent" defects but also with "correctable" ones. In the aim of studying structure of space described by database when reducing its dimension, we perform some experiments. First a reduction of dimensionality from 13 (raw dimensionality) to 2 of the database B was performed using SOM, CCA and CDA, in order to compare projection quality of these three techniques. Then the entire database C was projected into the obtained space in order to evaluate the pertinence of dimensionality reduction for discrimination between "correctable" and "abiding" defects. Finally a classification task, involving aforementioned databases and Multi-layer Perceptron artificial neural network, was carried out with and without dimensionality reduction phase with the aim to demonstrate usefulness of such pre-processing phase.

Table 1. Description of the three experiments supplying studied databases.

Database	Optical Device Identifiant	Cleaning	Number of studied microscopic fields	Correspondant studied area	Number of items in the learning database
A	1	No	1178	28 cm ²	3865
B	2	No	605	14 cm ²	1910
C	2	Yes	529	12,5 cm ²	1544

4 Experimental Results and Analysis

4.1 Quality of Projection

Dimensionality reduction has been performed using the three aforementioned techniques, SOM, ACC and CDA on database B. To compare the results of the three experiments, the 2-D projections issued from CCA and CDA were processed by a SOM, using the same shape of grid (20x8) as in the SOM experiment. An important point is that SOM is just used, in these two last cases, to perform a quantization and not for dimension reduction, since it works on a 2 dimension space. Therefore, we can directly compare dimension reduction ability of the different techniques by comparing these maps with map obtained by applying SOM's algorithm on raw data. The quality evaluation of non-linear projection of the data space onto the neurons grid space is performed by studying, for each pair of neurons, the dx distance between these two neurons in the data space, versus the dy distance between these two neurons in the grid space [20]. For each couple of neurons (i, j) we draw a point $(dy(i, j); dx(i, j))$ where $dx(i, j) = \|\bar{x}_i - \bar{x}_j\|$ and $dy(i, j) = \|\bar{y}_i - \bar{y}_j\|$. \bar{x}_k (resp. \bar{y}_k) is the vector of features corresponding to the k -th neuron in the data space (resp. in the grid space). If the topology of the data space is not well respected, dx is not related to dy and we obtain a diffuse cloud of points. On the contrary, if neurons organization is correct, the drawn points are almost arranged along a straight line.

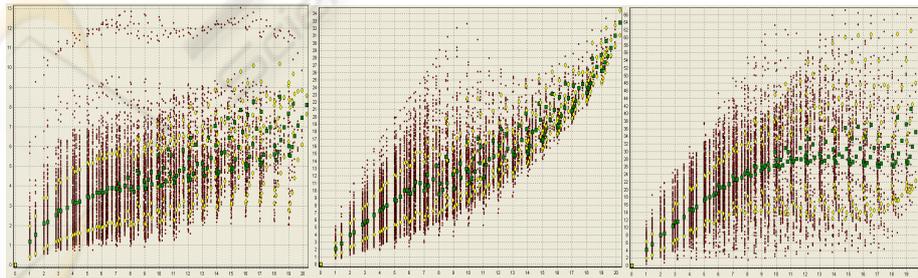


Fig. 2. dy - dx representation of the three obtained SOMs for database B (mean \square and standard deviation \diamond of dx are also represented). Left: SOM; middle: CCA; right: CDA.

First, in Figure 2, cloud of points is more diffuse for SOM than in the case of CCA, and the curve constituted by dx averages for each dy less uniformly monotonic. It reveals the fact that the CCA performs better than SOM, while approximately the same quantity is minimized. The cloud obtained for CDA is quite different because dy is related to curvilinear distance and not Euclidean one. The figure is however the same as for CCA for little dy value, because in these cases Euclidean distance is a good approximate of curvilinear one (and therefore distribution is locally linear).

4.2 Analysis of Possible Impact on Classification Tasks

We now consider the database C (only “permanent” defects) and project its items onto the three previously obtained SOMs. We perform also an equivalent experiment on raw data (13-dimension), using k-means algorithm with $k=20 \times 8=160$. Since k-means algorithm has identical behaviour as SOM, except concerning neighbourhood constraints, it has the same effect on projected items distribution but doesn’t allow visual representation. Projected items distribution after SOM (Figure 3), CCA (Figure 4) and CDA (Figure 5) dimension reduction are studied. In these figures, the equalized grey level depicts the number of projected items for each SOM’s cell (this number is also reported in the cell). In table 2 are reported some characteristic values of permanent defects distributions “homogeneity”: entropy and standard deviation of projected items number in each cell; number of empty or quasi-empty cells (<3 projected items).

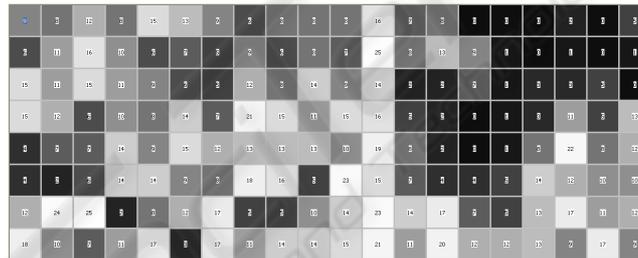


Fig. 3. Distribution of projected items in SOM map. (SOM reduction dimension).

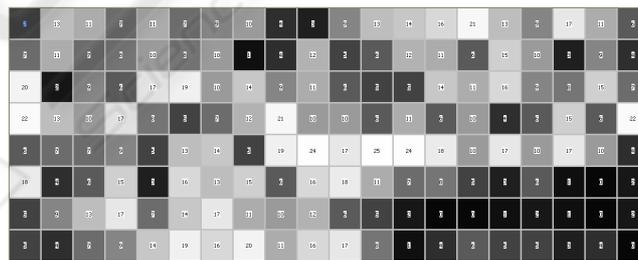


Fig. 4. Distribution of projected items in SOM map. (CCA reduction dimension).

Maps and numerical measurements for SOM and CCA are comparable and therefore these techniques are equivalent for the considered problem. CCA is however easier to

perform (no a priori knowledge or difficult choice) and provide more information (continuous projection). CDA offers the same advantages as CCA, but it seems to be more appropriate for pre-processing before classification. Corresponding map depicts indeed more specific “areas” for database C projected defects. This intuition is confirmed by numerical measurements: entropy is lower than in SOM and CCA cases (better organization), standard deviation is higher (better contrast between full and empty areas) and there are more quasi-empty cells. We think that this organization is a foremost guarantee for the dimension reduction to allow a better classification. We can also remark that results obtained with CDA are fairly similar as those with raw data; it shows that little information is lost while reducing dimensionality.

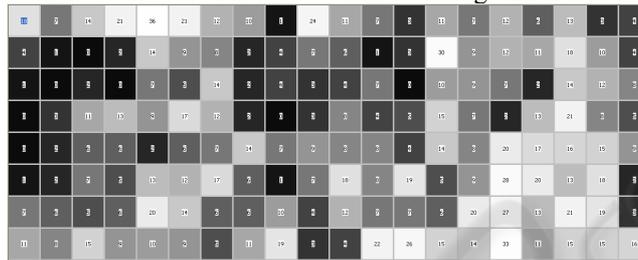


Fig. 5. Distribution of projected items in SOM map. (CDA reduction dimension).

Table 2. Different measurements characterizing the projections distribution of database C items (permanent defects).

Applied dimensionality reduction technique	Standard-deviation of projected defects distribution	Entropy of projected defects distribution	Number of empty cells	Number of cells with less than 3 defects
None	8.72	2.055	15	30
SOM	5.78	2.114	9	26
CCA	5.72	2.121	5	20
CDA	7.04	2.088	7	32

4.3 Validation on an Artificial Neural Network Based Classification

We studied a classification problem in order to evaluate pertinence of using dimension reduction before such task. First, we fixed item labels using obtained SOM with CDA dimension reduction (see Figure 5). Since database C wasn't completely constituted of “permanent” defects (according to an expert, some dusts and cleaning marks still remain), we chose to label all SOM cells with less than 5 projected items of database C as 1: “probably correctable defects”, and the others as -1: “probably permanent defects”. Then each item from database A and B was projected into the SOM and labelled in accordance with its belonging cell, obtaining databases described in Table 3. We performed a first experiment, training a multilayer perceptron with 13 input neurons, 35 neurons in one hidden layer, and 2 output neurons (13-35-2 MLP) artificial neural network using BFGS [21] with bayesian regularization algorithm with database 2. Then a second experiment was carried out, training a 2-25-2 MLP artificial neural network with database 2 after CDA 2-dimensional space reduction.

For these two experiments, training was achieved 20 times and the generalization ability of obtained neural networks was processed using database 1. Results are presented in Table 4. Since database 1 and database 2 came from different optical devices, these generalization results are significant. These results clearly prove that the considered classification problem can be simplified, when properly reformulated in a dimension lower than its raw dimensionality and in accord with its real dimensionality.

Table 3. Description of classification databases.

Database	Coming from database	Total number of items	Label 1 items	Label -1 items
1	A	3865	1046	2816
2	B	1910	489	1421

Table 4. MLP classification performances on database 1.

CDA Reduction Dimension	Training database dimensionality	Class 1 items Well-Recognized	Class -1 items Well-Recognized	Global Performance of good classification	Global Performance Standard Deviation
No	13	71.6 %	78.0 %	76.27 %	1.,37 %
Yes	2	87.4 %	96.7 %	94.16 %	0.87 %

5 Conclusion and Perspectives

A reliable diagnosis of aesthetic flaws in high-quality optical devices is a crucial task to ensure products' nominal specification and to enhance the production quality by studying the impact of the process on such defects. To ensure a reliable diagnosis, an automatic classification system is needed in order to discriminate the "correctable" defects from "abiding" ones. Unfortunately relevant data extracted from raw Nomarski image during defects detection phase are high dimensional. This can have harmful effect on behaviors of artificial neural networks which are suitable to perform such a challenging classification. Reducing the dimension of the data to a smaller value can decrease the problems related to high dimension. In this paper we have compared different techniques, SOM, CCA and CDA which permit such dimensionality reduction and evaluated their impact on classification tasks involving real industrial data. CDA seems to be the most suitable technique and we have demonstrated its ability to enhance performances in a synthetic classification task. Next phase of this work will deal with a classification task on data previously labeled by an expert.

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