Machine Learning evaluation of microscopy image segmentation methods: The case of Gaussian Mixture Models

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ABSTRACT

Multiphase materials are encountered in several areas of science and technology. Their properties are determined by the fraction of the phases (material compounds) constituting the composite material. Therefore, the quantitative characterization of phase fractions is highly demanded and has been the subject of extensive studies. To this end, a widely used technique is the segmentation of top-down back-scattered electron SEM (BSE-SEM) images given that different phases are depicted with pixel collections of different luminosity. Gaussian mixture models (GMM) are one the most popular and easily implemented methods to segment the BSE-SEM images through the deconvolution of their histograms. However, the accuracy and the limitations of their application have not been fully investigated. The aim of this paper is to design a neural-network approach to fill this gap and provide a fast tool for the automatic evaluation of the accuracy of GMM predictions for all material phases based on the inspection of the measured SEM image histogram alone. The proposed tool facilitates the decision-making process of an SEM user concerning the optimum choice of a segmentation method.

CCS CONCEPTS

• **Applied computing** → Physical sciences and engineering; Chemistry; • **Computing methodologies** → Machine learning; Neural networks.

KEYWORDS

Scanning Electron Microscopy, Back-scattered Electron Imaging, Multiphase Materials, Image Segmentation, Gaussian Mixture Model, Neural Network

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1 INTRODUCTION

During the last decades, the use of multiphase materials has been expanded in several technology sectors enabling new applications and providing solutions to current societal challenges (e.g., energy [1], health [2], and environment [3, 4]). At the same time, the theoretical understanding of the new properties and functionalities of these materials has attracted great interest. A key requirement in both theory and applications is the detailed knowledge of material structural morphology and especially of the co-existence of multiple material compounds (phases) within its bulk. Therefore, it is of primary concern the measurement and characterization of the fraction and morphology of phase components in a multiphase material. To this end, a wide spectrum of techniques has been developed [5, 6]. Among these, the SEM imaging based on the detection of back-scattered electron (BSE) signal provides a detailed depiction of the size and morphology of the different phases with nanometer resolution. To translate SEM images into a quantitative measurement of phase fractions, a segmentation process should be applied. It must be mentioned that distinction of phases in BSE-SEM images can be accomplished if phases correspond to different z-effective. GMM is a widely used and easily implemented technique to make segmentation through the deconvolution of the histogram of image pixel intensities [7]. However, as expected, GMM accuracy is not always justified, and the method has inherent limitations triggered by specific characteristics of SEM images which undermine the accuracy of its predictions. As part of previous work by our team [8], we studied systematically the dependence of GMM accuracy on specific collective parameters such as range, variance, and width defining the position and shape of phase distributions. To quantify the accuracy of GMM predictions for all distributions, we introduced a distribution similarity (DS) measure and calculated it for a large spectrum of the above-mentioned parameters. In particular,

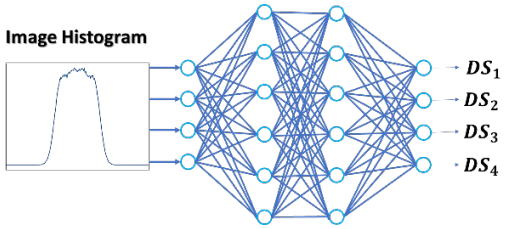

Figure 1: Schematic description of the neural network approach described in this paper. The input of the NN is a back-scattered electron image histogram and the output is a prediction of the GMM deconvolution success.

DS is defined by the equation 1):

$$DS = \min\left(\frac{OA}{PDA}, \frac{OA}{RDA}\right) \quad (1)$$

Where, OA is the overlapping area of predicted and real distribution, PDA is the area of predicted distribution and RDA is the area of real distribution.

The analysis has been based on the assumption that the distributions of pixel intensities belonging to all phases are known and can be used for the calculation of DS. However, in real-world problems, we face the inverse problem. We ignore the distribution of each phase separately and what we have from our measurements is the total distribution (histogram) of pixel intensities of the whole image including all phases. In our previous work, we provided some rules of thumb to guide an SEM user on the appropriateness of GMM-based segmentation of a specific image histogram. In this paper, we proceed to a more thorough analysis exploring the benefits of a neural network (NN) approach which takes as input the image histogram and output the DS values for all distributions (see Figure 1). The latter can be used as quantification of the success of GMM-based segmentation in the specific case.

In the following Section 2, we present the architecture of the developed NN along with the limited parameter space we are using to train and test it. The results of the application of the trained NN are presented in Section 3. In the same Section, we discuss the prospects of the method while the paper closes with the Conclusions and the design of future steps in Section 4.

2 METHODOLOGY – NEURAL NETWORK ARCHITECTURE

A synthetic dataset covering all probable configurations of phase histograms is very large to be considered. Therefore, in this preliminary work, a subspace of the total parameter space is investigated to test the application of a NN approach in the evaluation of GMM accuracy. This subspace is defined by the following constraints of histograms included in the dataset used in this work. Each synthetic histogram consists of four Gaussian distributions with mean values of equal distances while the variances of participant distributions are equal, and the weights are equal too. This small subspace is chosen to demonstrate how a NN can predict the accuracy of another machine learning method, while additionally may reveal differences in the predictability of internal distributions in respect

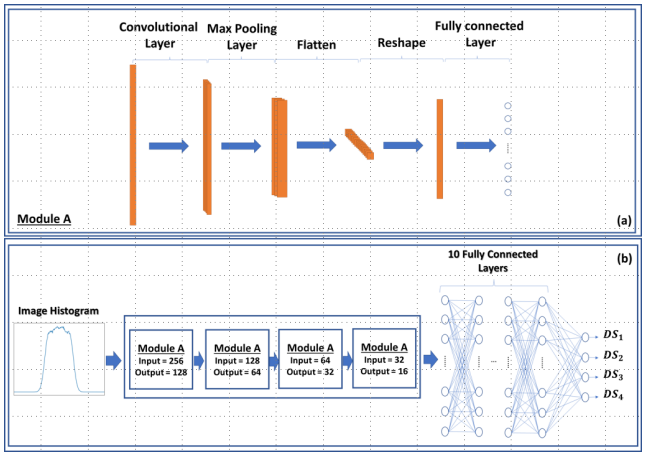

Figure 2: A brief description of the NN architecture. The first part of the network consists of four modules described in the (a) upper part of the figure where a convolutional layer is followed by a max-pooling layer, followed by a flatten layer, and finally, the output is reshaped and ends to a SeLu fully connected layer. This module is repeated four times reducing the size of the output by a factor of two each time. The second part of the NN contains 10 SeLu fully connected layers with 16 nodes each leading to a 4-nodes SeLu layer output.

to the external ones. The NN training is realized in Python using the Keras library [9].

The architecture of the NN can be separated into two parts as depicted in Figure 2. The first part consists of four sets of layers. In more detail, every set of this part (i.e., Module A) is composed of a one-dimensional convolutional layer, followed by a max-pooling layer, a flatten layer, and finally a fully connected layer. The convolutional kernel is set at 16 for all convolutional layers, without padding and the stride is equal to one. The nodes in the fully connected layers are set to be 128, 64, 32, and 16, respectively. The pooling size is equal to two whilst no padding occurs, and stride is one. In between these sets of layers, a reshaping is performed. The second part of the NN is composed of 10 fully connected layers consisting of 16 nodes each followed by a four-node fully connected layer. The Scale Exponential Linear activation Unit (SeLu) [10] is used as the activation function for all nodes while the mean squared error is selected as the loss function. Adam optimizer is also used as a stochastic gradient descent optimizer [11] and an early stopping occurs when the loss function of the validation set is not improved for 25 epochs. Finally, 80% of the dataset is used for the training, 10% for validation, and the remaining 10% is left for the testing of the model. The total size of the dataset consists of 241.006 histograms along with an equal number of 4-dimensional arrays composed of 4 DSs as emerges from GMM histogram deconvolution.

3 RESULTS

Using 10-fold cross-validation, the model can achieve an R^2 value just above 0.93 during the training phase while for the validation set, the average of R^2 saturates to 0.93. Figure 3a shows a representative

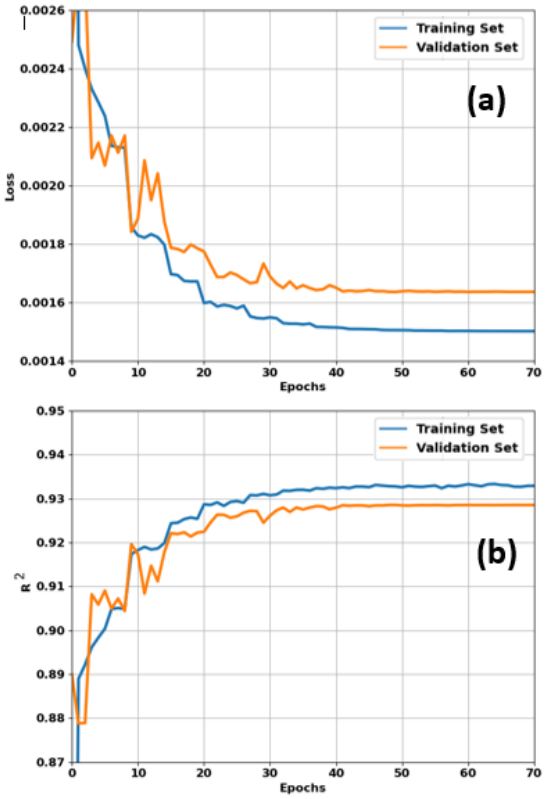

Figure 3: (a) Loss function versus epochs reveals that the NN has been successfully trained (b) R2 values with respect to the epochs of the training process indicate again that the model has reached an adequate level of training.

diagram of the loss function of both training and validation sets versus the number of epochs revealing that the model was trained over the data set, since both losses are stabilized for epochs>50. Additionally, the absence of any increase in the validation curve versus epochs is an indication that overfitting is avoided.

Moreover, Figure 3b displays the R^2 versus the number of epochs and justifies again that the model has reached a satisfactory level of training and that there is no overfitting.

A more detailed evaluation of the success of NN model predictions is illustrated in Figure 4, which depicts the true DS values with respect to predicted ones for all phase distributions. An interesting observation is that for low DS values the prediction of these values is a challenging task for the proposed NN. Deviations between predicted and true DSs are larger for the external distributions with reference to the internal ones. (cf. Figure 4 a, d and Figure 4b, c).

4 SUMMARY-CONCLUSIONS

In data analysis, it is very useful to know the accuracy of the predictions of an analysis method for the specific data set before applying it because it leads to saving time and achieving meaningful results. In this paper, we present preliminary results from the application of an NN-based approach to evaluate the accuracy of the GMM

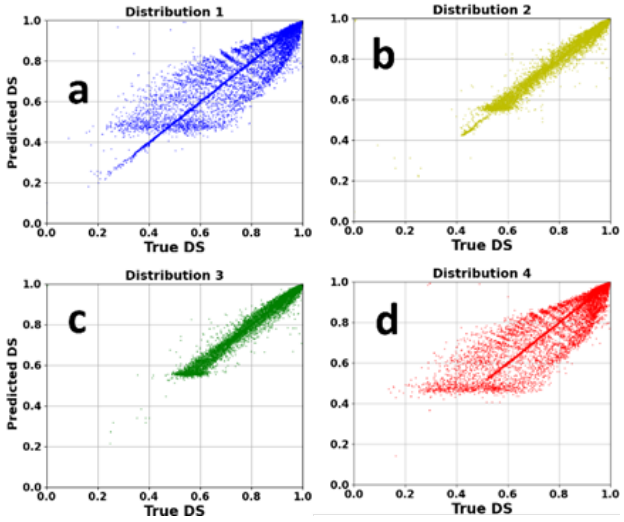

Figure 4: True DS values versus predicted ones reveal the incompetence of NN to correctly predict the success of low DS values.

method in the deconvolution of the histogram of an SEM image of a sample of multiphase material. The successful deconvolution can provide an accurate assessment of the fraction of the phases comprising the multiphase material.

To this end, we developed a NN method that consists of multiple layers and found that it is able to predict sufficiently the accuracy of the GMM-based segmentation for each material phase separately, especially at high DS values. Furthermore, we found that the NN-based predictions are worse in the evaluation of the GMM accuracy of external distributions rather than internal distributions. This result is in conformity with our previous work, where it has been shown that GMM is more accurate in the internal distributions rather than the external ones. It seems that NN can provide a useful ML tool to predict the accuracy of GMM predictions based on the analysis of image histogram alone.

The next steps of our work target to expand the NN method to a more extended parametric space leading to an enhanced training of NN with richer synthetic data. Finally, we plan to apply the methodology to real experimental images and compare it with other methods.

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