Spectral Classification of Microplastics using Neural Networks: Pilot Feasibility Study

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Keywords: Microplastics, FTIR Spectra, Spectroscopy, Neural Network, Deep Learning, Spectra Matching.

Abstract: Microplastics, i.e. synthetic polymers that have particle size smaller than 5 mm, are emerging pollutants that are widespread in the environment. In order to monitor environmental pollution by microplastics, it is necessary to have available rapid screening techniques, which provide the accurate information about the quality (type of polymer) and quantity (amount). Spectroscopy is an indispensable method, if precise classification of individual polymers in microplastics is required. In order to contribute to the topic of autonomous spectra matching when using spectroscopy, we decided to demonstrate the quality and efficiency of neural networks. We adopted three neural network architectures, and we tested them for application to spectra matching. In order to keep our study transparent, we use publicly available dataset of FTIR spectra. Furthermore, we performed a deep statistical analysis of all the architectures performance and efficiency to show the suitability of neural networks for spectra matching. The results presented at the end of this article indicated the overall suitability of the selected neural network architectures for spectra matching in microplastics classification.

1 INTRODUCTION

Plastic pollution has recently become a huge global problem. Worldwide plastics production reached about 367 million tons in 2020 (Kaul, 2021). Approximately 80 percent of produced plastic is disposed of as various kinds of waste (Chen et al., 2021). Plastic waste, that is improperly deposited, can be disintegrated into small pieces by sunlight, heat, physical abrasion, eventually directing to the particle size of microplastic (<5mm) (Xu et al., 2022).

These microplastics are receiving big interest from the scientific community as well as from international institutions, since the effect of microplastics on organisms and the environment is not yet clearly known (Rochman et al., 2013; Katare et al., 2022).

One of the open problems is the issue of monitoring of mikroplastics in environment. Only several long-term studies, which examine the evolution of microplastics pollution over the years, have been performed. This is caused especially due to the time and resource consuming process of repeated sample acquisition, laboratory preparation and evaluation. In some recent studies, the identification and detection of microplastics is performed by manual visual counting and sorting under a microscope, based on color, size, morphology etc. (Hanvey et al., 2017; Mukhanov et al., 2019). Furthermore, some authors propose advanced image analysis-based approaches, which are powerful in case of measuring and counting particles (Lorenzo-Navarro et al., 2020).

However, spectroscopy is an indispensable method, if precise classification of individual polymers in microplastics is required. Raman and Fourier transform infrared (FTIR) spectroscopy are the most common techniques for classifying the polymers in plastic particles (Cowger et al., 2020). Although both mentioned techniques provide exceptional accuracy, the application of them requires a complex sequence of steps, many of which are performed manually by default (Cabernard et al., 2018). A crucial step, which is evaluated manually in most cases, is spectra matching. Specifically, the Raman or SWIR spectrum of an examined sample needs to be preprocessed (filtering, baseline signals removal) and compared to a reference library of spectra, in order to classify

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Dolezel, P., Rolecek, J., Honc, D., Stursa, D. and Zanon, B.
Spectral Classification of Microplastics using Neural Networks: Pilot Feasibility Study.
DOI: 10.5220/0010986900003123
In *Proceedings of the 15th International Joint Conference on Biomedical Engineering Systems and Technologies (BIOSTEC 2022) - Volume 4: BIOSIGNALS*, pages 283-289
ISBN: 978-989-758-552-4; ISSN: 2184-4305

the polymer in the sample. Although this process is simple in theory, it is not easy to automatize it due to the large variability of the measured spectra. See Fig. 1 for four examples of high-density polyethylene FTIR spectrum measured by the same device. Note the differences in peak numbers, peak positions and peak heights.

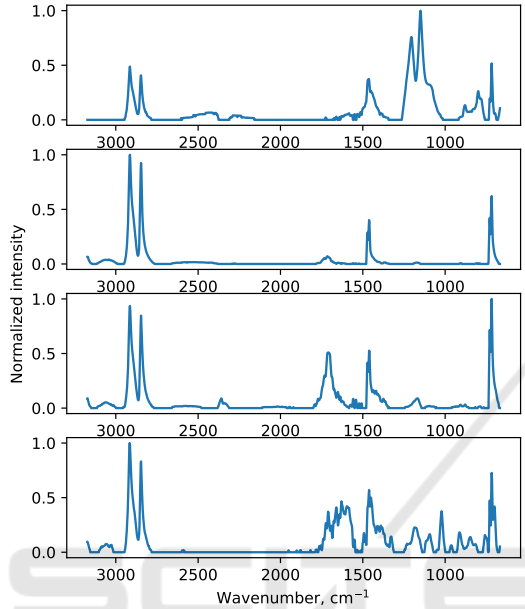

Figure 1: Four examples of high-density polyethylene FTIR spectrum measured by the same device. Note the differences in peak numbers, peak positions and peak heights. Despite the obvious differences, these spectra should be evaluated as one class.

Despite the obvious uncertainty of machine evaluation, several methods, that aim to replace the manual spectra matching, have been proposed. Lorenzo-Navarro et al. introduced a multi-step method composed from a segmentation step, feature extraction and classification. They considered and tested different feature extractors and classifiers, including machine learning and deep learning algorithms (Lorenzo-Navarro et al., 2020). Alternately, a hybrid fusion algorithm, that simultaneously combines high-level fusion with low- and mid-level fusion based on an ensemble of various classical classifiers, is proposed in (Chabuka and Kalivas, 2020). Finally, the authors (Cowger et al., 2021) offer a comprehensive software tool, which encapsulates a large number of tools to process and classify microplastic spectra. Moreover, this tool is ”open source” and can be rapidly adapted to include new techniques.

In order to contribute to the topic of autonomous spectra matching, we decided to demonstrate the quality and efficiency of convolutional neural networks (LeCun et al., 1999) and attention mechanism-based neural networks (Vaswani et al., 2017) for signal classification. Specifically, we intuitively understand the problem of spectra matching to be very similar to time series classification (see Fig. 2). It is well known that neural networks are a very effective tool for time series classification (Ismail Fawaz et al., 2019; Franklin and Muthukumar, 2022; Sikdar et al., 2022). Although some pilot studies have already considered convolutional neural networks as a tool for spectra matching (Ng et al., 2020), it is still open problem and more analyses have to be performed.

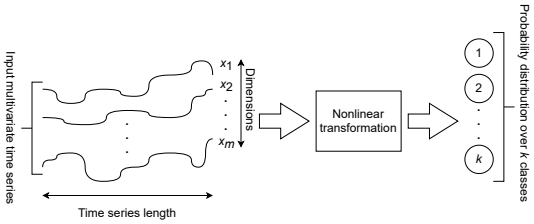

Figure 2: A general framefork for time series classification. A nonlinear transformation module processes the input time series and provides the probability of the input time series belonging to each class.

In this article, we adopt three neural network architectures, that have already proven successful for time series classification, and we test them for application to spectra matching. In order to keep our study transparent, we use publicly available dataset of FTIR spectra (Chabuka and Kalivas, 2020). Furthermore, we perform a deep statistical analysis of all the architectures performance and efficiency to show the suitability of neural networks for spectra matching.

2 MATERIALS AND METHODS

2.1 Neural Network Architectures

Many different architectures, from multilayer perceptron to long short-term memory recurrent neural network, have been already more or less successfully implemented for signal classification. We aimed at architectures with exceptional performance and acceptable response time for real-time implementation. Based on an extensive literature review, we selected (1) a variant of a fully-convolutional neural network classifier adapted from (Wang et al., 2017), (2) an implementation of a multi-scale convolutional neural network based on (Cui et al., 2016), and (3) an attention mechanism-based Transformer architecture presented in (Vaswani et al., 2017).

2.1.1 Fully-convolutional Neural Network Classifier

Fully convolutional neural networks provide efficiency and quality especially for semantic segmentation-related issues (Shelhamer et al., 2017). In this setting, a fully convolutional neural network is performed as a feature extractor, followed by a softmax layer. A number of neurons in the softmax layer is equal to the number of classes. The explicit graph of this architecture, as used in this contribution, is depicted in Fig. 3.

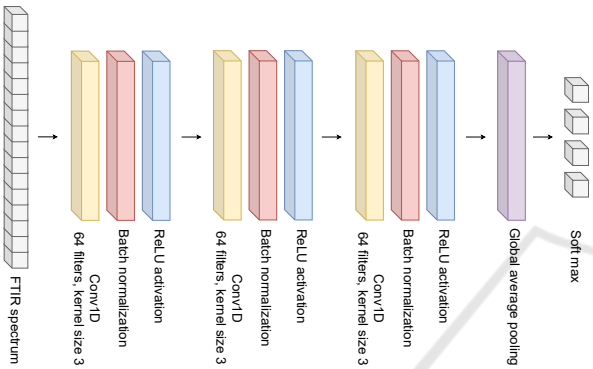

Figure 3: Architecture of a selected fully-convolutional neural network classifier.

2.1.2 Multi-scale Convolutional Neural Network

The multi-scalability of this network consists in its architecture. The first part of the architecture works in three parallel independent branches. Each branch implements a base module to extract features of different nature from the input, operating at different frequency scales. The outputs of all branches are concatenated and the resulting signal is processed by a softmax layer. The overall architecture, as we implemented it in our experiments, is depicted Fig. 4. The architecture of the base module is shown in Fig. 5. The kernel size of the convolutional layer varies from 8 (the upper module) to 24 (the lower module). The lower module input is the original FTIR spectrum, the middle module input is the spectrum downsized to one half, and the upper module input is the spectrum downsized to one third of the original.

2.1.3 Transformer Architecture

The idea of the Transformer architecture is to propose a topology based solely on attention mechanisms, dispensing with recurrence and convolutions entirely (Vaswani et al., 2017). The architecture was originally proposed to natural language processing, but it can be seamlessly adapted to spectra matching. The

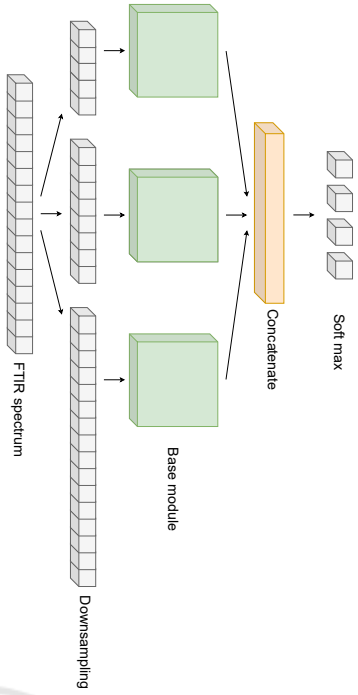

Figure 4: Overall architecture of our implementation of a multi-scale convolutional neural network.

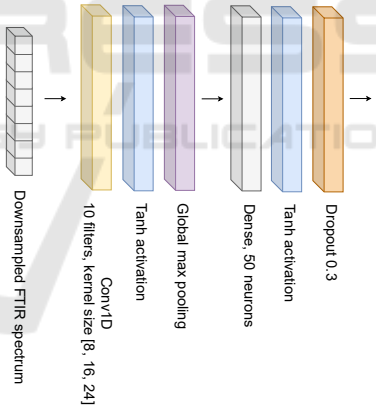

Figure 5: Base module for a multi-scale convolutional neural network.

key part of this architecture is a multi-head attention layer. Intuitively, this layer allows for attending to parts of the input sequence in various different ways, e.g. from the long-term dependency point of view and the short-term dependency point of view. We implemented a tiny version of this architecture, in order to keep a comparable size to the other selected architectures - see Fig. 6.

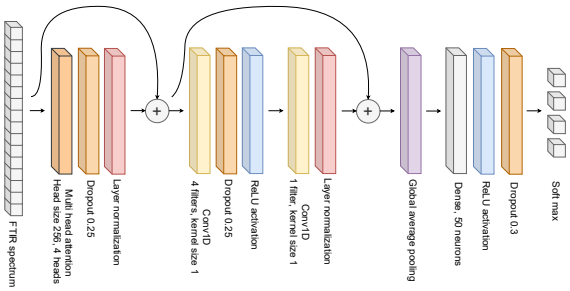

Figure 6: Our implementation based on the Transformer architecture.

2.2 Dataset

We adopted 272 FTIR spectra from (Chabuka and Kalivas, 2020). These spectra were acquired using Thermo Nicolet NEXUS 670 FTIR spectrophotometer with spectral resolution 4 cm^{-1}. The dataset includes 137 spectra of high-density polyethylene (HDPE) and 135 spectra of polyethylene terephthalate (PET), i.e. two balanced classes for classification. Each spectrum consists of 1300 points. Some examples are shown in Fig. 1 for high-density polyethylene and in Fig. 7 for polyethylene terephthalate.

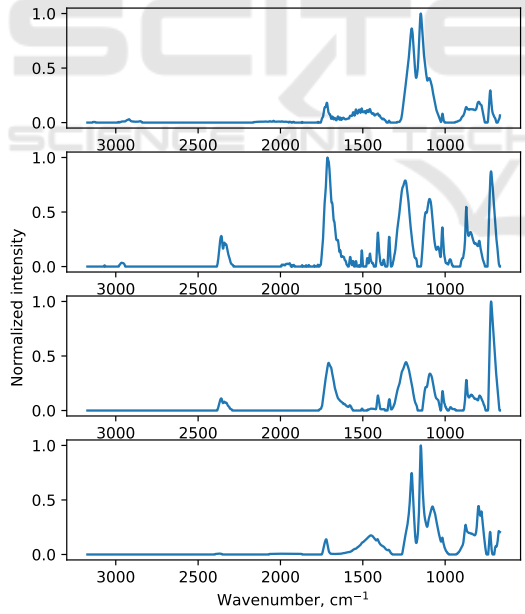

Figure 7: Four examples of polyethylene terephthalate FTIR spectrum.

The dateset was shuffled and divided into training set (160 samples), validation set (41 samples) and testing set (71 samples).

2.3 Training Details

The Adam algorithm was selected as an optimizer, since it is generally considered to provide acceptable performance in most of the cases (Kingma and Ba, 2014). Sparse categorical crossentropy loss function was used to evaluate training process. Initial weights were set randomly with Gaussian distribution. The training experiments were performed 100 times due to a stochastic character of training. For each training session, the instance, which performed best over validation set, was selected for further evaluation. All the parameters of the training are summarized in Table 1.

Table 1: Parameters of the training.

Input shape	1300 x 1
Training algorithm	Adam algorithm
Loss function	Sparse categorical crossentropy
Number of experiments for each architecture	100
Initialization	Normal distribution (mean = 0, std = 0.05)
Maximum epochs	500
Stopping criterion	Maximum epochs reached
Initial learning rate α	0.001
Exponential decay rate 1 β_1	0.9
Exponential decay rate 2 β_2	0.999

2.4 Evaluation Metrics

After training of all the considered architectures, every network was evaluated. From the training performance point of view, the courses of loss function over the training set and over the validation set during the training sessions were evaluated. Since 100 distinct training sessions were performed, the courses were depicted as sequences of box plots in relation to the epoch number.

From the classification quality point of view, the confusion matrix for each architecture was prepared. Again, the confusion matrix shows the average values including the standard deviation, since 100 training sessions for each architecture were performed.

Evaluation of the memory size and response time is also important, especially if the edge computing implementation is intended. Therefore, the size of the neural network architectures and their response times were also considered. The response times

of of the selected architectures were evaluated on a personal computer with Intel Core i5-8600K (3.6 GHz) CPU, internal memory 16 GB DDR4 330 (2666 MHz), video card NVIDIA PNY Quadro P5000 16 GB GDDR5 PCIe 3.0. The architectures were implemented using TensorFlow 2.7 using Windows 10 operating system.

3 RESULTS AND DISCUSSION

The selected architectures were trained and validated 100 times according to the procedure addressed above. In order to demonstrate training results, the courses of the sparse categorical cross entropy loss function over the training set and over the validation set are depicted in Fig. 8 for the fully-convolutional neural network classifier, in Fig. 9 for the multi-scale convolutional neural network, and in Fig. 10 for the Transformer architecture. The central lines in the box graphs, shown in the figures, are medians of loss function current values in relation to the epoch number; the edges of the boxes are 25^{th} and 75^{th} percentiles; and the whiskers extend to the most extreme data points (except outliers).

Consequently, the confusion matrices for each architecture over the testing set are presented in Table 2, in Table 3, and in Table 4. Each column of the matrices represents the instances in an actual class (HDPE or PET) while each row represents the instances in a predicted class. The values in brackets mean the standard deviation for each value.

Lastly, the sizes and the relative response times are shown in Table 5.

Table 2: Confusion matrix for the fully-convolutional neural network classifier. The values in brackets mean the standard deviation.

	HDPE actual	PET actual
HDPE predicted	32.95 (0.22)	1.41 (0.71)
PET predicted	0.05 (0.22)	36.59 (0.71)

Table 3: Confusion matrix for the multi-scale convolutional neural network. The values in brackets mean the standard deviation.

	HDPE actual	PET actual
HDPE predicted	33.00 (0.00)	1.35 (0.48)
PET predicted	0.00 (0.00)	36.65 (0.48)

All the presented results indicate the overall suitability of the selected neural network architectures for spectra matching. Looking at training performances, the fully-convolutional neural network classifier provided the slowest learning curve and additionally, the

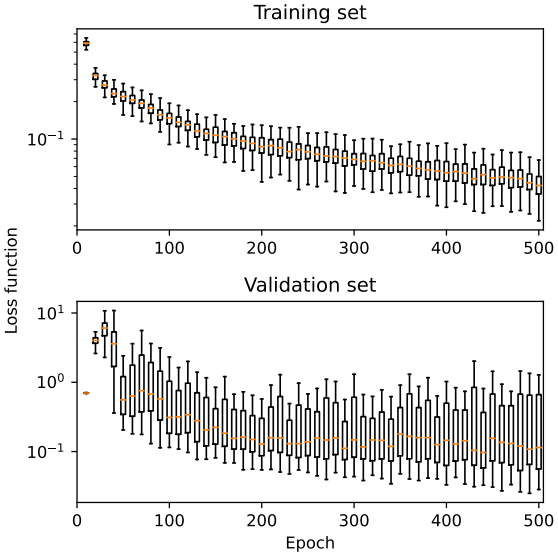

Figure 8: Training course for the fully-convolutional neural network classifier.

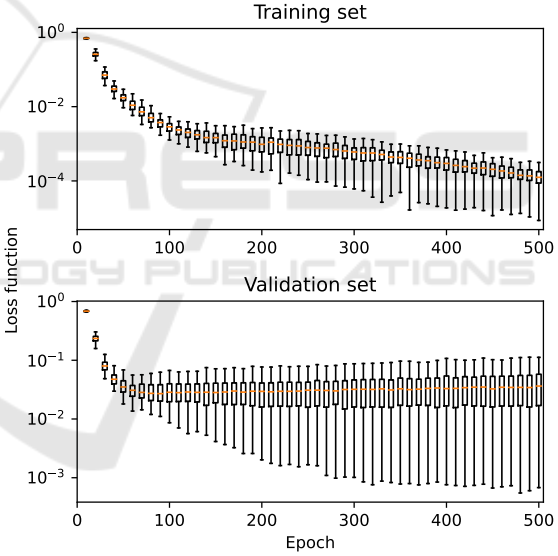

Figure 9: Training course for the multi-scale convolutional neural network.

generalization capability of this model was low - the evaluation over the validation set provided relatively high values with a large variance. The learning curve for the other two architectures was steep and stable, with the Transformer architecture in particular providing exceptionally good values of loss function over the validation set, with low variance.

The confusion matrices, which represent performance of each architecture over the testing set, provided results, that correspond with the training performance. The best performance was provided by the Transformer architecture, where, statistically, the

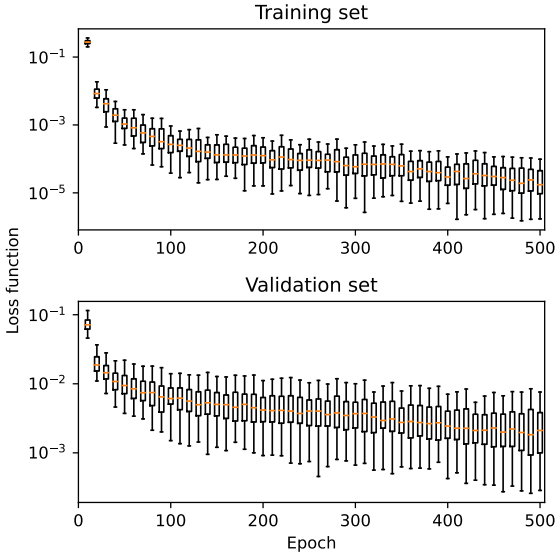

Figure 10: Training course for the Transformer architecture.

Table 4: Confusion matrix for the Transformer architecture. The values in brackets mean the standard deviation.

	HDPE actual	PET actual
HDPE predicted	33.00 (0.00)	0.82 (0.38)
PET predicted	0.00 (0.00)	37.18 (0.38)

classifier misclassified less than one spectrum from the testing set. The other two architectures performed a little worse. For the Transformer architecture, 18 training sessions (from 100) provided model, that did classify all the samples in the testing set correctly. For the other two architectures, each model provided at least one misclassified sample.

Looking at Table 5, the response times of each classifier are similar; the multi-scale convolutional neural network was about 20 percent slower than the other two architectures. Considering the memory sizes, all the architectures are smaller than 1 MB. Hence, they are very lightweight and can be considered for use in edge computing applications.

4 CONCLUSIONS

In this study, three selected neural network architectures are used to classify microplastics FTIR spectra. Although only a limited dataset with two types of polymer is used, the results look promising to implement neural network architecture for spectra matching.

The Transformer architecture was particularly successful with almost 20 percent of training sessions providing model, that classifies all the samples in the testing set correctly.

Table 5: Size and response times.

Architecture	Relative response time	Size (kB)
Fully-convolutional neural network classifier	1.00	372
Multi-scale convolutional neural network	1.18	94
Transformer architecture	1.05	940

The usage of neural networks for spectra matching generally brings major advantages in comparison to classical matching techniques. It greatly reduces the number of operations required for preprocessing, is not sensitive to noise and has good generalization capability. Moreover, lightweight neural networks are characterized by low computational power requirements, which makes them suitable for use in edge computing applications, such as portable spectroscopes.

In a future study, datasets with more classes are definitely suggested to be tested in order to justify the proposed work. With a dataset that covers all the most common plastics, it will be possible to determine the optimal neural network architecture with high accuracy and efficient response time.

ACKNOWLEDGEMENTS

The work was supported from ERDF/ESF "Cooperation in Applied Research between the University of Pardubice and companies, in the Field of Positioning, Detection and Simulation Technology for Transport Systems (PosiTrans)" (No. CZ.02.1.01/0.0/0.0/17_049/0008394).

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