Scientific Reports Title to see here

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ABSTRACT

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Please note: Abbreviations should be introduced at the first mention in the main text – no abbreviations lists. Suggested structure of main text (not enforced) is provided below.

Introduction

Plastic materials are an integral part of modern society due the sheer endless application possibilities. Yet, due to the lack of recycling measurements vast amounts of plastic waste end up uncontrollably in our environment. Numerous studies revealed to us the impact of this unstoppable plastic pollution: microplastics derived from plastic waste can be found marine lifeforms. Only recently, further studies found microplastics in human stool and the human placenta with unknown long-term effects.

To trace back the different pathways of microplastic into the human body, we need identification techniques that allow us to identify and classify plastic waste at different stages. Here, Raman and FTIR spectroscopy are commonly used in plastic pollution studies due to the availablity of commercial systems. At the same time, plastic pollution samples are highly diverse due to environmental influences and the sheer endless combinations to produce plastic. Due to the physical limitations of each aformentioned technqiue, it is forseeable that each technique only work for a subset of plastic waste. Consquently, additional techniques are required to cover in particular those plastic waste types are currently not covered. A recent study by Ornik et al. [XXXREF] demonstrated that photoluminescence is a suitable technique to identify plastics from other materials that occur in the riverine environment.

Compared to the previous techniques, photoluminescence (PL) stands out for its simplicity. A basic setup consists of only two components, namely a monochromatic laser and spectrometer, which makes it a globally accessible technique for microplastic identification. However, the simplicity of the basic setup also raises questions about the comparability of different spectral data. Even if a sample is measured by two setups with identical hardware, the acquired spectra can look different because of different alignments, sample sites or even scientific experiences. Thus, while measurements should always be taken at laboratory conditions, this cannot be always fulfilled and raises the question for other identification methods that can be used instead. One possible solution is to take advantage of the fact that large sets of data can be generated due to the simplicity of the setup. Once integrated in a library, computer algorithms and models can be developed to help unraveling the origins of the plastic sample.

Today, we have a choice over a vast amount of computational methods that could be used for plastic classification. Amongst them, machine learning models are the most popular ones with many established methods available to the public. Generating a machine learning model consists of two steps: first, we identify patterns on a selected dataset and second, we select a learning model to use these patterns and identify the plastic samples. Since different combinations of methods can be used to do both steps, it is not clear if the chosen method can work with high accuracies, i.e. the probability that a model based prediction is correct, in the presence of data heterogeneities due to experimental variations.

Here, we look at two different methods to identify patterns. The first one uses all information from a single spectrum while the second one uses a method known as signal dissection by correlation maximization (SDCM). The latter has the advantage that physically meaningful patterns can be extracted. Our study shows that, machine learning models based on SDCM are more robust towards experimental heterogoneities.

Results

Up to three levels of **subheading** are permitted. Subheadings should not be numbered.

Subsection

Example text under a subsection. Bulleted lists may be used where appropriate, e.g.

- First item
- Second item

Third-level section

Topical subheadings are allowed.

Discussion

The Discussion should be succinct and must not contain subheadings.

Methods

Experimental setup

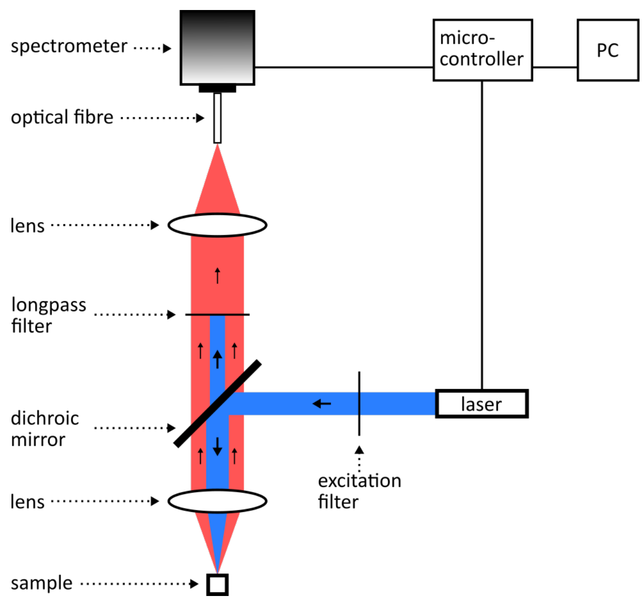

Figure 1. Diagram of the photoluminescence spectroscopy setup.

1 illustrates our experimental setup which we use to acquire the photoluminescence spectra. The beam path to excite the sample and induce photoluminescence emission is highlighted in blue. For the excitation, we use a beam with a central wavelength of 405 nm. This is achieved by using a laser that generates a beam with a central wavelength of 402 nm and a excitation filter to select our wavelength. A dichroic mirror directs the beam to a lens that focusses the beam on the sample's surface. The beam path of the emitted photoluminescence light is highlighted in red. Starting from the sample's surface, the emitted light is collected and collimated by the lens and passes through the dichroic mirror. To ensure that the excitation beam is completely removed from the emission path we use a longpass filter with a cut-on wavelength of 420 nm. Once filtered, the beam passes through a lens that focusses the light onto an optical fibre which directs the light to a spectrometer (LR2, Lasertack GmbH).

Both the laser and the spectrometer are controlled with a microcontroller which, in turn, is connected to a pc. This arrangement makes it possible to control the laser power, illumination time and the delay time to start acquiring the spectrum. The latter is set to 500 ms.

Sample Type	Number of Samples	Measurement 1		Measurement 2	
		Laser Power [mW]	Exposure Time [ms]	Laser Power [mW]	Exposure Time [ms]
Non-plastic	12	0.5–130	300	0.2–2.8	
Plastic (manufacturer)	26	5–130	300	0.5–100	300
Plastic (retail)	8	0.5–130	300–1500	0.5–104	300

Table 1. Legend (350 words max). Example legend text.

Samples and measurement parameters

Our spectral data set consists of 46 samples which contains non-plastic samples from the riverine and marine environment and plastics from manufacturers and retail products. For each sample, we acquire multiple spectra with two sets of parameters, namely laser power and illumination time. 1 gives a summary of all samples with the range of the measurement parameters used in this study.

References

1. Hao, Z., AghaKouchak, A., Nakhjiri, N. & Farahmand, A. Global integrated drought monitoring and prediction system (GIDMaPS) data sets. *figshare* http://dx.doi.org/10.6084/m9.figshare.853801 (2014).

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For data citations of datasets uploaded to e.g. *figshare*, please use the `howpublished` option in the bib entry to specify the platform and the link, as in the `Hao:gidmaps:2014` example in the sample bibliography file.

Acknowledgements (not compulsory)

Acknowledgements should be brief, and should not include thanks to anonymous referees and editors, or effusive comments. Grant or contribution numbers may be acknowledged.

Author contributions statement

Must include all authors, identified by initials, for example: A.A. conceived the experiment(s), A.A. and B.A. conducted the experiment(s), C.A. and D.A. analysed the results. All authors reviewed the manuscript.

Additional information

To include, in this order: **Accession codes** (where applicable); **Competing interests** (mandatory statement).

The corresponding author is responsible for submitting a competing interests statement on behalf of all authors of the paper. This statement must be included in the submitted article file.

Condition	n	p
A	5	0.1
B	10	0.01

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Figures and tables can be referenced in LaTeX using the ref command, e.g. Figure 2 and Table 2.

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