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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

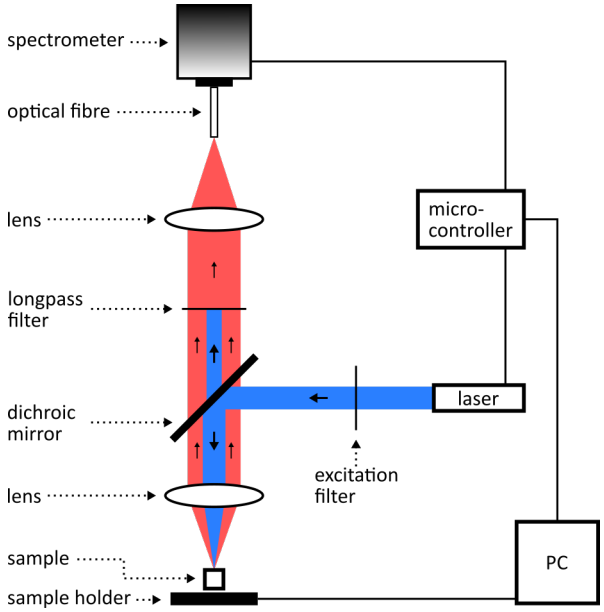

Figure 1. Diagram of the photoluminescence spectroscopy setup.

As an excitation source a blue laser diode with a central wavelength of 402 ± 3 nm. A band-pass filter was placed after the diode to narrow down the excitation to 405 ± 10 nm. To reflect the excitation beam on to the sample and to transmit the emitted light from the sample a 425 nm dichroic long-pass filter. An achromatic lens was placed between the sample and dichroic mirror, to focus the excitation beam on the sample which simultaneously also collimates the emission from the sample. Since the dichroic mirror wasn't sufficient in blocking the excitation light, an additional 420 nm long-pass filter after dichroic mirror was used to further block the excitation beam. A fiber coupling lens was placed after the filter to couple the PL emission in to the optical fiber. The optical fiber was then attached to an optical spectrometer (LR2 spectrometer from Lasertack, GmbH). The spectrometer covers a wavelength range from 200–1100 nm with <1 nm resolution. The integration time of spectrometer was set to a particular value. A microcontroller was used to regulate the laser power until sufficient PL signal was detected. If no signal was obtained at maximum out power of the laser the integration time of the spectrometer was increased. To compensate for non-uniformity in measurements due to undesired photobleaching at high powers, the spectrometer was turned on 500 ms after the laser using a microcontroller. Samples were placed on a two axis mototised stage to perform raster scanning. Before acquiring the PL spectra from samples, to eliminate any artifacts in the PL spectra a background spectrum was recorded by blocking the laser light, which was then subtracted from the PL spectra.

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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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.

Figure 2. Legend (350 words max). Example legend text.

Figures and tables can be referenced in LaTeX using the ref command, e.g. Figure 2 and Table 1.

Condition	n	p
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B	10	0.01

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