Exploitation of the maximum potential of fluorescence spectroscopy for water resource systems using Bayesian statistical approaches

Sandra Peer, Ottavia Zoboli, Anastassia Vybornova, Jörg Krampe, and Matthias Zessner
Institute for Water Quality and Resource Management, TU Wien, Austria (sandra.peer@tuwien.ac.at)

Fluorescence Spectroscopy is a very promising tool for the identification of dissolved organic material (DOM) in aquatic systems. It is rapid, sensitive and relatively inexpensive. Knowledge gaps and challenging interpretation of large and complex datasets are currently hindering the full exploitation of its potential. To cite only few of the most crucial challenges, different fluorophores can contribute to overlapping peaks in the Excitation Emission Matrix (EEM), peaks can be shifted or their intensity can be reduced or enhanced through different environmental factors, and more powerful data processing tools are required. EEM data are typically analyzed by means of Parallel Factor Analysis (PARAFAC), which is a powerful technique that will also be applied here. Nevertheless, PARAFAC and similar analytical tools have a range of limitations. Therefore, we propose to develop and test a novel systemic approach and Bayesian statistical techniques to overcome existing obstacles. Contrary to the above mentioned, Bayesian statistics allow integrating prior information within the analysis in a transparent, formal and reproducible way. In this field, a vast body of knowledge and data has been gathered, which can be formalized in the form of priors and be included in the interpretation of data to make the analysis more powerful and robust. We will explore different applications in an EEM dataset consisting of samples from well-studied water systems with diverse characteristics covering spatial and temporal variability.