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New deconvoluting algorithm offers new approach for mass spectrometry data compression **FREE**

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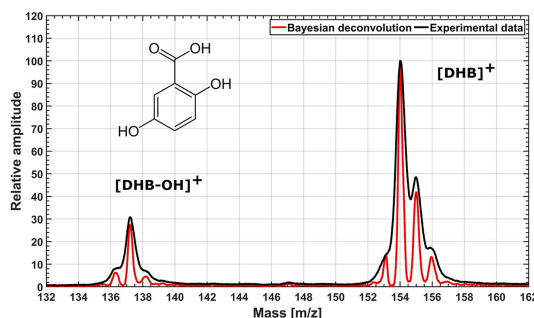


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Modifying the established Lucy-Richardson algorithm with Bayesian prior distributions increase convergence rate four-fold and doubles mass resolution.



Mass spectrometry (MS) has emerged as a promising new way to differentiate between healthy and unhealthy biological tissues. Maintaining a mass spectrometric database for such biomarkers from increasingly complex measurements requires a more efficient way to manage and compress the data. One new paper points a way forward for how to manage this data while still preserving its usefulness for studying biological tissues.

Pieterse et al. report findings from deconvoluting low-resolution time-of-flight data for MS experiments. By modifying the established Lucy-Richardson deconvolution algorithm with Bayesian prior distributions, the group was able to improve on the algorithm's performance when using a prior of second-differences in the signal.

In addition to implementing a novel stopping criterion and boosting mechanism, they demonstrated their new method by deconvoluting fragmentation peaks of 2,5-dihydroxybenzoic acid matrix and a benzyltriph-nylphosphonium thermometer ion.

"We feel that this new approach to analyzing MS data is going to make a major difference in handling the huge amount of data and assignments in the coming advances in resolution in spatially resolved MS," said author Cornelius Pieterse.

The new method increases the rate of convergence by more than four-fold compared to the standard algorithm. It accomplishes this while preserving peak amplitude ratios of a similar fraction of the total peaks, as well as doubling the mass resolution, which provides a way for researchers to quantify spectra more accurately.

The group next looks to test their method on other types of datasets, including MS images for spatially resolving single cells, where an analytical tool tailored for higher performance is vital.

Source: "Rapid deconvolution of low-resolution time-of-flight data using Bayesian inference," by Cornelius L. Pieterse, Michiel B. de Kock, Wesley D. Robertson, Hans C. Eggers, and R. J. Dwayne Miller, *Journal of Chemical Physics* (2019). The article can be accessed at <https://doi.org/10.1063/1.5129343>.

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