The PTW package: Global Parametric Time Warping in R

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Chemometric analyses of chromatograms and spectra are often hampered by misalignments due to small changes in experimental parameters (column ageing in chromatography, pH differences in NMR, etc.). Several computational techniques have been proposed to correct for such shifts, notably Correlation Optimized Warping (COW[1]) and Parametric Time Warping (PTW[2]) which have become popular during the last years.

The widespread use of multivariate detection methods in chromatography and the development of new 'hybrid' or 'hyphenated' techniques like GC-MS and LC-NMR demand the development of global alignment methods, that use the multivariate nature of the detector to their advantage. An example of such a technique is COW-CODA[3], an expansion of COW including the selection of high-quality chromatographic traces by the COmponent Detection Algorithm (CODA[4]).

PTW can also be modified to make it capable of performing global alignments. Here we present the **PTW** package, containing an R impletation of the Parametric Time Warping algorithm, based on the original implementation by Eilers[2]. The algorithm has been expanded to include:

- an optional global alignment making full use of multivariate detection methods;
- the use of optimization methods from the **stats** package, enhancing the search for the optimal alignment beyond the original steepest descent method;
- a number of measures for assessing the alignment quality;
- a method for selecting the best traces to use for alignment based on an enhanced version of CODA;
- a number of visualization options.

References

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