The rpm package: Aligning LC/MS mass spectra with R

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multidimensional
image
processing
group

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Overview

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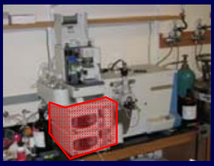
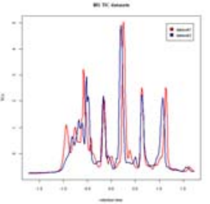
- LC/MS
  - liquid chromatography
  - mass spectrometry
- total ion current (TIC)
  - non-linear distortions
  - alignment for inter-sample comparability
- challenge
  - landmark-free
  - robustness





Methods

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- Robust Point Matching (RPM) [1]
  - matches two point sets $\{x_i\}$ and $\{v_a\}$
  - alternating approach
    - estimate correspondence matrix
    - estimate transformation f: $\{v_a\} \rightarrow \{x_i\}$
  - annealing steps
- adaption to LC/MS data
  - warping constrained to LC domain
  - new distance metric for correspondence estimation
  - additional slope information

[1] Chui H, Rangarajan A (2002)

Results

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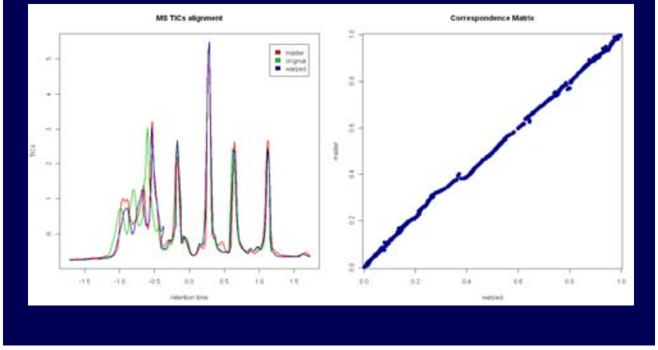

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