

on the full two-dimensional data, Figure 2 shows the alignments applied to the TICs and also the two-dimensional data, using the optimal value of λ .

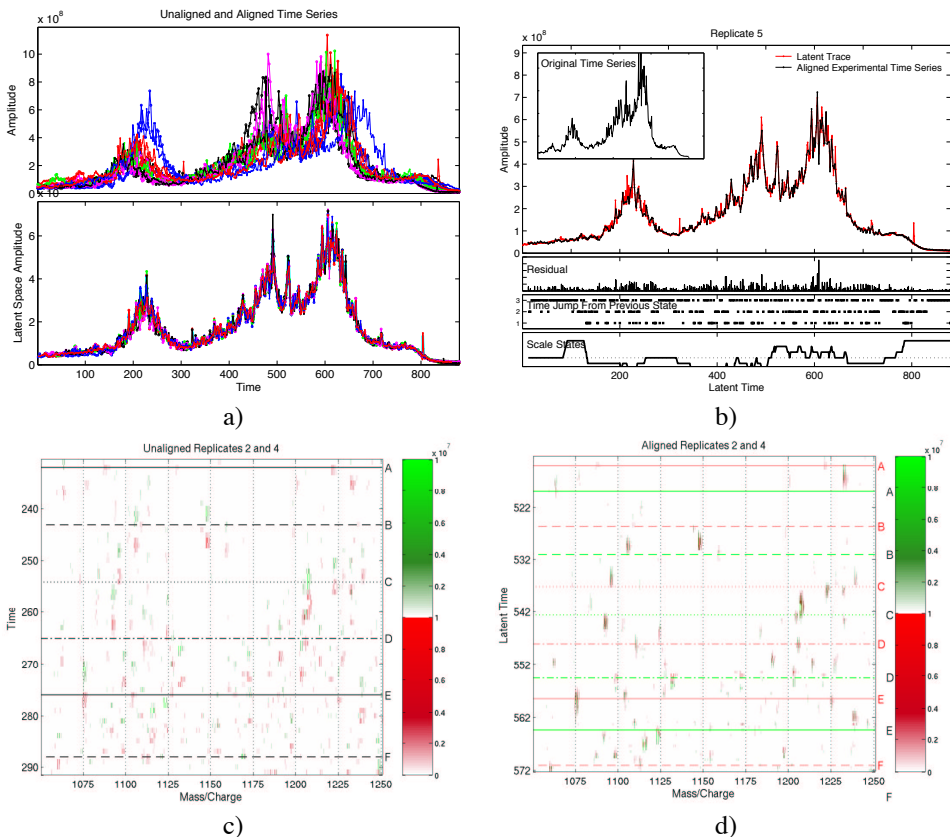


Figure 2: Figure 2: a) Top: 13 Replicate pre-processed TICs as described in Section 4), Bottom: same as top, but aligned with CPM (the learned latent trace is also shown). b) The fifth TIC replicate aligned to the learned latent trace (inset shows the original, unaligned). Below are three strips showing, from top-to-bottom, i) the error residual, ii) the number of time states moved between every two states in the Viterbi alignment, and iii) the local scaling applied at each point in the alignment. c) A portion of the two-dimensional LC-MS data from replicates two (in red) and four (in green). d) Same as c), but after alignment (the same one dimensional alignment was applied to every Mass/Charge value). Marker lines labeled A to F show how time in c) was mapped to latent time using the Viterbi alignment.

We also trained our model on five different sets of LC-MS data, each consisting of human blood serum. We used no smoothing and found the results visually similar in quality to the first data set.

To ensure convergence to a good local optimum and to speed up training, we pre-processed the LC-MS data set by coarsely aligning and scaling each time series as follows: We 1) translated each time series so that the center of mass of each time series was aligned to the median center of mass over all time series, 2) scaled the abundance values such that the sum of abundance values in each time series was equal to the median sum of abundance values over all time series.

We also used our model to align 10 speech signals, each an utterance of the same sentence