Factor analysis techniques in single-particle aerosol mass spectrometry

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Single-particle aerosol mass spectrometry

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The figure is from
Thomson, D.S., M.E. Schein, and D.M. Murphy, Particle analysis by laser mass spectrometry WB-57 instrument overview, Aerosol Science and Technology, 33, 153-169, 2000. Please see Figure 1.

The challenge

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The figure is from
Murphy, D. M., A. M. Middlebrook, and M. Warshawsky, Cluster analysis of data from the Particle Analysis by Laser Mass Spectrometry (PALMS) instrument, *Aerosol Sci. Technol.*, 37, 382-391, 2003.

Principal component analysis

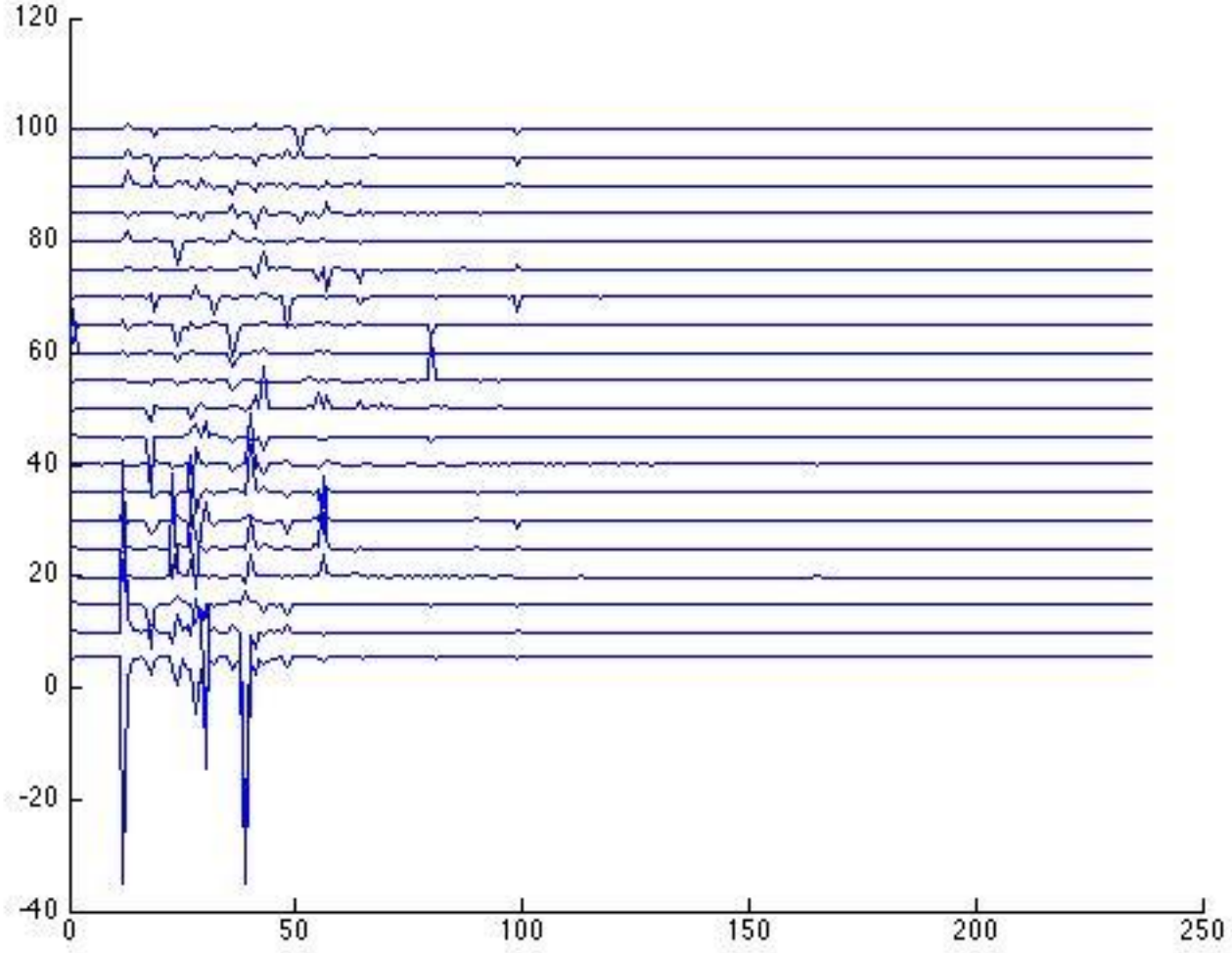
Probabilistic PCA: PCA together with EM to handle large data sets and missing values. Algorithm written by Jakob Verbeek, et al. 2002.

If y is a data vector and x is a vector of principal components,

- E-step: estimate x vectors and missing values of y

- M-step: maximize the expected joint log-likelihood of x and y

Principal component analysis



Independent component analysis

1. Starts with the principal components derived from the previous algorithm.

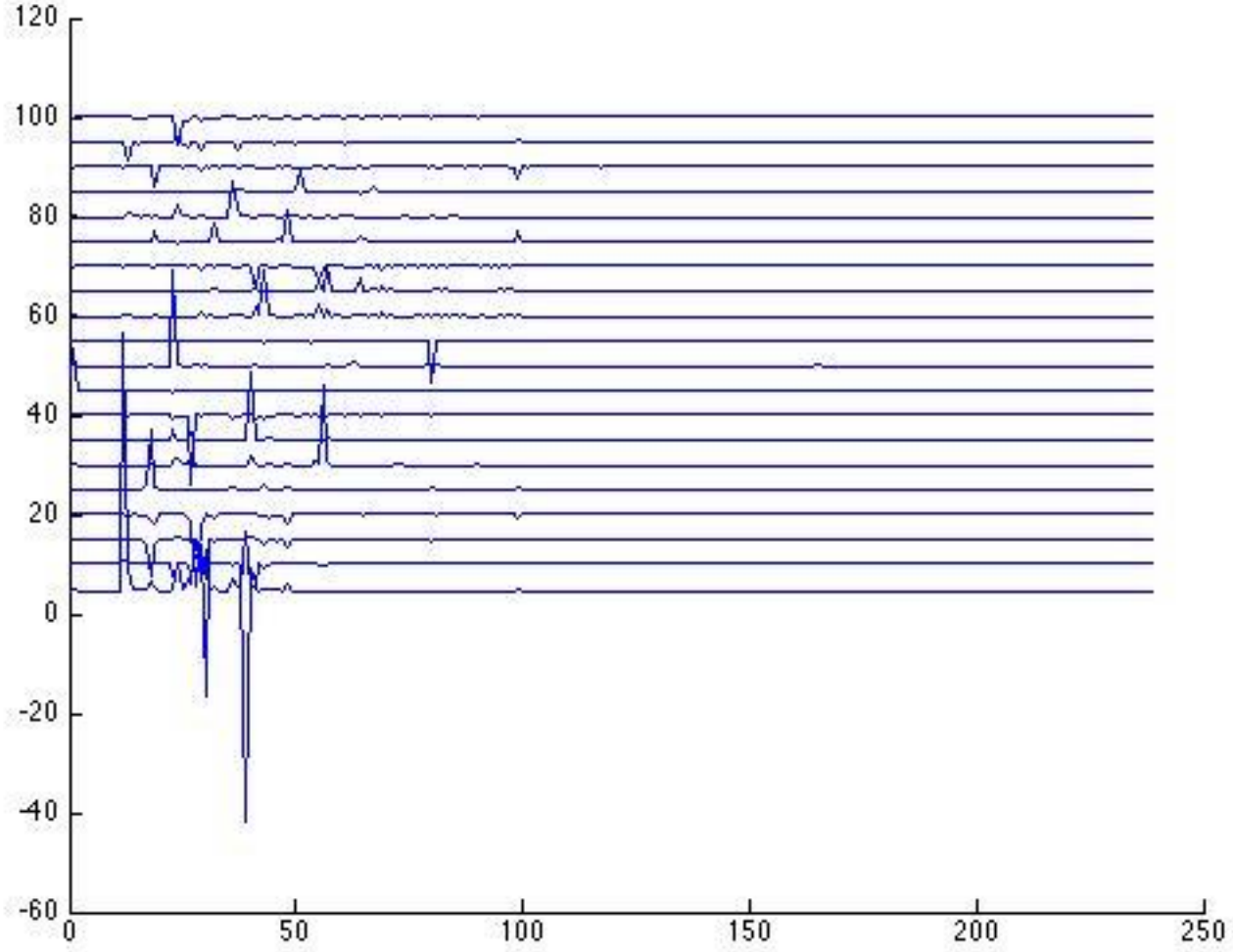
1. Assumes non-Gaussian distributions, maximizes the kurtosis for randomly-generated weighing factors.

2. Decorrelates and re-normalizes factors after every iteration:

$$w_{p+1} = w_{p+1} - \sum_{j=1}^{p} w_{p+1}^{T} w_j w_j$$

$$w_{p+1} = w_{p+1} / \sqrt{w_{p+1}^{T} w_{p+1}}$$

Independent component analysis



Non-negative matrix factorization

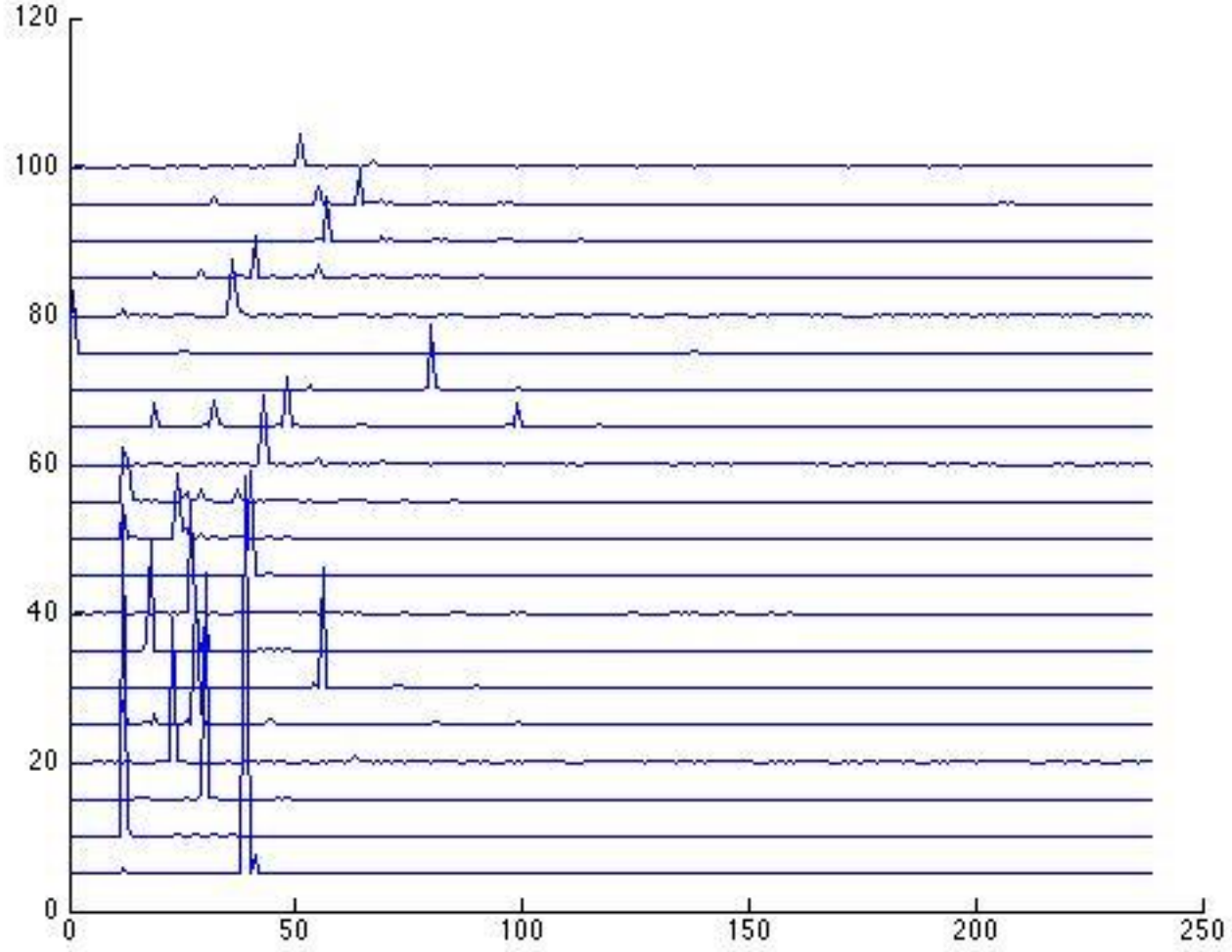
1. Factors an *n*-by-*m* matrix A into nonnegative factors W (*n*-by-k) and H (k-by-*m*).

2. Starting with random W and H, iteratively minimize the residual:

$$D = \sqrt{\frac{\|A - WH\|_F}{nm}}$$

3. Re-normalize W and H.

Non-negative matrix factorization



Future work

1. Try a different way of measuring non-gaussianity in the ICA algorithm (negentropy)

2. Combine ICA and NNMF?

3. Validate results with laboratory data and analyze multiple aircraft flights

4. Clustering algorithms?

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