3-D Factorization of Mass Spectral Datasets

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Open Mic Time
A data matrix is decomposed into an arbitrary number of factors, each of which is represented by a constant mass spectrum and a contribution time series. There is usually some residual of fit.
What about 3D datasets?

- Particle Size
- Desorption Temp
- Retention Time

AMS  PToF
AMS + Thermal denuder
“T”GO
MOVI-CIMS
TAG
Options for factorization of 3D matrices

Ulbrich et al., Atmos. Meas. Tech. Discuss., 2011

Input Matrix

\[
\begin{align*}
\text{Input Matrix} & = \text{Factor 1} + \text{Factor 2} + \ldots + \text{Residual Matrix} \\
& = \begin{cases}
\text{Constant Spectrum} & \text{Constant Size Distribution} \\
\text{Contribution Time Series} & \\
\text{Time-Evolving Spectrum} & \text{Time-Evolving Size Distribution}
\end{cases}
\end{align*}
\]

Chemical component has fixed size distribution

Chemical component has changing size distribution

3-vector model

Vector-matrix model

(showing 1 of 3 types)