Nonnegative **u**nimodal **M**atrix **F**actorization

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1. Introduction and motivation
2. Algorithm
3. Theory
4. Some fancy pictures
5. Summary

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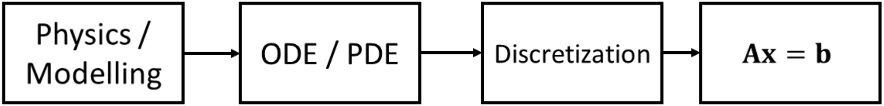
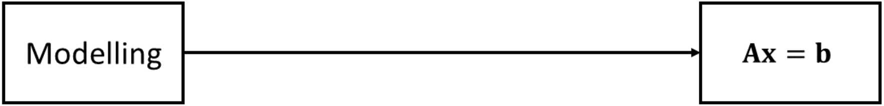
Scientific computing



A is ``*structured*'': tri-diagonal, symmetric, ...

Machine Learning / Data Mining / Data Science



A is ``*structured*'' in other sense

Structural factorization

- Factorize data into (low-rank) factors with **structural constraints**.

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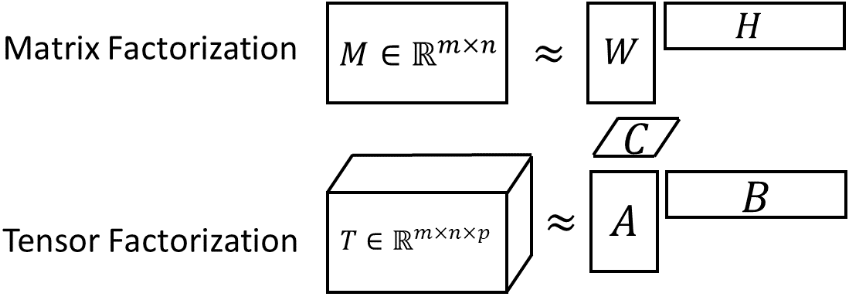

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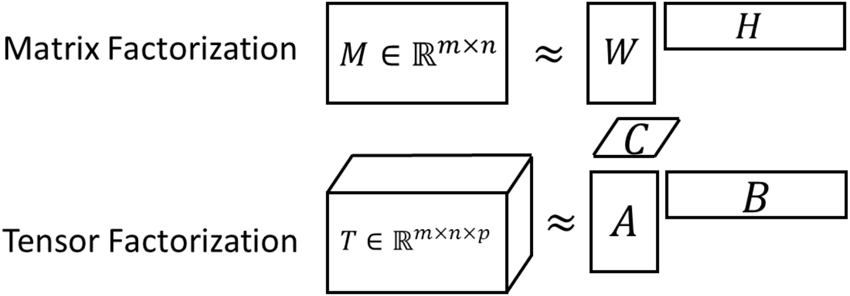

- This talk: **unimodal structure.**

Unimodality

- A vector $\mathbf{a} = [a_1 \ a_2 \ \dots \ a_m]$ is unimodal if

$$\underbrace{a_1 \leq a_2 \leq \cdots \leq}_{\text{increasing head}} \ a_p \ \underbrace{\geq a_{p+1} \geq \cdots \geq a_m}_{\text{decreasing tail}}.$$

- Nonnegative Unimodality (Nu) $=$ Def. of u $+$ nonnegativity

$$0 \leq a_1 \leq a_2 \leq \cdots \leq a_p \geq a_{p+1} \geq \cdots \geq a_m \geq 0. \qquad \text{(Nu)}$$

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- Nonnegative Unimodality (Nu) = Def. of u + nonnegativity

$$0 \leq a_1 \leq a_2 \leq \cdots \leq a_p \geq a_{p+1} \geq \cdots \geq a_m \geq 0. \qquad \text{(Nu)}$$

- A vector $\mathbf{x}$ is Nu:

$$\mathbf{x} \in \mathbb{R}^m \text{ is Nu} \iff \exists p \in [m] \text{ s.t. } 0 \leq x_1 \leq \cdots \leq x_p \geq \cdots \geq x_n \geq 0.$$

Some Nu vectors

$$0 \le a_1 \le a_2 \le \cdots \le a_p \ge a_{p+1} \ge \cdots \ge a_m \ge 0. \qquad \text{(Nu)}$$

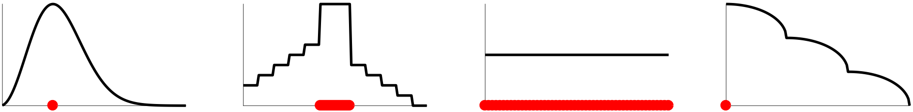

Figure: Four Nu vectors. Black: the plot of the sequence. Red: the locations of p.

- p can be unique or non-unique
- p can be any integer in $\{1, 2, \ldots, m\}$.

Nonnegative unimodal factorization

- Factorize data into (low-rank) factors with **Nu constraints**.
- Examples
  - Factorize a matrix $\mathbf{M}$ into product $\mathbf{WH}$ such that the columns of $\mathbf{W}$ are Nu + (other constraints).
  - Factorize a tensor $\mathcal{T}$ into product $\mathcal{G} \times_1 \mathbf{A} \times_2 \mathbf{B} \times_3 \mathbf{C}$ such that the columns of $\mathbf{A}$ are Nu + (other constraints).

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- Questions
  - Why consider Nu? — Application motivation
  - How to formulate Nu and how to solve it? — Algorithm / Optimization
  - What is known about this model? — Theory / Linear Algebra

Motivation: some data are Nu

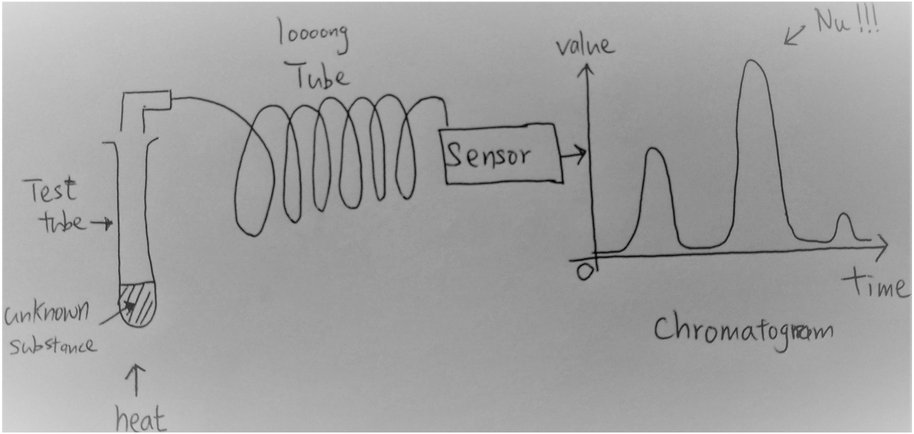

Figure: Chromatography.

Characterization of Nu set

- A vector $\mathbf{x} \in \mathbb{R}^m$ is Nu:

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- Notations
  - $\mathbf{x} \in \mathcal{U}_+^m$ means $\mathbf{x} \in \mathbb{R}^m$ is Nu
  - $\mathbf{x} \in \mathcal{U}_+^{m,p}$ means $\mathbf{x} \in \mathbb{R}^m$ is Nu with known p

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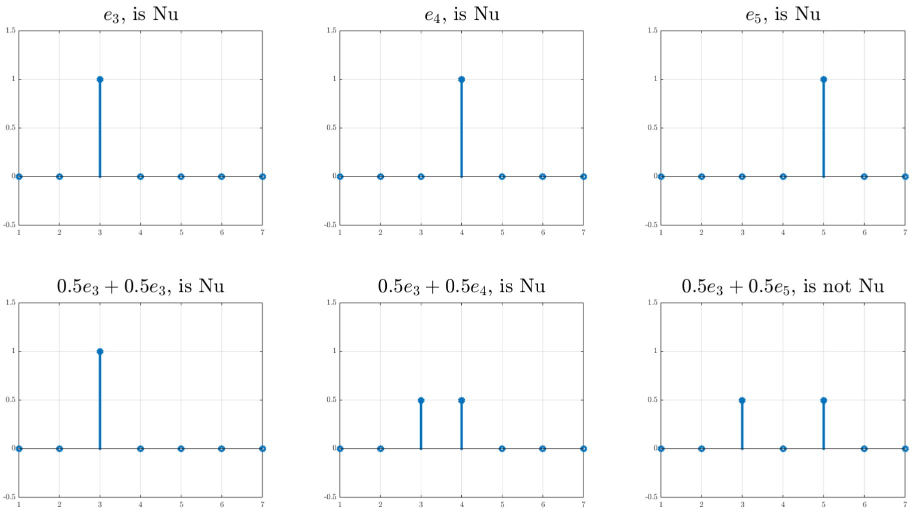
- Facts
  - $\mathcal{U}_+^{m,p}$ is a convex set.
  - $\mathcal{U}_+^m = \bigcup_k \mathcal{U}_+^{m,k}$
  - $\mathcal{U}_+^m$ is **non**convex.
    Example: $\mathbf{e}_i$ and $\mathbf{e}_j$ are Nu but $\lambda \mathbf{e}_i + (1-\lambda)\mathbf{e}_j$ is not Nu if $|i-j| \geq 2$.

$\mathbf{e}_i$ and $\mathbf{e}_j$ are Nu but $0.5\mathbf{e}_i + 0.5\mathbf{e}_j$ is not Nu if $|i-j| \geq 2$.



The set $\mathcal{U}_+^{m,p} \cup \mathcal{U}_+^{m,p+1}$ is convex

$$\mathbf{x} \in \mathbb{R}^m \text{ is Nu} \quad \iff \quad \exists p \in [m] \text{ s.t. } \mathbf{x} \in \mathcal{U}_+^{m,p} \cup \mathcal{U}_+^{m,p+1}$$

$$\iff \quad \begin{cases} 0 & \leq & x_1 \\ x_1 & \leq & x_2 \\ & \vdots & \\ x_{p-1} & \leq & x_p \\ & & \\ x_{p+1} & \geq & x_{p+2} \\ & \vdots & \\ x_{m-1} & \geq & x_m \\ x_m & \geq & 0 \end{cases}$$

"Nu membership characterized by a system of monic inequalities".

$$\mathbf{x} \in \mathcal{U}_+^{m,p} \cup \mathcal{U}_+^{m,p+1} \iff \begin{cases} 0 & \leq & x_1 \\ x_1 & \leq & x_2 \\ & \vdots & \\ x_{p-1} & \leq & x_p \\ x_{p+1} & \geq & x_{p+2} \\ & \vdots & \\ x_{m-1} & \geq & x_m \\ x_m & \geq & 0 \end{cases} \iff \mathbf{U}_p\mathbf{x} \geq \mathbf{0}$$

$$\mathbf{U}_p = \begin{pmatrix} \underbrace{\begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}_{p\times p}}_{\mathbf{D}_{p\times p}} & \mathbf{0}_{p\times(m-p)} \\ \mathbf{0}_{(m-p)\times p} & \mathbf{D}^\top_{(m-p)\times(m-p)} \end{pmatrix}.$$

NuMF

- GIVEN $\mathbf{M} \in \mathbb{R}_+^{m \times n}$ and $r \in \mathbb{N}$,
  FIND $\mathbf{W} \in \mathbb{R}^{m \times r}$ and $\mathbf{H} \in \mathbb{R}^{r \times n}$ by solving

$$\text{minimize } \frac{1}{2}\|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2 \quad \text{subject to} \quad \begin{aligned} &\mathbf{H} \geq \mathbf{0}, \\ &\mathbf{w}_j \in \mathcal{U}_+^m \text{ for all } j \in [r], \\ &\mathbf{w}_j^\top \mathbf{1}_m = 1 \text{ for all } j \in [r], \end{aligned}$$

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- Apply the characterization:

$$\text{minimize } \frac{1}{2}\|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2 \quad \text{subject to} \quad \begin{aligned} &\mathbf{H} \geq \mathbf{0}, \\ &\mathbf{U}_{p_j}\mathbf{w}_j \geq \mathbf{0} \text{ for all } j \in [r], \\ &\mathbf{w}_j^\top \mathbf{1}_m = 1 \text{ for all } j \in [r], \end{aligned}$$

where integers $p_1, p_2, \ldots, p_r$ are unknown!

How to solve: BCD

$$\min_{\substack{\mathbf{W},\mathbf{H}\\ p_1,\ldots,p_j}} \frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 \ \text{ s.t. } \mathbf{H}\geq \mathbf{0},\ \mathbf{U}_{p_j}\mathbf{w}_j\geq \mathbf{0},\ \mathbf{w}_j^\top \mathbf{1}_m = 1,\ \forall j\in[r].$$

- Subproblem on $\mathbf{H}$ is simple.

$$\min_{\mathbf{H}} \frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 \ \text{ s.t. } \mathbf{H}\geq \mathbf{0}.$$

- Main difficulty comes from subproblem on $\mathbf{W}$.

Subproblem on $\mathbf{W}$

$$\min_{\mathbf{W},p_1,\ldots,p_j} \frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 \;\text{ s.t. }\; \mathbf{U}_{p_j}\mathbf{w}_j \geq \mathbf{0},\; \mathbf{w}_j^\top \mathbf{1}_m = 1,\; \forall j \in [r].$$

- Problem involves integer variables and is nonconvex.
- The subproblem on a column of $\mathbf{W}$ (in the HALS framework) is

$$\min_{\mathbf{w}_i,p_i} \frac{\|\mathbf{h}^i\|_2^2}{2}\|\mathbf{w}_i\|_2^2 - \langle \mathbf{M}_i {\mathbf{h}^i}^\top, \mathbf{w}_i\rangle + c \;\text{ s.t. }\; \mathbf{U}_{p_i}\mathbf{w}_i \geq \mathbf{0},\; \mathbf{w}_i^\top \mathbf{1} = 1,$$

which is a linearly-constrained quadratic program.

What is HALS= column-wise block coordinate descent

$$
\begin{aligned}
\frac{1}{2}\|\mathbf{M}-\mathbf{W}\mathbf{H}\|_F^2 &= \frac{1}{2}\Big\|\mathbf{M}-\sum_{j=1}^{r}\mathbf{w}_j\mathbf{h}^j\Big\|_F^2 \\
&= \frac{1}{2}\Big\|\underbrace{\mathbf{M}-\sum_{j\neq i}\mathbf{w}_j\mathbf{h}^j}_{:=\mathbf{M}_i}-\mathbf{w}_i\mathbf{h}^i\Big\|_F^2 \\
&= \frac{1}{2}\|\mathbf{M}_i-\mathbf{w}_i\mathbf{h}^i\|_F^2 \\
&= \text{a quadratic function on } \mathbf{w}_i
\end{aligned}
$$

Subproblem on a column of $\mathbf{W}$

$$\min_{\mathbf{w}_i, p_i} \frac{\|\mathbf{h}^i\|_2^2}{2} \|\mathbf{w}_i\|_2^2 - \langle \mathbf{M}_i {\mathbf{h}^i}^\top, \mathbf{w}_i \rangle \ \text{ s.t. } \mathbf{U}_{p_i} \mathbf{w}_i \geq \mathbf{0}, \ \mathbf{w}_i^\top \mathbf{1} = 1,$$

- A linearly-constrained quadratic program.
- Brute-force approach: solve this problem on all (even) p, pick the best one as p_i.
- Brute-force is slow if m is large, only OK if m sufficiently small. We need acceleration!

Speed up the brute-force algorithm for large m

- Speed up 1: solve the subproblem using Nesterov's accelerated projected gradient.
- Speed up 2: reduce the search space for p_i's.
  - By guessing the location of p_i's
  - By dimension reduction: **multi-level / multi-grid method**
    - Multi-grid preserves Nu: a theorem with proof in 3 sentences!
    - Other dimension reduction techniques such as PCA or Gaussian sampling do not work here as they destroy the Nu.

APG: Accelerated Projected Gradient

The subproblem on a column of $\mathbf{W}$ (**with** p_i **fix**)

$$\min_{\mathbf{w}_i} \frac{\|\mathbf{h}^i\|_2^2}{2}\|\mathbf{w}_i\|_2^2 - \langle \mathbf{M}_i {\mathbf{h}^i}^\top, \mathbf{w}_i \rangle \ \text{ s.t. } \ \mathbf{U}_{p_i}\mathbf{w}_i \geq \mathbf{0}, \ \mathbf{w}_i^\top \mathbf{1} = 1.$$

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- The constraint $\left\{\mathbf{U}_{p_i}\mathbf{w}_i \geq \mathbf{0}, \;\; \mathbf{w}_i^\top \mathbf{1} = 1\right\}$ is hard to project.

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$$\min_{\mathbf{w}_i} \frac{\|\mathbf{h}^i\|_2^2}{2}\|\mathbf{w}_i\|_2^2 - \langle \mathbf{M}_i \mathbf{h}^{i\top}, \mathbf{w}_i \rangle \ \text{ s.t. } \ \mathbf{U}_{p_i}\mathbf{w}_i \geq \mathbf{0}, \ \mathbf{w}_i^\top \mathbf{1} = 1.$$

- The constraint $\left\{ \mathbf{U}_{p_i}\mathbf{w}_i \geq \mathbf{0}, \ \mathbf{w}_i^\top \mathbf{1} = 1 \right\}$ is hard to project.
- Transform the problem via $\mathbf{y} = \mathbf{U}\mathbf{w}$:

$$\min_{\mathbf{y}} \frac{1}{2}\left\langle \|\mathbf{h}^i\|_2^2 \mathbf{U}_{p_i}^{-\top}\mathbf{y},\, \mathbf{y} \right\rangle - \left\langle \mathbf{U}_{p_i}^{-\top}\mathbf{M}_i \mathbf{h}^{i\top},\, \mathbf{y} \right\rangle \text{ s.t. } \mathbf{y} \geq \mathbf{0},\, \mathbf{y}^\top \mathbf{U}_{p_i}^{-\top}\mathbf{1} = 1$$

or equivalently

$$\min_{\mathbf{y}} \frac{1}{2}\langle \mathbf{Q}\mathbf{y}, \mathbf{y} \rangle - \langle \mathbf{p}, \mathbf{y} \rangle \ \text{ s.t. } \ \mathbf{y} \geq \mathbf{0}, \ \mathbf{y}^\top \mathbf{b} = 1.$$

- Once we get $\mathbf{y}^*$, we get $\mathbf{w}_i^*$ by $\mathbf{y} = \mathbf{U}\mathbf{w}$.

APG on solving $\mathbf{y}$

- The key is the projection onto the irregular simplex: given a point $\mathbf{z}$

$$P(\mathbf{z}) = \operatorname*{argmin}_{\mathbf{y}} \frac{1}{2}\|\mathbf{y}-\mathbf{z}\|_2^2 \text{ s.t. } \mathbf{y} \geq \mathbf{0}, \mathbf{y}^\top \mathbf{b} = 1.$$

- Optimal sol.: solving the partial Lagrangian

$$\mathbf{y}^* \overset{(*)}{=} \min_{\mathbf{y}\geq\mathbf{0}} \max_{\nu} \underbrace{\frac{1}{2}\|\mathbf{y}-\mathbf{z}\|_2^2 + \nu(\mathbf{y}^\top\mathbf{b}-1)}_{L(\mathbf{y},\nu)} = [\mathbf{z}-\nu^*\mathbf{b}]_+,$$

with closed-form solution given by soft-thresholding, where the Lagrangian multiplier ν^* is the root of a piece-wise linear equation

$$\sum_{i=1}^{m} \max\left\{0, z_i - \nu b_i\right\} b_i = 1,$$

which takes $\mathcal{O}(m)$ to $\mathcal{O}(m\log m)$ to solve by sorting the break points $\frac{z_i}{b_i}$. After sorting, the magical-one-line-code is

```
nu = max((cumsum(z.*b)-1)./(cumsum(b.*b)));
```

(*): The problem satisfies the Slater's condition, i.e., the feasible set has a non-empty relative interior, which guarantees strong duality.

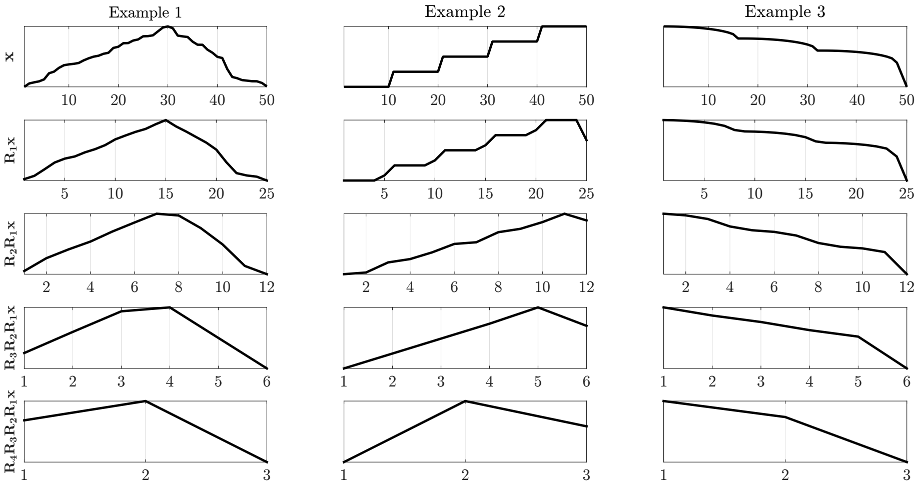
Multi-grid

- Idea: instead of working on $\mathbf{w}$, work on $\mathbf{R}_N \dots \mathbf{R}_1 \mathbf{w}$ with smaller search space of p.

- Restriction $\mathbf{R} \in \mathbb{R}_+^{m_1 \times m}$ changes $\mathbf{x} \in \mathbb{R}_+^m$ to $\mathbf{R}\mathbf{x} \in \mathbb{R}_+^{m_1}$ with $m_1 < m$.

$$\mathbf{R}(a,b) = \begin{bmatrix} a & b & & & & & \\ & b & a & b & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & b & a & b & \\ & & & & & b & a \end{bmatrix}, \begin{array}{c} a > 0, b > 0, \\ a + 2b = 1. \end{array}$$

- **Key fact**: if $\mathbf{x}$ is NU, then $\mathbf{R}\mathbf{x}$ is Nu.


Example 1
Example 2
Example 3
x
R_1x
R_2R_1x
$R_3R_2R_1x$
$R_4R_3R_2R_1x$

Theorem: if $\mathbf{x}$ is Nu, then $\mathbf{Rx}$ is Nu.

- The 3-sentence-proof:
  1. $\mathbf{R}$ can be expressed as a sum

     $$\underbrace{\begin{bmatrix} a & b & & & \\ & b & a & b & \\ & & & b & a \end{bmatrix}}_{\mathbf{R}} = \underbrace{\begin{bmatrix} a & 0 & & & \\ & 0 & a & 0 & \\ & & & 0 & a \end{bmatrix}}_{\mathbf{A}} + \underbrace{\begin{bmatrix} 0 & b & & & \\ & & 0 & b & \\ & & & & 0 \end{bmatrix}}_{\mathbf{B}} + \underbrace{\begin{bmatrix} 0 & & & & \\ & b & 0 & & \\ & & & b & 0 \end{bmatrix}}_{\mathbf{C}}$$

     so $\mathbf{Rx} = \mathbf{Ax} + \mathbf{Bx} + \mathbf{Cx}$.

  2. $\mathbf{A}, \mathbf{B}, \mathbf{C}$ are sampling operators picking the odd or even indices of $\mathbf{x}$, so $\mathbf{Ax}$, $\mathbf{Bx}$ and $\mathbf{Cx}$ are all Nu.

  3. The sum $\mathbf{Ax} + \mathbf{Bx} + \mathbf{Cx}$ is Nu because their p values differ at most 1.

- Theorem (formally): let $\mathbf{x} \in \mathcal{U}_+^{m,p}$ with p is even[1] and $\mathbf{R} \in \mathbb{R}^{m_1 \times m}$ defined as in page 16. Then $\mathbf{y} = \mathbf{Rx} \in \mathcal{N}_+^{m_1,p_y}$ with $\mathcal{N}_+^{m,p} = \mathcal{U}_+^{m,p} \cup \mathcal{U}_+^{m,p+1}$ and $p_y \in \{\lfloor \frac{p}{2} + 1 \rfloor, \lfloor \frac{p}{2} \rfloor\}$.

[1] If p is odd, by considering the vector $[0, \mathbf{x}]$ does not change the unimodality and increases p by one.

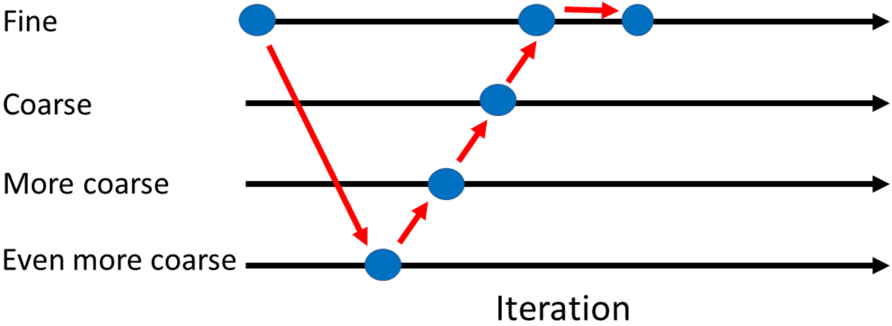
The whole algorithm (in words) for NuMF($\mathbf{M}, r$)

Steps:

1. Restriction $\mathbf{M}^{[N]} = \mathbf{R}_N \dots \mathbf{R}_1 \mathbf{M}$ and $\mathbf{W}_0^{[N]} = \mathbf{R}_N \dots \mathbf{R}_1 \mathbf{W}_0$
2. Solve NuMF on coarse grid:
$$[\mathbf{W}_*^{[N]}, \mathbf{H}_*, \mathbf{p}_*^{[N]}] \leftarrow \mathrm{NuMF}(\mathbf{M}^{[N]}, \mathbf{W}_0^{[N]}, \mathbf{H}_0)$$
by brute-forcing the p_i and using APG on subproblem on $\mathbf{W}$.
3. Interpolate: $[\mathbf{W}_0, \mathbf{p}_0] \leftarrow \mathrm{Interpolate}(\mathbf{W}_*^{[N]}, \mathbf{p}_*^{[N]})$.
4. Solve NuMF on the original fine grid:
$$[\mathbf{W}_*, \mathbf{H}_*, \mathbf{p}_*] \leftarrow \mathrm{NuMF}(\mathbf{M}, \mathbf{W}_0, \mathbf{H}_0, \mathbf{p}_0)$$
without brute-forcing p_i.

* step 1-4 can be repeated several times: V-cycle, W-cycle, blablabla.

Not really a multigrid but multi-level algorithm



Identifiability: when does solving NuMF give a unique sol?

- Definition: for $\mathbf{x} \in \mathbb{R}^m_+$, $\text{supp}(\mathbf{x}) := \{i \in [m] \mid x_i \neq 0\}$.
- $\forall$ Nu vectors, supp is a closed-interval $[a, b]$ $\because$ no "internal zeros".
- Interactions between two Nu vectors $\mathbf{x}, \mathbf{y}$:
  let $\text{supp}(\mathbf{x}) = [a_x, b_x]$ and $\text{supp}(\mathbf{y}) = [a_y, b_y]$,
  - Strictly disjoint: $a_x > b_y + 1$.
  - Adjacent: $a_x = b_y + 1$.
  - Disjoint = strictly disjoint $\cup$ adjacent
  - Overlap: not disjoint
  - Partial overlap: supports overlap but $\text{supp}(\mathbf{x}) \overset{\subsetneq}{\underset{\supsetneq}{}} \text{supp}(\mathbf{y})$
  - Complete overlap: $\text{supp}(\mathbf{x}) \subseteq \text{supp}(\mathbf{y})$
- Current research status: identifiability for the first two cases.

Identifiability of the strictly disjoint case

Theorem

Assumes $\mathbf{M} = \bar{\mathbf{W}}\bar{\mathbf{H}}$. *Solving NuMF recovers* $(\bar{\mathbf{W}}, \bar{\mathbf{H}})$ *if*

1. $\bar{\mathbf{W}}$ *is Nu and all the columns have strictly disjoint support.*
2. $\bar{\mathbf{H}} \in \mathbb{R}_+^{r \times n}$ *has* $n \geq 1$, $\|\bar{\mathbf{h}}^i\|_\infty > 0$ *for* $i \in [r]$.

Proof *Assume there is another solution* $(\mathbf{W}^*, \mathbf{H}^*)$ *that solves the NuMF. The columns* $\bar{\mathbf{w}}_j$ *contribute in* $\mathbf{M}$ *a series of disjoint unimodal components. For the solution* $\mathbf{W}^*\mathbf{H}^*$ *to fit* $\mathbf{M}$, *each* $\mathbf{w}_i^*$ *has to fit each of these disjoint component in* $\mathbf{M}$, *and hence* $\mathbf{W}^*$ *recovers* $\bar{\mathbf{W}}$ *up to permutation. There is no scaling ambiguity here because of the normalization constraints* $\mathbf{w}_i^\top \mathbf{1} = 1$. *Moreover,* $\mathbf{W}^*$ *and* $\bar{\mathbf{W}}$ *have rank* r, *since their columns have disjoint support, and hence* $\mathbf{H}^*$ *and* $\bar{\mathbf{H}}$ *are uniquely determined (namely, using the left inverses of* $\mathbf{W}^*$ *and* $\bar{\mathbf{W}}$*), up to permutation.*

Note: this theorem holds for $r \geq n$. You can have a $r = 1000$ factorization with $n = 1$.

Demixing two non-fully overlapping Nu vectors

- Given non-zero vectors $\mathbf{x}, \mathbf{y}$ in $\mathcal{U}_+^m$ with partial overlap supports, if $\mathbf{x}, \mathbf{y}$ are generated by two non-zero Nu vectors $\mathbf{u}, \mathbf{v}$ as

$$\mathbf{x} = a\mathbf{u} + b\mathbf{v} \text{ and } \mathbf{y} = c\mathbf{u} + d\mathbf{v}$$

  with nonnegative coefficients a, b, c, d, then either

$$\mathbf{u} = \mathbf{x}, \mathbf{v} = \mathbf{y} \text{ or } \mathbf{u} = \mathbf{y}, \mathbf{v} = \mathbf{x}.$$

- Let $\mathbf{X} = \mathbf{U}\mathbf{Q}$, where $\mathbf{X} := [\mathbf{x}, \mathbf{y}]$, $\mathbf{U} := [\mathbf{u}, \mathbf{v}]$ and $\mathbf{Q} := \begin{bmatrix} a & c \\ b & d \end{bmatrix} \geq \mathbf{0}$.
  What we show: $\mathbf{Q}$ is a permutation matrix.

Sketch of the proof

- $\mathbf{x}, \mathbf{y}$ are Nu with partial-overlap supports imply
  - $\mathbf{u}, \mathbf{v}$ are linearly independent: $\mathbf{U}$ is rank-2
  - $\mathbf{x} \neq 0$, $\mathbf{y} \neq 0$ and $\mathbf{x}, \mathbf{y}$ are linearly independent: $\mathbf{X}$ is rank-2
  - non-zero indices

$$\begin{aligned} \operatorname{supp}(\mathbf{x}) \nsubseteq \operatorname{supp}(\mathbf{y}) &\implies \exists i^* \in [m] \text{ s.t. } x_{i^*} > 0, y_{i^*} = 0, \\ \operatorname{supp}(\mathbf{y}) \nsubseteq \operatorname{supp}(\mathbf{x}) &\implies \exists j^* \in [m] \text{ s.t. } y_{j^*} > 0, x_{j^*} = 0. \end{aligned} \tag{1}$$

- $\mathbf{X}, \mathbf{U}$ are rank 2 imply $\mathbf{Q}$ is rank-2, hence

$$\mathbf{U} = \mathbf{X}\mathbf{Q}^{-1} = \mathbf{X} \begin{bmatrix} d & -c \\ -b & a \end{bmatrix} \frac{1}{ad - bc}, \quad ad - bc \neq 0. \tag{2}$$

  Put i^*, j^* from (1) into (2), together with the fact that $\mathbf{x}, \mathbf{y}, \mathbf{u}, \mathbf{v}$ are nonnegative give $\mathbf{Q}^{-1} \geq \mathbf{0}$.

- $\mathbf{Q} \geq \mathbf{0}$ and $\mathbf{Q}^{-1} \geq \mathbf{0}$ imply $\mathbf{Q}$ is the permutation of a diagonal matrix with positive diagonal, where the diagonal matrix here is $\mathbf{I}$.

Fancy picture: multi-grid saves 75% time with 2-layer

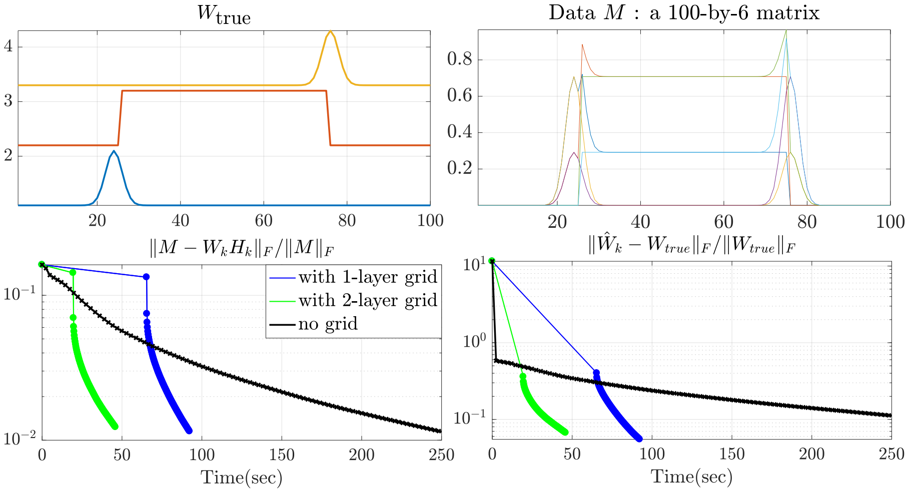
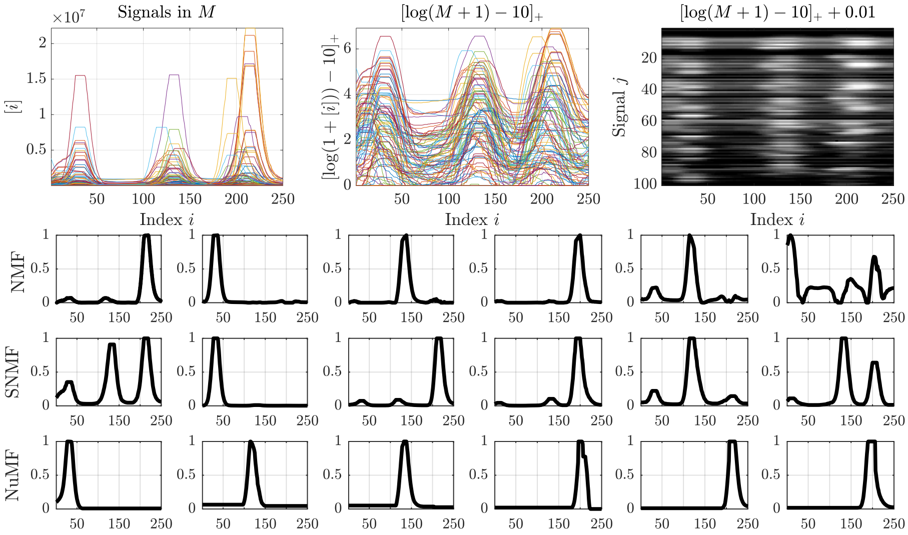
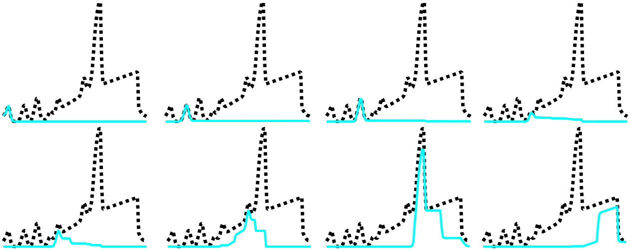


Figure: Experiment on a toy example. All algorithms run 100 iterations with same initialization. For algorithms with MG, the computational time taken on the coarse grid are also taken into account, as reflected by the time gap between time 0 and the first dot in the curves.

Fancy picture: on Belgian beers



Fancy picture: on $r > n$



- On a data vector in $\mathbb{R}_+^{947}$ (black) with $r = 8 > 1 = n$.
- Cyan curves are the components $\mathbf{w}_i h_i$.
- Relative error $\|\mathbf{M} - \mathbf{WH}\|_F / \|\mathbf{M}\|_F = 10^{-8}$.
- The first two peaks in the data satisfy Theorem 1, NuNMF identifies them perfectly.
- For the other peaks: supports overlap, decomposition not unique.
- Identifiability on overlapping supports: future research.

Open problems related to multigrid

- How to further improve the time efficiency?
- Uneven grid?
- Adaptive multigrid?

Last page - summary

- NuMF: motivation, modeling, algorithm, identifiability
- Not discussed
  - The log-concavity
  - Guessing location of p
  - Identifiability of NuMF for Nu vectors with adjacent support.
  - The traditional non-NuMF approach used in analytical chemistry
  - Minimum-volume NuMF?
- References
  - Chapter 5 of my thesis "Nonnegative Matrix and Tensor Factorizations: Models, Algorithms and Applications".
  - **A**, Gillis, Vandaele and De Sterck, "Nonnegative Unimodal Matrix Factorization", to be presented in ICASSP21.
- Slide, paper, code available at angms.science

The end