Nonnegative Matrix and Tensor Factorizations: Models, Algorithms and Applications

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Overview

1 Introduction

- 2 Part I: Minimum volume NMF
- 3 Part II: NuMF
- 4 Part III: HER
- 5 Summary of contributions

About myself, and acknowledgments

I spent 9 years learning how to know you don't know.



I acknowledge:

- My boss Nicolas Gillis
- Jury members
 - Xavier Siebert (UMONS), Thierry Dutoit (UMONS), Laurent Jacques (UCL), Francois Glineur (UCL), Lieven De Lathauwer (KUL)
- Colleagues and friends Nicolas, Pierre, Hien, Arnaud, Valentin, Maryam, Tim, Francois Punit, Jeremy, Junjun, Christophe, Flavia

About this "talk"

- ▶ 3 main parts to cover the 8 chapters of the thesis.
 - Ch1 Introduction
 - Ch2 NMF with minimum volume: minvol NMF
 - Ch3 Minvol NMF on hyperspectral unmixing
 - Ch4 Minvol NMF on audio source separation
 - Ch5 NMF with unimodality: NuMF
 - Ch6 Tensor algebra and factorization
 - Ch7 Heuristic extrapolation with restarts
 - Ch8 Conclusion
- ► Highly compressed. → details in the thesis
- Only core ideas and eye-catching items.

Overview



2 Part I: Minimum volume NMF

3 Part II: NuMF

For non-NMF people : why NMF ?

Interpretability

NMF beats similar tools (PCA, SVD, ICA) due to the interpretability on non-negative data.

Model correctness

NMF can find ground truth (under certain conditions).

Mathematical curiosity

NMF is related to some serious problems in mathematics.

• My boss tell me to do it.

(New) It is cool.

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Thunder-fast review of NMF



and $r \in \mathbb{N}$

Output $\mathbf{H} \in \mathbb{R}^{r \times n}_+$ $\mathbf{W} \in \mathbb{R}^{m \times r}_+$ fulfilling some properties ...

Thunder-fast review of NMF



NMF

Numerical optimization

minimize
$$\frac{1}{2} \|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2$$
 subject to $\mathbf{W} \ge 0$ and $\mathbf{H} \ge 0$.

NMF

Numerical optimization

minimize
$$\frac{1}{2} \|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2$$
 subject to $\mathbf{W} \ge 0$ and $\mathbf{H} \ge 0$.

Regularized model

 $\min_{\mathbf{W},\mathbf{H}} \frac{1}{2} \|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2 + g(\mathbf{W}) \text{ s.t. } \mathbf{W} \ge 0, \mathbf{H} \ge 0 \text{ and other constraints.}$

• Notation: hide $\mathbf{W} \ge 0$, $\mathbf{H} \ge 0$.

The details I skipped

- Popularity of NMF in research
- The nonnegative rank
- ► How NMF is used in application
- How NMF problems are solved
- HALS
- Solution space of NMF
- NMF is NP-hard
- Separable NMF
- How to solve Separable NMF
- Successive Projection Algorithm
- ... see chapter 1 of the thesis!

Geometry of $\mathbf{M}=\mathbf{W}\mathbf{H}$



Figure: Nested cone geometry of NMF: blue cone \subseteq red cone \subseteq green cone.

Minimum volume NMF

$$\min_{\mathbf{W},\mathbf{H}} \ \frac{1}{2} \|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2 + \lambda \mathcal{V}(\mathbf{W}) \text{ subject to some constraints.}$$

What is "volume"?

▶ Lemma 2.1.1 (p.17 in thesis) If $\mathbf{W} \in \mathbb{R}^{m \times r}_+$ is full rank, then

 $\sqrt{\det(\mathbf{W}^{\top}\mathbf{W})}$

is the volume of $\mathrm{conv}\big([0\ \mathbf{W}]\big)$ in the column space of $\mathbf{W},$ up to a constant factor.

Proof idea: Gram-Schmidt orthogonalization and SVD.

Figure illustration.

What is "volume"?

$$\det(\mathbf{W}^{\top}\mathbf{W}) = \|\mathbf{w}_1\|_2^2 \cdot \left\|\mathbf{P}_1^{\perp}\mathbf{w}_2\right\|_2^2 \left\|\mathbf{P}_{1,2}^{\perp}\mathbf{w}_3\right\|_2^2 \dots \left\|\mathbf{P}_{1,\dots,r-1}^{\perp}\mathbf{w}_r\right\|_2^2,$$

where $\mathbf{P}_{\mathbf{a}}^{\perp} = \mathbf{I} - \frac{\mathbf{a}\mathbf{a}^{\top}}{\|\mathbf{a}\|_2^2}$ is the projector on span^{\perp}(\mathbf{a}),

$$\begin{array}{rclcrcl} \mathbf{P}_{1}^{\perp} &=& \mathbf{P}_{\mathbf{a}_{1}}^{\perp}, && \mathbf{a}_{1} = \mathbf{w}_{1} \\ \mathbf{P}_{1,2}^{\perp} &=& \mathbf{P}_{1}^{\perp} \mathbf{P}_{\mathbf{a}_{2}}^{\perp}, && \mathbf{a}_{2} = \mathbf{P}_{1}^{\perp} \mathbf{w}_{2} \\ \mathbf{P}_{1,2,3}^{\perp} &=& \mathbf{P}_{1,2}^{\perp} \mathbf{P}_{\mathbf{a}_{3}}^{\perp}, && \mathbf{a}_{3} = \mathbf{P}_{1,2}^{\perp} \mathbf{w}_{3} \\ &\vdots &\vdots && \\ \mathbf{P}_{1,...,r-1}^{\perp} &=& \mathbf{P}_{1,2,...,r-2}^{\perp} \mathbf{P}_{\mathbf{a}_{r-1}}^{\perp}, && \mathbf{a}_{r-1} = \mathbf{P}_{1,2,...,r-2}^{\perp} \mathbf{w}_{r-1}. \end{array}$$

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Some volume functions for $\min_{\mathbf{W},\mathbf{H}} \frac{1}{2} \|\mathbf{M} - \mathbf{W}\mathbf{H}\|_F^2 + \lambda \mathcal{V}(\mathbf{W})$

Name	Definition	$\lng\circ\boldsymbol{\sigma}(\mathbf{W})$
Determinant (det)	$\mathcal{V}_{det}(\mathbf{W}) = \det\left(\mathbf{W}^\top \mathbf{W}\right)$	$\prod_{i=1}^r \sigma_i^2$
log-determinant (logdet)	$\mathcal{V}_{\text{logdet}}(\mathbf{W}) = \log \det \left(\mathbf{W}^\top \mathbf{W} + \delta \mathbf{I}_r \right)$	$\sum_{i=1}^{r} \log \left(\sigma_i^2 + \delta\right)$
Frobenius norm squared	$\mathcal{V}_{\mathrm{F}}(\mathbf{W}) = \ \mathbf{W}\ _F^2$	$\sum_{i=1}^{r} \sigma_i^2$
Nuclear norm	$\mathcal{V}_*(\mathbf{W}) = \ \mathbf{W}\ _*$	$\sum_{i=1}^{r} \sigma_i$
Smooth Schatten- p norm	$\mathcal{V}_{p,\delta}(\mathbf{W}) = \operatorname{Tr}\left(\mathbf{W}^{ op}\mathbf{W} + \delta \mathbf{I}_r ight)^{rac{p}{2}}$	$\sum_{i=1}^{r} (\sigma_i^2 + \delta)^{\frac{p}{2}}$

New theory developed in the thesis: Identifiability of a minvol (N)MF

▶ Theorem 2.1.1 Let $\mathbf{M} = \mathbf{W}\mathbf{H}$ where $\mathbf{H} \in \mathbb{R}^{r \times n}_+$ satisfies the SSC, $\mathbf{W} \in \mathbb{R}^{m \times r}$ satisfies $\mathbf{W}^\top \mathbf{1}_m = \mathbf{1}_r$ and rank $(\mathbf{M}) = r$. Then the (exact) solution of

argmin W.H	$\mathcal{V}_{det}(\mathbf{W})$	% Det-volume
s.t.	$\mathbf{M}=\mathbf{W}\mathbf{H}$	% Matrix factorization
	$\mathbf{H} \ge 0$	% Nonnegativity
	$\mathbf{W}^ op 1_m = 1_r$	$\%$ Normalization of col. of ${f W}$

is essentially unique.

► Significance: justify the use of minvol NMF in application.

Illustration

http://angms.science/eg_SNPA_ini.gif

The details I skipped

- Details of the formulation of the minvol NMF
- Motivation of minvol NMF
- Details on the volume regularizer
- Comparing the volume regularizer
- Parameter tuning
- Rank deficiency case
- The proof of the identifiability theorem
- How to solve minvol NMF
- Computational cost of the algorithm
- Convergence analysis of the algorithm
- ... see chapter 2 of the thesis!

Hyperspectral Unmixing

row

·col







Minvol NMF on Hyperspectral Unmixing



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Ref.











minvolNMF







Water















Vegetation





























0.4

0.3

0.2

0.1





 Dirt















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The details I skipped

- Details of the hyperspectral image
- Pure-pixel assumption
- Performance metrics for ranking algorithms
- Parameter tuning and experiment setup
- Details of many experimental results
 - minvol NMF >> SPA, MVC-NMF and RVolMin on synthetic and real datasets.
 - ► minvol NMF with V_{det} and V_{logdet} are the top two methods among the tested methods.
- ... see chapter 3 of the thesis!



Illustration



https://www.youtube.com/watch?v=1BrpxvpghKQ

Correct identification of the note sequence



How does it work?



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Assumptions on applying minvol NMF on audio data

On using minvol NMF to estimate the source $\ensuremath{\mathbf{s}}$:

- A1 No time delay in the mixing.
- A2 Linear mixing model.
- A3 Sources are balanced.

A4 Additive mixture
$$\mathbf{V} = \sum_i |\mathbf{S}_i|$$
.

- A5 $|S_i|$ are well approximated by nonnegative rank-1 matrices.
- A6 Reconstructed components are consistent.
- A7 The data has no outlier.

Violating any one of these assumptions leads to errors, or ... new research opportunities!

On the consistency assumption



Figure: Illustrating the consistency issue of decomposing a time-frequency matrix. Here the NMF result W_1H_1 is consistent as the matrix Y while the result W_2H_2 is not. 30/53

The details I skipped

- Details of the audio source separation process
- ► Time frequency transform
- β -divergence and β -divergence NMF
- Assumptions on applying NMF on audio data
- Parameter tuning and experiment setup
- Details of experimental results... see chapter 4 of the thesis!

Overview

1 Introduction

2 Part I: Minimum volume NMF









Nonnegative unimodality

▶ A vector \mathbf{x} is nonnegative unimodal $\exists p \in [m]$ such that

 $0 \le x_1 \le x_2 \le \cdots \le x_p$ and $x_p \ge x_{p+1} \ge \cdots \ge x_m \ge 0$.

 $\begin{array}{l} \mathcal{U}^m_+ \text{: the set of Nu vectors in } \mathbb{R}^m \\ \mathcal{U}^{m,p}_+ \text{: the set of Nu vectors in } \mathcal{U}^m_+ \text{ with tonicity change at } p. \end{array}$

Examples



Characterizing the Nu set

$$\underbrace{\mathbf{x} \in \mathcal{U}_{+}^{m}}_{\text{"x is unimodal"}} \iff \exists p \text{ s.t. } \mathbf{x} \in \underbrace{\mathcal{U}_{+}^{m,p} \cup \mathcal{U}_{+}^{m,p+1}}_{\text{a convex set}} \iff \begin{cases} 0 \leq x_{1} \\ x_{1} \leq x_{2} \\ \vdots \\ x_{p-1} \leq x_{p} \\ x_{p+1} \geq x_{p+2} \\ \vdots \\ x_{m-1} \geq x_{m} \\ x_{m} \geq 0 \end{cases}$$

Union of two systems of monic inequalities.

Characterizing the Nu set

$$\begin{array}{cccccccc} 0 & \leq & x_1 \\ x_1 & \leq & x_2 \\ & \vdots \\ x_{p-1} & \leq & x_p \\ x_{p+1} & \geq & x_{p+2} \end{array} \iff \mathbf{U}_p \mathbf{x} \geq 0 \\ & \vdots \\ x_{m-1} & \geq & x_m \\ & x_m & \geq & 0 \end{array}$$



NuMF

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

How to solve it?

- There are r integer unknowns p_1, \ldots, p_r
- ► Idea to solve it: brute force
- Improvement: accelerated projected gradient, peak detection, multi-grid

New theory developed in the thesis: Restriction operator preserves Nu

▶ Theorem 5.2.1 Let $\mathbf{x} \in \mathcal{U}_+^m$ and $\mathbf{R} \in \mathbb{R}^{m \times m'}$ with the structure

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

then $\mathbf{y} = \mathbf{R}\mathbf{x} \in \mathcal{U}_{+}^{m'}$. Furthermore, if $\mathbf{x} \in \mathcal{U}_{+}^{m,p}$ where p is even, then $\mathbf{y} \in \mathcal{U}_{+}^{m,p_y}$ with $p_y \in \left\{ \begin{array}{c} \frac{p}{2} - 1, \frac{p}{2}, \frac{p}{2} + 1 \right\}$.

 Significance: justify the use of Multi-grid as a dimension reduction step in solving NuMF. New theory developed in the thesis:

- 3 theorems related to identifiability of NuMF
 - ► **Theorem 5.3.1** Informally, if w_i are Nu and have strictly disjoint support, then the sol. of NuMF is essentially unique.

• Specialty of the theorem: it works with $n \ge 1$, even if r > n.

- Theorem 5.3.2 Informally, if w_i are Nu and have strictly disjoint support, H satisfies the independent sensing condition, then the (exact) sol. of NuMF is essentially unique.
- ► Theorem 5.3.3 Informally, given $\mathbf{x}, \mathbf{y} \in \mathcal{U}_{+}^{m}$ s.t. $\operatorname{supp}(\mathbf{x}) \not\subseteq^{\not\subseteq} \operatorname{supp}(\mathbf{y})$. If \mathbf{x} , \mathbf{y} can be generated by two non-zero Nu vectors \mathbf{u} , \mathbf{v} as $\mathbf{x} = a\mathbf{u} + b\mathbf{v}$ and $\mathbf{y} = c\mathbf{u} + d\mathbf{v}$, then the only possibilities are either $\mathbf{u} = \mathbf{x}$, $\mathbf{v} = \mathbf{y}$ or $\mathbf{u} = \mathbf{y}$, $\mathbf{v} = \mathbf{x}$.



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The details I skipped

- Details of the accelerated projected gradient
- Details of the peak detection
- Details of multi-grid
- Details of the identifiability results ... see chapter 5 of the thesis!

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HER

► A framework for accelerating algo. for solving NMF, NTF and CPD.



- Key ideas
 - Extrapolation with restart.
 - Cheap computation by making use of computed component in the update.
- ► Many numerical evidences on the effectiveness of HER.

Extrapolation? Why?



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Algorithm 8 HER

- 1: Input: a nonnegative N-way tensor
- 2: Output: nonnegative factors $\mathbf{A}^{(1)}, \mathbf{A}^{(2)}, \dots, \mathbf{A}^{(N)}$.
- 3: Initialization: Choose $\beta_0 \in (0, 1), \eta \geq \bar{\gamma} \geq \gamma \geq 1$ and 2 sets of initial factor matrices $(\mathbf{A}_0^{(1)}, \dots, \mathbf{A}_0^{(N)})$ and $(\hat{\mathbf{A}}_0^{(1)}, \dots, \hat{\mathbf{A}}_0^{(N)})$. Set $\bar{\beta}_0 = 1$ and k = 1.
- 4: for $k = 1, \ldots$ until some criteria is satisfied do
- 5: **for** i = 1, ..., N **do**
- 6: **Update step** Let $\mathbf{A}_{k}^{(i)}$ be an exact/inexact solution of

$$\min_{\mathbf{A}^{(i)} \ge 0} F\left(\hat{\mathbf{A}}_{k}^{(1)}, \dots, \hat{\mathbf{A}}_{k}^{(i-1)}, \mathbf{A}^{(i)}, \hat{\mathbf{A}}_{k-1}^{(i+1)}, \dots, \hat{\mathbf{A}}_{k-1}^{(N)}\right).$$
(7.1)

7: Extrapolation step

$$\hat{\mathbf{A}}_{k}^{(i)} = \left[\mathbf{A}_{k}^{(i)} + \beta_{k-1}(\mathbf{A}_{k}^{(i)} - \mathbf{A}_{k-1}^{(i)})\right]_{+}.$$
(7.2)

9: Compute
$$\hat{F}_k := F\left(\hat{\mathbf{A}}_k^{(1)}, \hat{\mathbf{A}}_k^{(2)}, \dots, \hat{\mathbf{A}}_k^{(N-1)}, \mathbf{A}_k^{(N)}\right).$$

- 10: **if** $\hat{F}_k > \hat{F}_{k-1}$ **then** 11: Set $\hat{\mathbf{A}}_k^{(i)} = \mathbf{A}_k^{(i)}, \forall i \in [N]$ 12: Set $\bar{\beta}_k = \beta_{k-1}, \quad \beta_k = \beta_{k-1}/\eta.$ % abandon the sequence $\hat{\mathbf{A}}_k^{(i)}$ % Update $\bar{\beta}$, decrease $\bar{\beta}$
- 13: else

14: Set
$$\mathbf{A}_{k}^{(i)} = \hat{\mathbf{A}}_{k}^{(i)}, \forall i \in [N].$$

15: Set $\bar{\beta}_{k} = \min\{1, \bar{\beta}_{k-1}\bar{\gamma}\}, \quad \beta_{k} = \min\{\bar{\beta}_{k-1}, \beta_{k-1}\gamma\}.$

- 16: end if
- 17: end for

% keep the sequence $\hat{\mathbf{A}}_{k}^{(i)}$ % Increase $\bar{\beta}$ and β



Results

See thesis: Chapter 7, p.113- p.125.

- ► The discussion of HER in the original form for solving NMF problem.
- ► The details of HER on NMF and NTF problems.
- Other similar algorithms.
- ... see chapter 7 of the thesis!

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- 5 Summary of contributions



Summary of contributions: the modeling aspect

- Minvol NMF
 - ► It generalizes *Separable NMF*, an important class of NMF.
 - \blacktriangleright Minvol NMF with $\mathcal{V}_{\rm det}$ is identifiable under the SSC condition.
 - Minvol NMF is empirically superior than other approaches.
 - ► Minvol NMF with nuclear norm: new model.

- NuMF
 - Proposed a brute-force heuristic to solve it, with acceleration by APG, peak detection and a dimension reduction step based on a multi-grid method.
 - The multi-grid method preserves unimodality.
 - ► 3 identifiability theorems of NuMF in 3 special cases.

Summary of contributions: the algorithm aspect

- A generic framework named HER on accelerating both exact and inexact BCD type of algorithms in solving NMF, NTF and CPD.
- ► Many empirical evidences on the effectiveness of HER.
- ► The benefits of HER:
 - ► it can accelerate any BCD algorithm
 - it extrapolates the variable sequence without increasing the per-iteration computational cost of the algorithm
 - ► the auxiliary extrapolation sequence it produces is always feasible.
- The main shortcomings of HER are: no theoretical convergence guarantee; requires parameter tuning.
- Apart from HER, we provided efficient algorithms for solving minvol NMF and NuMF.

Summary of contributions: the application aspect

 Geography Hyperspectral unmixing in remote sensing.

 Music Audio blind source separation.

 Chemistry Chromatography - mass spectrometry

The end

PhD Thesis:

Nonnegative Matrix and Tensor Factorizations: Models, Algorithms and Applications Available online: https://angms.science/doc/PhDThesis.pdf Errata: https://angms.science/doc/PhDThesisErrata.pdf slide: https://angms.science/doc/PhDPublicDefSlide.pdf

Works during the PhD period

green = journal paper, black = conference paper

- 1. A., and Gillis, Volume regularized non-negative matrix factorizations, WHISPERS18
- 2. A., and Gillis, Algorithms and comparisons of nonnegative matrix factorizations with volume regularization for hyperspectral unmixing, JSTAR, 19
- A., and Gillis, Accelerating nonnegative matrix factorization algorithms using extrapolation, Neural Computation, 19
- A., Cohen and Gillis, Accelerating approximate nonnegative canonical polyadic decomposition using extrapolation, GRETSI19
- Leplat, Gillis, Siebert and A., Séparation aveugle de sources sonores par factorization en matrices positives avec pénalité sur le volume du dictionnaire, GRETSI19
- 6. Leplat, A. and Gillis, Minimum-volume rank-deficient nonnegative matrix factorizations, ICASSP19
- 7. Leplat, Gillis and A., Blind Audio Source Separation with Minimum-Volume Beta-Divergence NMF, TSP, 20
- A., Cohen, Le and Gillis, Extrapolated Alternating Algorithms for Approximate Canonical Polyadic Decomposition, ICASSP20
- 9. A., Cohen, Gillis and Le, Accelerating Block Coordinate Descent for Nonnegative Tensor Factorization, NLAA, under review, 20
- 10. A., Gillis, Vandaele and De Sterck, Nonnegative Unimodal Matrix Factorization, submitted to ICASSP (NEW)