Nonnegative Matrix Factorization

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Data Science Book Series

Nonnegative matrix factorization (NMF) in its modern form has become a standard tool in the analysis of high-dimensional data sets. This book provides a comprehensive and up-to-date account of the most important aspects of the NMF problem and is the first to detail its theoretical aspects, including geometric interpretation, nonnegative rank, complexity, and uniqueness. It explains why understanding these theoretical insights is key to using this computational tool effectively and meaningfully.

Nonnegative Matrix Factorization

- is accessible to a wide audience and is ideal for anyone interested in the workings of NMF,
- discusses some new results on the nonnegative rank and the identifiability of NMF, and
- makes available MATLAB codes for readers to run the numerical examples presented in the book.

Graduate students starting to work on NMF and researchers interested in better understanding the NMF problem and how they can use it will find this book useful. It can be used in advanced undergraduate and graduate-level courses on numerical linear algebra and on advanced topics in numerical linear algebra and requires only a basic knowledge of linear algebra and optimization.

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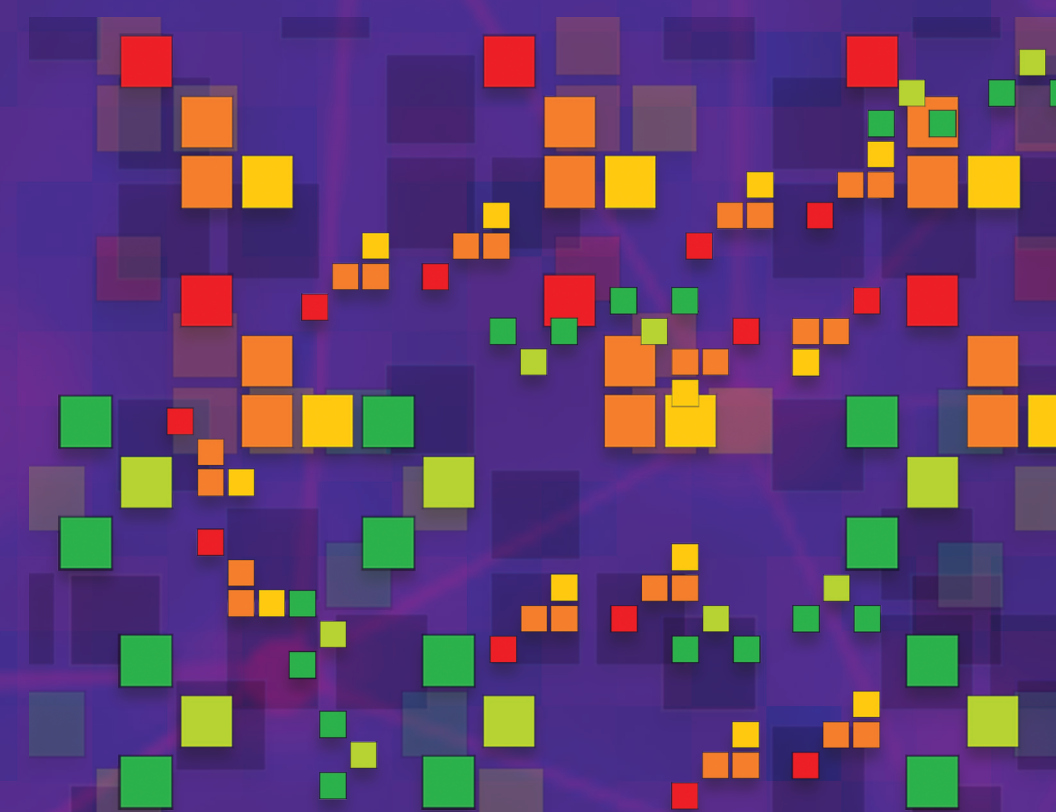

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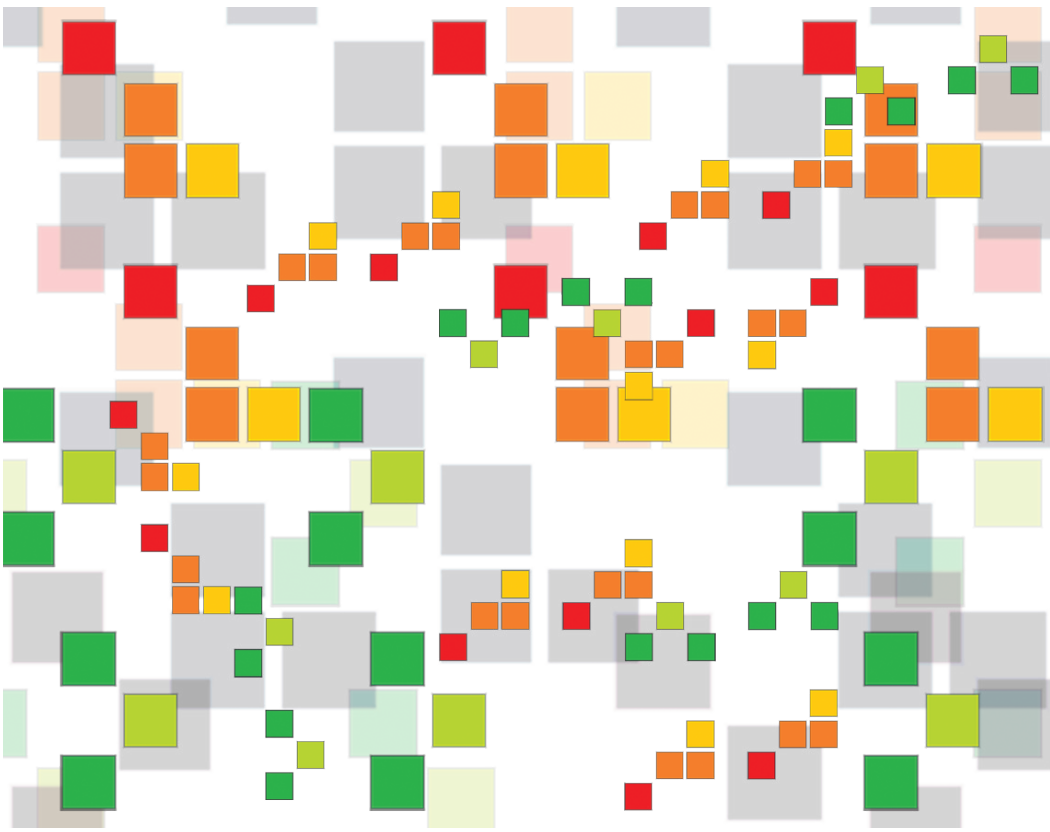
Nonnegative Matrix Factorization



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Pour Aline, Elinor, et Rose

Contents

Preface

Identifying the underlying structure of a data set and extracting meaningful information is a key problem in data analysis. Simple and powerful methods to achieve this goal are *linear dimensionality reduction* (LDR) techniques, which are equivalent to low-rank matrix approximations (LRMA). Examples of LDR techniques are principal component analysis (PCA), independent component analysis, sparse PCA, robust PCA, low-rank matrix completion, and sparse component analysis. The reason for the success of this type of methods is that, although simple, they are applicable in a wide range of applications such as recommender systems, model-order reduction and system identification, clustering, image analysis, and blind source separation, to cite a few.

Among LRMA techniques, nonnegative matrix factorization (NMF) requires the factors of the low-rank approximation to be componentwise nonnegative. This makes it possible to interpret them meaningfully, for example when they correspond to nonnegative physical quantities. Applications of NMF include extracting parts of faces (such as eyes, noses, and lips) in a set of facial images, identifying topics in a set of documents, learning hidden Markov models, extracting materials and their abundances in hyperspectral images, separating audio sources from their mixture, detecting communities in large networks, analyzing medical images, and decomposing gene expression microarrays.

Aim of the book The aim of this book is to provide a comprehensive account of the most important aspects of the NMF problem:

- Theoretical aspects: the nonnegative rank, the nonuniqueness/identifiability of NMF solutions, the geometric interpretation of NMF, and computational complexity issues.

- Models: choice of the objective function and regularizations, link with well-known techniques such as k-means, and use of additional constraints such as orthogonality or symmetry.

- Algorithms: heuristic algorithms using standard nonlinear optimization schemes such as block coordinate descent methods, and provably correct algorithms under appropriate assumptions.

- Applications: they include image analysis, document classification, hyperspectral unmixing, audio source separation, topic modeling, and community detection.

This book is accessible to a wide audience. In particular it is intended for people who want to know about the workings of NMF. It also aims to give more insights to practitioners so that they can use NMF meaningfully. To read this book, basic knowledge of linear algebra and optimization is needed.

Why is this book important? Although NMF has been studied extensively for the last 20 years, there is currently only one book on the topic, by Cichocki et al. [98] (2009) which is already more than 10 years old. It focuses on iterative algorithms and applications, and many aspects of NMF are not covered in that book—especially since many important results have been obtained in the last 10 years.[1]

The aim of this book is to fill in this gap by providing more insights into the theoretical aspects of NMF. These are key to be able to use NMF effectively and meaningfully in practice. This will allow the reader to make better use of NMF as a computational tool. This book is aimed at researchers who want to understand the NMF problem; for example,

- You do not know (much) NMF and want to discover this problem, why and how it works, and what it can be used for. This book would be ideal for example for a master's or Ph.D. student starting to work on NMF.

- You are using NMF for applications but you would like to understand better its subtly difficult aspects such as its computational complexity, its geometric interpretation, or its nonuniqueness/identifiability issues. Also, you would like to know about the state-of-the-art algorithms.

- You are already rather familiar with NMF but have not yet studied all of its aspects (for example you would like to know more about the nonnegative rank, or the nonuniqueness of NMF solutions). This book will allow you to delve into different aspects of the NMF problem and will give you useful references.

Moreover, this book contains a few new results not present in the literature (as far as I know): bounds on the nonnegative rank under rank-one perturbations (Theorem 3.3), the study of the generic value of the nonnegative rank (Section 3.3.2), the identifiability of orthogonal NMF (Section 4.3.2), and a necessary condition for the sufficiently scattered condition, a crucial notion when studying the uniqueness of NMF solutions (see Theorem 4.28).

MATLAB code All algorithms and numerical experiments presented in this book are available from `bookstore.siam.org/di02/bonus`. When we discuss an algorithm, or display results from a numerical experiment, the corresponding MATLAB file will be indicated using

```
[Matlab file: Name of file]
```

It can be found in the folder of the corresponding chapter. Hence the interested reader can easily find the corresponding MATLAB file. To provide a better view of all the NMF algorithms available with this book, there is an *exception* for NMF algorithms: they can all be found in the folder [algorithms]. For example, the separable NMF algorithms presented in Chapter 7 can be found in the folder [algorithms/separable NMF], although the numerical experiments presented in Chapter 7 can be found in the folder [Chapter 7 - Separable NMF].

All tests in this book are performed using MATLAB R2019b on a laptop Intel Core i7-7500U CPU @2.9GHz, 24GB RAM.

How to use this book The book is organized so that it is possible to read only subsets of the chapters depending on the reader's interests. The book was written so that each chapter is

[1] Such as the identifiability results based on the sufficiently scattered condition (Chapter 4), and the polynomial-time algorithms for separable NMF (Chapter 7).

as self-contained as possible. Each chapter can be thought of as a survey on the corresponding topic. Moreover, each chapter ends with take-home messages that summarize and highlight the important results covered in the chapter. The book is organized as follows.

Chapter 1 serves as an introduction and the problem definition. It contains the description of four key applications of NMF that will be used throughout the book as illustrations. It also contain a historical account of the problem explaining when, why, and how the NMF problem came about. Then the book is divided into two parts.

Part I. *Exact factorizations* The first part considers the Exact NMF problem: given the nonnegative input matrix X and a factorization rank r, find nonnegative factors W with r columns and H with r rows such that $X = WH$. Chapter 2 discusses theoretical aspects of Exact NMF and in particular its geometric interpretation; this is crucial to design algorithms but also to use NMF meaningfully in practice. Section 2.1 on the geometric interpretation of NMF is useful to understand Chapters 4 and 7. The second part of this chapter discusses a more constrained NMF problem where the first factor W is required to have the same rank as the input matrix, which is referred to as restricted Exact NMF, and its link with a geometric problem, namely, the nested polytope problem. The third part of the chapter discusses the computational complexity of these problems. Chapter 3 digs into theoretical aspects of the nonnegative rank (the smallest r such that an Exact NMF exists): its properties, its lower and upper bounds, and its link with extended formulations of polytopes and with communication complexity. Chapter 4 discusses the identifiability issues when using NMF in practice. In fact, NMF decompositions are in general not unique, while most applications are looking for the unique ground truth underlying factors. This chapter explains how to recover the true factors, and under which conditions it is possible. Section 4.2 focuses on uniqueness conditions for the plain NMF model, while Section 4.3 discusses regularized NMF models, namely, orthogonal, separable, minimum-volume, and sparse NMF, that lead to unique decompositions under milder conditions.

Part II. *Approximate factorizations* The second part of the book considers approximate NMF decompositions, where $WH \approx X$, which we refer to as NMF for short as it is the standard in the literature. Chapter 5 discusses several important variants of the NMF model that use additional constraints, regularizations, and different objective functions; for example symmetric NMF which requires $W = H^\top$. As discussed in Chapter 4, considering such variants in practice is key to obtain unique solutions. This chapter also discusses different models that are closely related to NMF such as k-means and probabilistic latent semantic analysis/indexing (PLSA/PLSI). Chapter 6 discusses the computational complexity of NMF, which is NP-hard[2] in general. Chapter 7 considers NMF under the separability assumption, referred to as separable NMF, where the columns of the first factor W can be found among the columns of X. Although it is a strong assumption, it makes sense in several applications. Moreover, it allows us to provably solve NMF efficiently, that is, in polynomial time, and renders the solution unique, hence resolving two key issues of NMF (NP-hardness and identifiability). This chapter presents the main algorithms for separable NMF, discusses their robustness to noise, and compares them on several synthetic data sets. Chapter 8 focuses on iterative heuristic algorithms to compute NMF solutions. The state-of-the-art algorithms for NMF are presented; they are based on standard optimization techniques. We also discuss convergence guarantees and provide some numerical comparisons. Chapter 9 presents three more applications of NMF, as well as pointers to more applications.

[2]NP-hardness of a problem implies that unless P=NP, there exists no algorithm running in a number of operations polynomial in the size of the input that solves the problem.

Disclaimer The book presents the NMF problem from my own perspective and is clearly biased toward my own work and research interests. I apologize for not discussing or referring to many relevant works (that I am either unfamiliar with or unaware of). This book is a summary of my current knowledge about NMF and is by no means comprehensive. Any feedback on the book is more than welcome and is highly encouraged.

Tensors The NMF model can be directly generalized to tensors, in which case it is referred to as nonnegative tensor factorization (NTF) or nonnegative canonical polyadic decomposition (nonnegative CPD). It is out of the scope of this book to discuss this important extension, and we stick to the matrix case. However, one should keep this connection in mind as results from the matrix case can be used in the tensor case. For example, NP-hardness results for NMF (see Chapter 6) directly apply to NTF since NTF is a generalization of NMF, and NMF algorithms based on the block coordinate descent framework described in Chapter 8 directly extend to NTF. We refer the interested reader to [283, 98, 418] and the references therein for more details on tensor factorizations.

Acknowledgments Writing this book would not have been possible without the many fruitful collaborations I have been lucky to have over the years. In particular, I am grateful to my two mentors, François Glineur, who introduced me to NMF (the topic of my master's thesis in 2007), and Steve Vavasis, who welcomed me as a postdoc at the University of Waterloo. I have also been lucky that many enthusiastic researchers joined me in Mons: Arnaud, Punit, Andersen, Jérémy, Valentin, Hien, Junjun, François, Nicolas^2, Tim, Christophe, Pierre, and Maryam.

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Writing a book on NMF has been in the back of my mind for several years, but I thank Andersen Ang and Jennifer Pestana, who motivated me and pushed me to finally undertake this endeavor.

I would like to thank the SIAM editorial team, who have done a wonderful job improving the book through their reviewing and copyediting. It was a pleasure collaborating with them on this project.

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I thank my family and my friends.

Notation

Sets of scalars, vectors, matrices

$\mathbb{R}$	set of real numbers
$\mathbb{R}_+$	set of nonnegative real numbers
$\mathbb{R}_{++}$	set of positive real numbers
$\mathbb{R}^n$	set of real column vectors of dimension n
$\mathbb{R}^{m\times n}$	set of real m-by-n matrices
$\mathbb{R}^n_+$	set of nonnegative real column vectors of dimension n
$\mathbb{R}^{m\times n}_+$	set of m-by-n nonnegative real matrices
$\mathbb{S}^n$	set of n-by-n symmetric matrices
$\mathbb{S}^n_+$	set of n-by-n positive semidefinite matrices
$\mathbb{S}^n_{++}$	set of n-by-n positive definite matrices
$\mathfrak{C}^n$	set of n-by-n copositive matrices
$\mathfrak{C}^n_+$	set of n-by-n completely positive matrices
$\mathcal{C}$	second-order cone $\left\{x \in \mathbb{R}^r \mid e^\top x \geq \sqrt{r-1}\|x\|_2\right\}$
$\mathcal{C}^*$	second-order cone $\left\{x \in \mathbb{R}^r \mid e^\top x \geq \|x\|_2\right\}$, the dual of $\mathcal{C}$ (p. 113)
Δ^n	unit simplex of dimension n, that is, $\Delta^n = \{x \in \mathbb{R}^n \mid x \geq 0, \sum_{i=1}^n x_i = 1\}$
$\mathcal{S}^n$	convex hull of the unit simplex and the origin, that is, $\mathcal{S}^n = \{x \in \mathbb{R}^n \mid x \geq 0, \sum_{i=1}^n x_i \leq 1\}$

Submatrices, transpose and inverse

x_i of $x(i)$	ith entry of the vector x
$A_{i:}$ or $A(i,:)$	ith row of A
$A_{:j}$ or $A(:,j)$	jth column of A
A_{ij} or $A(i,j)$	entry at position (i,j) of A
$A(I,J)$	submatrix of A with row (resp. column) indices in I (resp. J)
$[A\ B; C\ D]$	We use Matlab notation: $[A\ B; C\ D] = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$
$A^\top$	transpose of the matrix A, $(A^\top)_{ij} = A_{ji}$
A^{-1}	inverse of the square matrix A, $A^{-1}A = AA^{-1} = I$
$A^{-\top}$	inverse of the transpose of the square matrix A, that is, $A^{-\top}A^\top = A^\top A^{-\top} = I$

Special vectors and matrices

0	matrix of zeros of appropriate dimension
$0_{m\times n}$	m-by-n matrix of zeros
I_n	identity matrix of dimension n
I	identity matrix of appropriate dimension
e	vector of all ones of appropriate dimension
e_k	kth unit vector with $e_k(k) = 1$ and $e_k(i) = 0$ for all $i \neq k$, that is, $e_k = I(:, k)$

Norms

$\\|.\\|_1$	ℓ_1 norm, $\\|x\\|_1 = \sum_{i=1}^n \|x_i\|$, $x \in \mathbb{R}^n$ componentwise matrix ℓ_1 norm, $\\|A\\|_1 = \sum_{i,j} \|A_{i,j}\|$, $A \in \mathbb{R}^{m\times n}$
$\\|.\\|_2$	vector ℓ_2 norm, $\\|x\\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$, $x \in \mathbb{R}^n$ matrix ℓ_2 norm, $\\|A\\|_2 = \max_{x\in\mathbb{R}^n, \\|x\\|_2=1} \\|Ax\\|_2$, $A \in \mathbb{R}^{m\times n}$
$\\|.\\|_F$	Frobenius norm, $\\|A\\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n A_{ij}^2}$, $A \in \mathbb{R}^{m\times n}$
$\\|.\\|_\infty$	vector ℓ_∞ norm, $\\|x\\|_\infty = \max_{1\leq i\leq n} \|x_i\|$, $x \in \mathbb{R}^n$ componentwise matrix ℓ_∞ norm, $\\|A\\|_\infty = \max_{i,j} \|A_{i,j}\|$, $A \in \mathbb{R}^{m\times n}$
$\\|.\\|_0$	ℓ_0 "norm," $\\|x\\|_0 = \big\|\{i \| x_i \neq 0\}\big\|$, $x \in \mathbb{R}^m$
$\\|.\\|_{1,q}$	matrix $\ell_{1,q}$ norm, $\\|A\\|_{1,q} = \sum_{i=1}^m \\|A(i,:)\\|_q$, $A \in \mathbb{R}^{m\times n}$

Inequalities

$A \geq 0$	A is a nonnegative matrix, that is, $A(i,j) \geq 0$ for all i, j
$A \geq B$	This means $A - B \geq 0$
$A \succeq 0$	A is a PSD matrix
$A \succeq B$	$A - B$ is a PSD matrix

Functions and sets on matrices

$\langle .,. \rangle$	Euclidean scalar product, that is, for $A, B \in \mathbb{R}^{m\times n}$, $\langle A, B\rangle = \sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}B_{ij}$,
$\sigma_i(A)$	ith singular values of matrix A, in nondecreasing order
$\sigma_{\max}(A)$	largest singular value of A, that is, $\sigma_1(A)$
$\sigma_{\min}(A)$	smallest singular value of $A \in \mathbb{R}^{m\times n}$, that is, $\sigma_{\min(m,n)}(A)$
$\kappa(A)$	condition number of A, $\kappa(A) = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$
$\det(A)$	determinant of A
$\mathrm{tr}(A)$	trace of A, that is, sum of its diagonal entries
$\mathrm{diag}(.)$	For $a \in \mathbb{R}^n$, $A = \mathrm{diag}(a) \in \mathbb{R}^{n\times n}$ is a diagonal matrix such that $A_{ii} = a_i$ for all i For $A \in \mathbb{R}^{n\times n}$, $a = \mathrm{diag}(A) \in \mathbb{R}^n$ is the vector containing the diagonal entries of A
$\overline{A}$	$\overline{A}$ is the matrix A without the last row
$\mathrm{rank}(A)$	rank of A
$\mathrm{rank}_+(A)$	nonnegative rank of A (p. 55)
$\mathrm{rank}_+^*(A)$	restricted nonnegative rank of A (p. 35)
cp-rank(A)	completely positive rank of A (p. 79)
k-rank(A)	Kruskal rank of A (p. 151)
$\mathrm{cone}(A)$	conical hull of the columns of A (p. 20)
$\mathrm{conv}(A)$	convex hull of the columns of A (p. 21)
$\mathrm{col}(A)$	column space of A (p. 21)
$\mathrm{aff}(A)$	affine hull of the columns of A (p. 21)
$A \circ B$	componentwise multiplication between A and B, that is, $(A \circ B)_{ij} = A_{ij}B_{ij}$
$\frac{[A]}{[B]}$	componentwise division between A and B, $\left(\frac{[A]}{[B]}\right)_{ij} = \frac{A_{ij}}{B_{ij}}$
$A^{\circ a}$	componentwise exponent of matrix A by the scalar a, that is, $A^{\circ a}(i,j) = A(i,j)^a$ for all i,j
$\mathrm{supp}(A)$	support (index set of nonzero entries) of matrix A, that is, $\mathrm{supp}(A) = \{(i,j) \mid A(i,j) \neq 0\}$
$\omega(A)$	fooling set bound for A (p. 64)
$\mathrm{bin}(A)$	$\mathrm{bin}(A)$ is the binarization of A, that is, the nonzero entries of A are set to 1 (p. 70)
$\mathrm{rank}_{01}(A)$	this is the Boolean rank of $\mathrm{bin}(A)$ (p. 70)
$\mathrm{rc}(A)$	rectangle covering bound for A (p. 72)
$\mathrm{rrc}(A)$	refined rectangle covering bound for A (p. 73)

Miscellaneous

$a{:}b$	set $\{a, a+1, \ldots, b-1, b\}$ (for a and b integers with $a \leq b$)
$[a, b]$	closed interval for reals $a \leq b$
(a, b)	open interval for reals $a \leq b$
∇f	gradient of the function f
$\nabla^2 f$	Hessian of the function f
$\lceil . \rceil$	$\lceil x \rceil$ is the smallest integer greater or equal to $x \in \mathbb{R}$
$\lfloor . \rfloor$	$\lfloor x \rfloor$ is the largest integer smaller or equal to $x \in \mathbb{R}$
$\backslash$	subtraction of two sets, that is, $R \backslash S$ is the set of elements that are in R but not in S
$\lvert . \rvert$	cardinality of a set, $\lvert S \rvert$ is the number of elements in S
k-sparse	the vector x is k-sparse if it has k nonzero entries, that is, $\lvert \operatorname{supp}(x) \rvert = k$
$\mathbb{P}(x)$	probability of the event $X = x$
$\mathbb{E}(X)$	expected value of a random variable X
$\mathcal{N}(\mu, \sigma)$	normal distribution of mean μ and standard deviation σ
$\mathcal{U}(a, b)$	uniform distribution in the interval $[a, b]$
$f(x) = \mathcal{O}(g(x))$	Big $\mathcal{O}$ notation: there exists K and x_0 such that $f(x) \leq K g(x)$ for all $x \geq x_0$
$f(x) = o(g(x))$	small o notation: $\lim_{x \to +\infty} \frac{f(x)}{g(x)} = 0$
$f(x) = \Omega(g(x))$	Big Omega notation, equivalent to $g(x) = \mathcal{O}(f(x))$
$f(x) = \Theta(g(x))$	Big Theta notation, equivalent to $f(x) = \mathcal{O}(g(x))$ and $f(x) = \Omega(g(x))$
$\min_{x \in \mathcal{X}} f(x)$	minimum value of $f(x)$ over the feasible set $\mathcal{X}$
$\operatorname{argmin}_{x \in \mathcal{X}} f(x)$	set of minimizers of $f(x)$ over the feasible set $\mathcal{X}$

Abbreviations

w.l.o.g.	without loss of generality
i.i.d.	independently and identically distributed
w.r.t.	with respect to

Acronyms

Page number indicates where the acronym is first defined.

2-BCD	two-block coordinate descent (p. 261)
ADMM	alternating direction method of multipliers (p. 289)
ANLS	alternating nonnegative least squares (p. 281)
BCD	block coordinate descent (p. 266)
BSUM	block successive upper-bound minimization (p. 268)
EDM	Euclidean distance matrix (p. 64)
Exact NMF	exact nonnegative matrix factorization (p. 19)
FAW	fast anchor words (p. 230)
FPGM	fast projected gradient method (p. 288)
HALS	hierarchical alternating least squares (p. 283)

Acronyms (continued)

HU	hyperspectral unmixing (p. 7)
IS	Itakura–Saito (p. 162)
KKT	Karush–Kuhn–Tucker (p. 264)
KL	Kullback–Leibler (p. 161)
k-sparse MF	k-sparse matrix factorization (p. 151)
LDR	linear dimensionality reduction (p. 1)
LP	linear programming (p. 249)
LRMA	low-rank matrix approximation (p. 1)
min-vol	minimum-volume (p. 138)
MLP	multiple linear programs (p. 249)
MM	majorization-minimization (p. 265)
MVE	minimum-volume ellipsoid (p. 237)
MU	multiplicative updates (p. 270)
NMF	nonnegative matrix factorization (p. 4)
NMU	nonnegative matrix underapproximation (p. 176)
NNLS	nonnegative least squares (p. 280)
NPP	nested polytope problem (p. 36)
ONMF	orthogonal NMF (p. 136)
PCA	principal component analysis (p. 2)
PGM	projected gradient method (p. 287)
PLSA	probabilistic latent semantic analysis (p. 189)
PLSI	probabilistic latent semantic indexing (p. 189)
PMF	positive matrix factorization (p. 4)
PPI	pure-pixel index (p. 247)
PSD	positive semidefinite (p. 79)
RE-NMF	restricted Exact NMF (p. 35)
SD-LP	self-dictionary via linear programming (p. 254)
SMCR	self-modeling curve resolution (p. 12)
SNPA	successive nonnegative projection algorithm (p. 232)
SPA	successive projection algorithm (p. 223)
SSC	sufficiently scattered condition (p. 104)
SSM	stochastic sequential machine (p. 13)
SVD	singular value decomposition (pp. 2, 196)
symNMF	symmetric NMF (p. 178)
tri-NMF	nonnegative matrix trifactorization (p. 181)
tri-symNMF	symmetric nonnegative matrix trifactorization (p. 181)
TSP	traveling salesman problem (p. 15)
VCA	vertex component analysis (p. 232)
WLRA	weighted low-rank matrix approximation (p. 3)

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Chapter 1

Introduction

In this chapter, we elaborate on the main reason why nonnegative matrix factorization (NMF) became a popular and standard tool in data analysis, namely because NMF is an easily interpretable linear dimensionality reduction technique for nonnegative data (Section 1.1). After providing a formal definition of NMF, the notation, and the terminology (Section 1.2), we illustrate the ability of NMF to extract meaningful components in nonnegative data sets with four applications: feature extraction in images, hyperspectral unmixing, text mining, and audio source separation[3] (Section 1.3). The last part of the chapter provides a historical overview of how NMF came about (Section 1.4). In each chapter of this book, we conclude with some take-home messages (Section 1.5).

1.1 ▪ Linear dimensionality reduction techniques for data analysis

Most works on NMF are motivated by its applicability in data analysis, more precisely, by the capability of NMF to automatically extract meaningful information in a data set. Extracting the underlying structure within data sets is one of the central problems in data science, and numerous techniques exist to perform this task. One of the oldest approaches is linear dimensionality reduction (LDR). LDR represents each data point as a linear combination of a small number of basis elements. Mathematically, given a data set of n data points $x_j \in \mathbb{R}^m$ $(1 \leq j \leq n)$, LDR looks for a small number r of basis vectors $w_k \in \mathbb{R}^m$ $(1 \leq k \leq r)$ such that each data point is well-approximated by a linear combination of these basis vectors, that is,

$$x_j \approx \sum_{k=1}^{r} w_k h_{kj} \quad \text{for all } j,$$

where the h_{kj}'s are scalars; see Figure 1.1 for an illustration in three dimensions with $m = 3$, $r = 2$, and $n = 50$.

LDR is equivalent to low-rank matrix approximation (LRMA):

$$\underbrace{[x_1, x_2, \dots, x_n]}_{X \in \mathbb{R}^{m \times n}} \approx \underbrace{[w_1, w_2, \dots, w_r]}_{W \in \mathbb{R}^{m \times r}} \underbrace{[h_1, h_2, \dots, h_n]}_{H \in \mathbb{R}^{r \times n}},$$

[3] Sections 1.1 and 1.3 follow closely the introductions from [189, 190, 191].

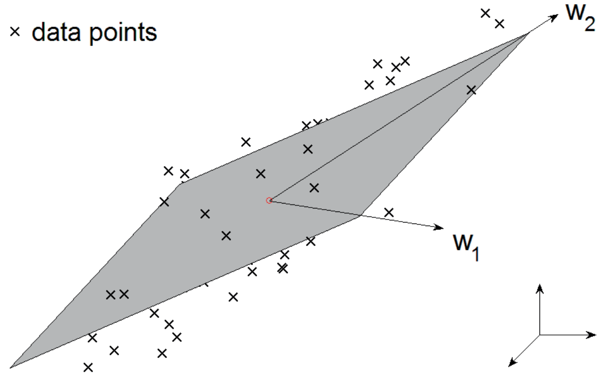


Figure 1.1. *Illustration of LDR: approximation of three-dimensional data points with a two-dimensional subspace generated by* w_1 *and* w_2.

where

- each column of the matrix $X \in \mathbb{R}^{m\times n}$ is a data point, that is, $X(:,j) = x_j$ for $1 \leq j \leq n$;
- each column of the matrix $W \in \mathbb{R}^{m\times r}$ is a basis element, that is, $W(:,k) = w_k$ for $1 \leq k \leq r$; and
- each column of $H \in \mathbb{R}^{r\times n}$ contains the coordinates of a data point $X(:,j)$ in the basis W, that is, $H(:,j) = h_j$ for $1 \leq j \leq n$.

Hence LDR provides a rank-r approximation WH of X, and each data point is mapped into the basis W using the corresponding column of H:

$$x_j \approx W h_j \quad \text{for all } j.$$

Typically, the number of basis vectors is much smaller than the ambient dimension m and the number of data points n, that is, $r \ll \min(m,n)$. This allows LDR and LRMA to compress the data, which is achieved for $r < \frac{mn}{m+n}$ since X contains mn entries, while W and H contain only $mr + nr$ entries.[4] Note that if the input matrix is sparse, with $\mathrm{nnz}(X)$ nonzero entries, compression requires $r < \frac{\mathrm{nnz}(X)}{m+n}$.

In order to compute W and H given X and r, one needs to define an error measure. For example, when the solution (W,H) minimizes the sum of the squares of the entries of the residual $X-WH$, that is, the squared Frobenius norm of the residual $\|X-WH\|_F^2 = \sum_{i,j}(X-WH)_{ij}^2$, LRMA is equivalent to principal component analysis (PCA) [266] which can be computed via the singular value decomposition (SVD) [216]. LRMA is a workhorse in numerical linear algebra, with the SVD being a central technique, and is closely related to the eigenvalue decomposition and factorizations such as Cholesky, QR, and LU, to cite a few. LRMA is at the heart of many fields in applied mathematics and computer science, for example in

- statistics, data analysis, and machine learning to perform regression, prediction, clustering, classification, and noise filtering [266, 144];
- numerical linear algebra to solve linear systems of equations [216];

[4]The factorization WH only has $(m+n-1)r$ degrees of freedom due to the scaling degree of freedom of the columns of W and rows of H, that is, $W(:,k)H(k,:) = (\alpha W(:,k))(H(k,:)/\alpha)$ for any $\alpha \neq 0$ and any k; see Chapter 4.

- signal and image processing to perform blind source separation [104, 87];
- graph theory to cluster the vertices of a graph [94];
- optimization to gain computational efficiency [68]; and
- systems theory and control to perform model-order reduction and system identification [341].

Although PCA has been around for more than 100 years, LRMA models have gained momentum in the last 20 years. The reason is mostly twofold: (i) data analysis has become more and more important due to the recent deluge of data in many different areas (the big data era), and (ii) despite a simple model, LRMA is very powerful since many high-dimensional data sets are well-approximated by low-rank matrices [458]. LRMA models are used to compress the data, filter the noise, reduce the computational effort for further manipulation of the data, or to directly identify hidden structure in a data set; see for example the survey [457]. Many variants of LRMA have been developed over the last few years [422]. They differ in two key aspects:

1. The error measure can vary and should be chosen depending on the noise statistic assumed on the data. For example, PCA uses least squares, that is, it minimizes $\|X - WH\|_F^2$, which implicitly assumes independently and identically distributed (i.i.d.) Gaussian noise.

   If data is missing or if weights are assigned to the entries of X (for example because the noise is not identically distributed over the entries of X), the problem can be cast as a weighted low-rank matrix approximation (WLRA) problem that minimizes $\sum_{i,j} P_{i,j}(X - WH)_{i,j}^2$ for some nonnegative weight matrix P, where $P_{i,j} = 0$ when the entry at position (i, j) is missing [434]. Note that if P contains entries only in $\{0, 1\}$, then the problem is also referred to as PCA with missing data or low-rank matrix completion with noise. WLRA is widely used in recommender systems [32, 287] for predicting the preferences of users for a given product based on the product's attributes and user preferences, such as in the Netflix prize competition; see [35] and Section 9.5.

   If the sum of the absolute values of the entries of the error $\sum_{i,j} |X - WH|_{i,j}$ is used as the error measure, we obtain yet another variant more tolerant to outliers; this is closely related to robust PCA [73, 212]. It can be used, for example, for background subtraction in video sequences where the noise (the moving objects) is assumed to be sparse while the background has low rank (the background does not change much between consecutive images in video sequences).

2. Different constraints can be imposed on the factors W and H. These constraints depend on the application at hand and allow, for example, for meaningful interpretation of the factors.

   For example, the k-means problem, which is the problem of finding a set of r centroids w_k ($1 \leq k \leq r$) such that the sum of the distances between each data point and the closest centroid is minimized, is equivalent to LRMA where the factor H is required to have a single nonzero entry in each column that is equal to one, so that the columns of W are the cluster centroids.

   If instead one wants to explain each data point using as few basis vectors as possible, each column of the matrix H should contain as many zero entries as possible. This LRMA variant is referred to as sparse component analysis [221] and is closely related to dictionary learning [5, 455] and sparse PCA [115]. It yields a more compact and easily interpretable decomposition.

NMF, an LDR technique for nonnegative data Among LRMA models, nonnegative matrix factorization (NMF) requires the factor matrices W and H to be componentwise nonnegative, which we denote $W \geq 0$ and $H \geq 0$. These nonnegativity constraints play an instrumental role in various applications as they allow one to extract meaningful and interpretable components in nonnegative data sets. For example, in some applications, the entries in W and H can be interpreted as physical quantities. Before presenting four such applications in Section 1.3, let us first define the NMF problem rigorously.

1.2 ▪ Problem definition

Let us formally define the NMF problem and discuss some of its aspects.

Problem 1.1 (Nonnegative matrix factorization). *Given a nonnegative matrix $X \in \mathbb{R}^{m \times n}_+$, a factorization rank r, and a distance measure $D(.,.)$ between two matrices, compute two nonnegative matrices $W \in \mathbb{R}^{m \times r}_+$ and $H \in \mathbb{R}^{r \times n}_+$ such that $D(X, WH)$ is minimized, that is, solve*

$$\min_{W \in \mathbb{R}^{m \times r}_+, H \in \mathbb{R}^{r \times n}_+} D(X, WH). \tag{1.1}$$

Terminology NMF in its modern form was first referred to as positive matrix factorization (PMF) by Paatero and Tapper [371] in 1994, but this name has not been used much, most likely because "positive" means strictly larger than zero, while NMF usually generates a factor with many zeros entries; see the discussion below in the paragraph Sparsity. The name NMF became standard after the paper of Lee and Seung published in 1999 [303]; see Section 1.4 for the historical overview of NMF. In most data analysis applications (see Section 1.3 and Chapter 9), the solution (W, H) is only an approximation of the data matrix X; hence $X \neq WH$ as with most applications using LRMA mentioned in Section 1.1. This is due to the presence of noise and the linear model being, in most cases, only an approximate model ("All models are wrong but some are useful" as mentioned by George Box[5] in 1976). Therefore, the use of the term "factorization" might be misleading since it usually refers to an exact decomposition $X = WH$. Hence some authors have argued that it would, for example, make more sense to refer to (1.1) as nonnegative matrix approximation [433]. However, in this book we subscribe to the widely accepted standard that the name NMF refers to the associated approximation problem, and we will further specify when we are considering the exact factorization, $WH = X$, by calling it Exact NMF. Exact NMF is important in linear algebra as it allows us to compute the nonnegative rank of a matrix X, denoted $\text{rank}_+(X)$, which is the smallest r such that an Exact NMF of X exists; see Chapters 2 and 3.

Objective function The objective function of the NMF problem is defined as

$$D\colon \mathbb{R}^{m \times n}_+ \times \mathbb{R}^{m \times n}_+ \mapsto \mathbb{R}_+ \text{ given by } (A, B) \mapsto D(A, B)$$

and is also referred to as the error measure. The choice of this function is crucial when designing LRMA models and often depends on the assumptions made about the noise statistics. It may greatly influence the solution (W, H) and leads to rather different optimization problems; see

[5] `https://en.wikipedia.org/wiki/All_models_are_wrong` (consulted May 27, 2020).

Chapter 8. Most error measures give the same importance to each entry of the data matrix X and hence have the form

$$D(A, B) = \sum_{i,j} d(A_{ij}, B_{ij})$$

for some function $d\colon \mathbb{R}_+ \times \mathbb{R}_+ \mapsto \mathbb{R}_+$ such that $d(x, y) = 0$ if and only if $x = y$. A standard choice is $d(x, y) = (x - y)^2$ which leads to $D(X, WH) = \|X - WH\|_F^2$. There are two main reasons for this choice: (1) it corresponds to the assumption of i.i.d. Gaussian noise which is reasonable for many data sets, and (2) it leads to a smooth optimization, which is easier to handle (see Chapter 8 for a discussion). We refer the reader to Section 5.1 for a discussion on the choice of D in the context of NMF.

Choice of the symbols In the linear algebra community, authors consistently use the symbols $A = U\Sigma V^\top$ to represent the SVD of matrix A. However, in the NMF literature, there is no consensus on the choice of the symbols used for the data matrix X and the factor matrices (W, H), and many combinations of symbols exist; examples include $V \approx WH$ [303], $X \approx CS^\top$ [263], $A \approx BC$ [433], $X \approx UV$ [478], $Y \approx AX$ [98], $X \approx WH$ [189], or $X \approx WH^\top$ [170]. In this book we choose the notation $X \approx WH$.

Transpose: $\boldsymbol{WH}$ vs. $\boldsymbol{WH}^\top$ In the numerical linear algebra community, most authors would likely prefer the use of $X \approx WH^\top$, similarly as for the SVD that uses $U\Sigma V^\top$ (see Section 6.1.1), as it preserves the symmetry by transposition, that is, $X \approx WH^\top$ if and only if $X^\top \approx HW^\top$. However, we choose $X \approx WH$ for the following reason. When interpreting NMF as an LDR technique, which is the main motivation behind NMF, the columns of H play the role of the coefficients of the columns of X in the subspace spanned by the columns of W since $X(:, j) \approx WH(:, j)$ for all j. In other words, there is a one-to-one correspondence between the high-dimensional columns of X and their low-dimensional representations as the columns of H. We believe this is the reason why it is the most common choice in the NMF literature.

NMF variants The problem (1.1) is the formulation of the standard NMF problem. However, it is important to keep in mind that there exist many variants of this problem. Moreover, as we will argue in Chapter 4, it is in general crucial to consider such variants in practice to obtain unique decompositions and be able to identify the true underlying factors that generated the data. Some variants use regularization in order to obtain solutions with some structure, such as sparsity; see Sections 4.3.4 and 5.3. Other variants use additional constraints; for example symmetric NMF (symNMF) requires $H = W^\top$, and orthogonal NMF (ONMF) requires H to have orthogonal rows (see Section 5.4).

Sparsity Because of the nonnegativity constraints, NMF solutions (W, H) are expected to contain zero entries and hence to naturally have some degree of sparsity; see for example Figures 1.2, 1.4, 1.6, and 1.8 in the next section. Mathematically, this is explained by the first-order optimality conditions of a smooth optimization problem with nonnegativity constraints

$$\min_{x \in \mathbb{R}^n} f(x) \quad \text{such that} \quad x \geq 0,$$

which are given by

$$x \geq 0, \quad \nabla f(x) \geq 0, \quad \text{and} \quad x_i(\nabla f(x))_i = 0 \text{ for all } i.$$

This enforces $x_i = 0$ whenever $(\nabla f(x))_i > 0$; see Section 8.1.2 for more details. In some applications, one might need to obtain even sparser solutions, which requires the use of additional constraints or regularization; see Chapters 4 and 5.

Applications In the next section, we describe four important applications of NMF in data analysis (see Chapter 9 for other NMF applications). However, it is important to stress that *NMF is not motivated only by its use as an LDR technique for data analysis*; see in particular the historical overview in Section 1.4. Another important motivation is exact factorizations. In particular, the nonnegative rank of a nonnegative matrix X, denoted $\mathrm{rank}_+(X)$, is the smallest r such that there exists an Exact NMF $X = WH$ where W has r columns and H has r rows; see Chapters 2 and 3 for more details. An application where the nonnegative rank has had tremendous impact is in the study of the extension complexity of polytopes; see Section 3.6.

1.3 ▪ Four applications of NMF in data analysis

In this section, we describe four important applications of NMF that will be used throughout the book as illustrative examples. They show that NMF is a particularly meaningful LRMA model as it leads to interpretable decompositions. In Chapter 9, we review other applications of NMF.

1.3.1 ▪ Feature extraction in a set of images

Given a set of gray-scale images of the same dimensions, let us construct the matrix X such that each column of X corresponds to a vectorized gray-level image. Vectorization means that the two-dimensional images are transformed into a long one-dimensional vector, for example, by stacking the columns of the image on top of each other.[6] This means that each row of X corresponds to the same pixel location among the images. The entry of X at position (i, j), that is, $X(i, j)$, is equal to the intensity of the ith pixel within the jth image, which is nonnegative. As explained in Section 1.1, factorizing X with NMF as $X \approx WH$ where $W \geq 0$ and $H \geq 0$ provides an LDR where the columns of W form a basis for the columns of X. Because W is nonnegative, its columns can be interpreted as basis images: the columns of W are vectors of pixel intensities whose linear combinations allow us to approximate each input image. Moreover, because of the nonnegativity constraints on the weight matrix H, no cancellation is possible between the basis images to reconstruct all the input images. Hence these basis images typically correspond to localized features that are shared among the input images, and the entries of H indicate which input image contains which feature. For example, if the columns of X are facial images, the columns of W correspond to facial features such as eyes, noses, mustaches, and lips. Figure 1.2 illustrates such a decomposition and shows that NMF is able to extract a part-based representation of a set of facial images. Note that to obtain such decompositions, the images need to be well-registered/aligned (for example, pixels corresponding to noses should be located at the same position in the input images).

Another example is the synthetic swimmer data set [138], where the columns of X are vectorized images of a swimmer whose four limbs take four different positions for a total of $n = 256$ images; see Figure 1.3. For an NMF of rank 17, the columns of W correspond to the body and the limbs in the 16 different positions; see Figure 1.4.

Remark 1.1 (Uniqueness, minimality, and sparsity). *The decomposition shown in Figure 1.4 is not minimal, that is, there exists an Exact NMF with fewer basis elements. In particular, there exist several Exact NMFs with factorization rank 16: for example the body can be put together with the limbs in all positions with an intensity of 1/4 (since each image in the data set contains four limbs), or the body can be put together with one limb in its four positions with an intensity of 1 (since each image in the data set contains each limb in one position). Hence the Exact NMF of rank 16 of this data set is not unique; see Chapter 4 for a discussion*

[6] In MATLAB, this is achieved via the function `vec`.

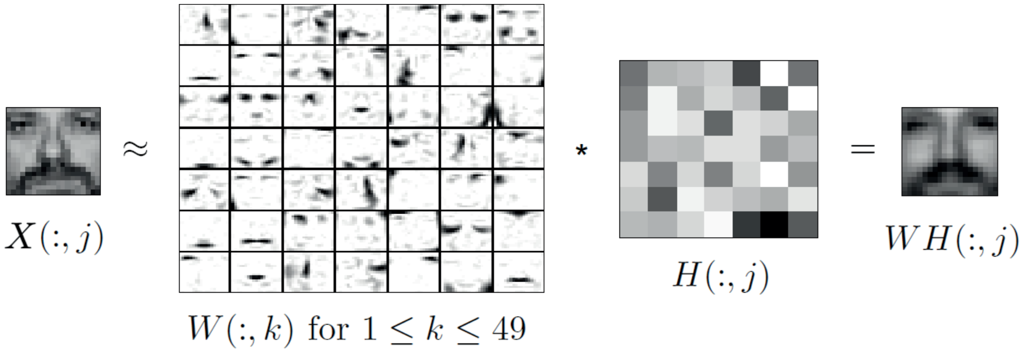


Figure 1.2. *NMF applied on the CBCL face data set with $r = 49$ (2429 images with 19×19 pixels each), as in the seminal paper of Lee and Seung [303]. On the left is a column of X reshaped as an image. In the middle are the 49 columns of the basis W reshaped as images and displayed in a 7×7 grid and the reshaped column of H in the same 7×7 grid that shows which features are present in that particular face. On the right is the reshaped approximation $WH(:,j)$ of $X(:,j)$ as an image. [`Matlab file: CBCL.m`].*

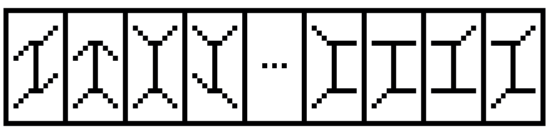


Figure 1.3. *Sample images of the swimmer data set.*

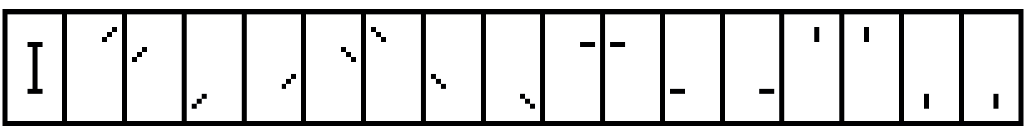


Figure 1.4. *NMF basis images for the swimmer data set. [`Matlab file: Swimmer.m`].*

on this important issue. However, additional constraints on the decomposition may make it unique. For example, the decomposition of rank 17 from Figure 1.4 can be obtained as the unique decomposition using sparse NMF; see Section 4.3.4. It can also be obtained with separable NMF (Chapter 7), minimum-volume NMF (Section 4.3.3), ONMF (Section 4.3.2), or nonnegative matrix underapproximation (NMU; Section 5.4.5).

1.3.2 ▪ Blind hyperspectral unmixing

A hyperspectral image measures the intensity of the light within a scene for many different wavelengths, typically between 100 and 200 wavelengths; see for example [427] for a gentle introduction to hyperspectral imaging. Hence, for each pixel, a vector of intensities is recorded that is equal to the fraction of light reflected by that pixel depending on the wavelength; this is referred to as the spectral signature of the pixel. Given a hyperspectral image, the goal of blind hyperspectral unmixing (blind HU) is to recover the materials present in an image, referred to as the endmembers, and their proportions in each pixel, referred to as abundances. Under the

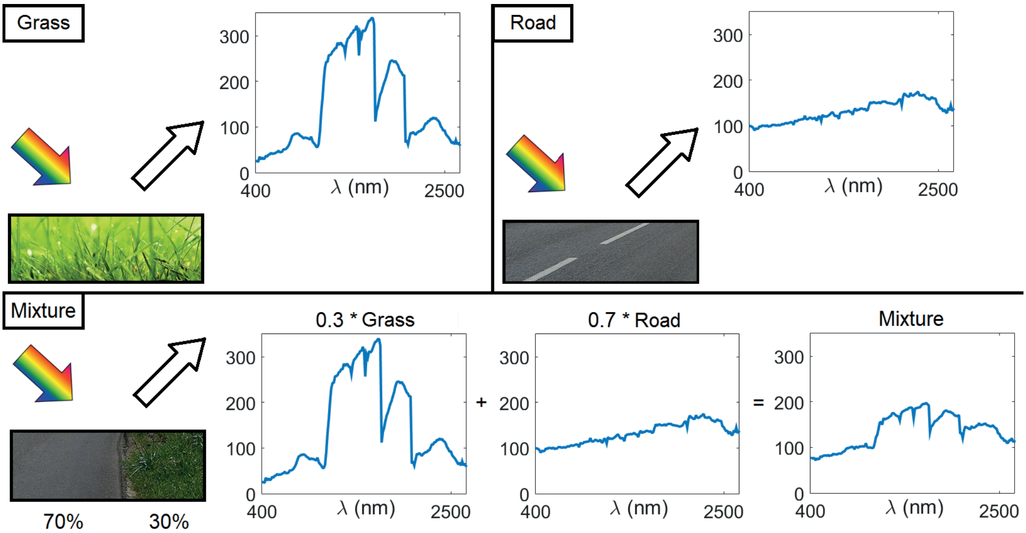


Figure 1.5. *Linear mixing model for hyperspectral imaging.*

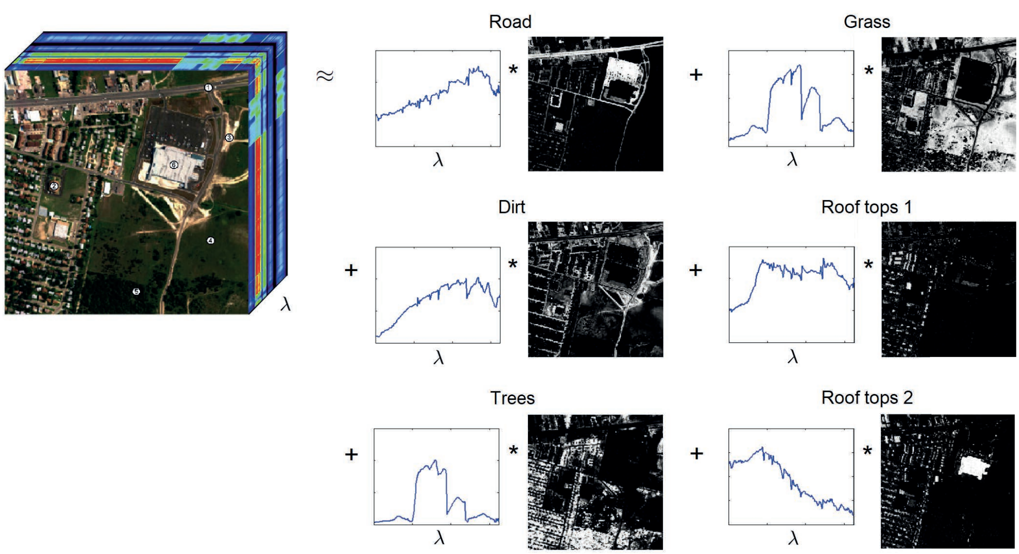


Figure 1.6. *Blind HU of an urban image taken above the Walmart in Copperas Cove, Texas, using NMF with $r = 6$ (162 spectral bands, 307 × 307 pixels). This is the so-called Urban data set. Each factor corresponds to the spectral signature of an endmember (a column of W) with its abundance map (a row of H, reshaped as an image on the figure), where light tones represent high abundances. The Urban hyperspectral image is mostly made up of six materials, namely road, grass, trees, dirt, and roof tops 1 and 2. In particular, the rank-6 NMF above explains more than 95% of the data, that is, $\|X - WH\|_F \leq 0.05\|X\|_F$. Image adapted from [191].* `[Matlab file: Urban.m]`.

linear mixing model, the spectral signature of a pixel is equal to the linear combination of the spectral signatures of the materials it contains. For example, if a pixel contains 30% grass and 70% road surface, its spectral signature is equal to 0.3 times the spectral signature of the grass plus 0.7 times the spectral signature of the road surface; see Figure 1.5 for an illustration. Hence letting each column of the matrix X be the spectral signature of a pixel, blind HU boils down to the NMF of matrix X. In fact, NMF decomposes X as

$$X(:,j) \approx \sum_{k=1}^{r} W(:,k)H(k,j),$$

where the columns of W are the spectral signatures of the endmembers, while the entries of H give the abundance of each endmember in each pixel; see Figure 1.6 for an illustration of NMF on the widely used Urban data set.

1.3.3 ▪ Text mining: topic recovery and document classification

Let each column of the matrix X correspond to a document, that is, a nonnegative vector of word counts. For example, the entry of X at position (i,j) can be the number of times word i appears in document j. The matrix X can also be constructed in different, more sophisticated ways, for example, with the term frequency-inverse document frequency (tf-idf) [389]. This is the so-called bag of words model where the positions of the words in a document are not taken into account. The NMF of X provides the model

$$X(:,j) \approx \sum_{k=1}^{r} W(:,k)H(k,j),$$

where the nonnegative columns of W can also be interpreted as bags of words, that is, as vectors of word count. Since the number of columns of W is much smaller than the number of columns of X ($r \ll n$), each column of W must be used to reconstruct many documents. Moreover, because of the nonnegativity of H, no cancellation is possible, and hence each column of W must contain words that appear simultaneously in these documents. In practice, it has been observed that the columns of W correspond to different topics; see Figure 1.7 for an illustration. Moreover, the columns of the factor H indicate the importance of the topics discussed in the corresponding documents.

Remark 1.2. *We will provide more details on topic modeling and its link with NMF later in the book. In Section 5.5.4, we will show the equivalence between NMF and probabilistic latent semantic analysis/indexing (PLSA/PLSI) which is a simple probabilistic topic model. In Section 5.4.9.1, we will discuss the limitations of NMF for topic modeling and describe a better suited NMF model for this task.*

1.3.4 ▪ Audio source separation

Given an audio signal recorded from a single microphone, its magnitude spectrogram can be constructed as follows. The signal is split into small time frames with some overlap (usually 50%), and each frame is multiplied by some window function (such as the Hamming window) to avoid artifacts due to the truncation of the signal. Each column of X is obtained by taking the short-time Fourier transform of each time frame. More precisely, the entry of X at position (i,j) is the magnitude of the Fourier coefficient for the jth time frame at the ith frequency. Given such

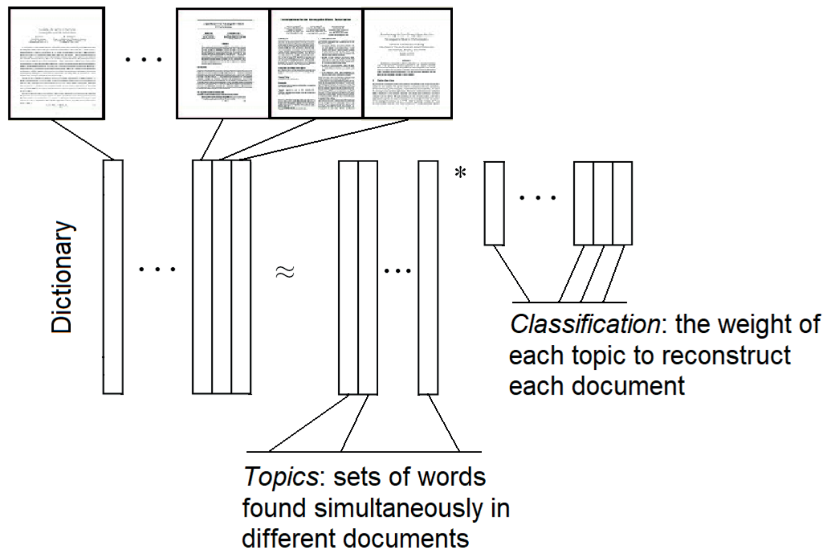


Figure 1.7. *Illustration of NMF for text mining: extraction of topics, and classification of each document with respect to these topics. The columns of X are sets of words, with $X(i, j)$ being the importance of word i in document j. Because H is nonnegative, these sets are approximated as the union of a smaller number of sets defined by the columns of W that correspond to topics.*

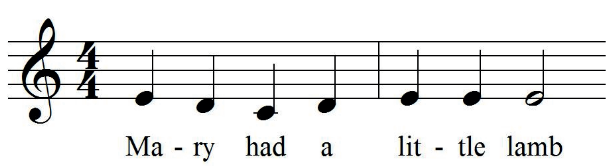
a signal, the goal is to blindly separate the sources that compose the signal, for example, separate the voice and the instruments in a song. Under the two following assumptions, this separation problem is yet another NMF problem:

1. The spectrogram of the mixture is a nonnegative linear combination of the spectrogram of the sources. Nonnegativity means that sound cancellation is neglected. Linearity is a natural model; nonlinear effects, such as the saturation of the microphone or reverberations of the sound, are not taken into account.

2. The spectrograms of the sources have low rank. This has been validated on many experiments and makes sense physically. For example, the spectrogram of an instrument is composed of rank-one factors made of the signature of each note in the frequency domain along with its activation over time.

We refer the interested reader to [158] and the references therein for more information on this model.

Let us use a simple monophonic signal for illustrative purposes, namely a piano recording of "Mary Had a Little Lamb," whose musical score is shown below.



The sequence is composed of three notes, C_4, D_4, and E_4, that activate as follows: E_4, D_4, C_4, D_4, E_4, E_4, E_4. For this data set, the three main sources are the piano notes whose spectrograms

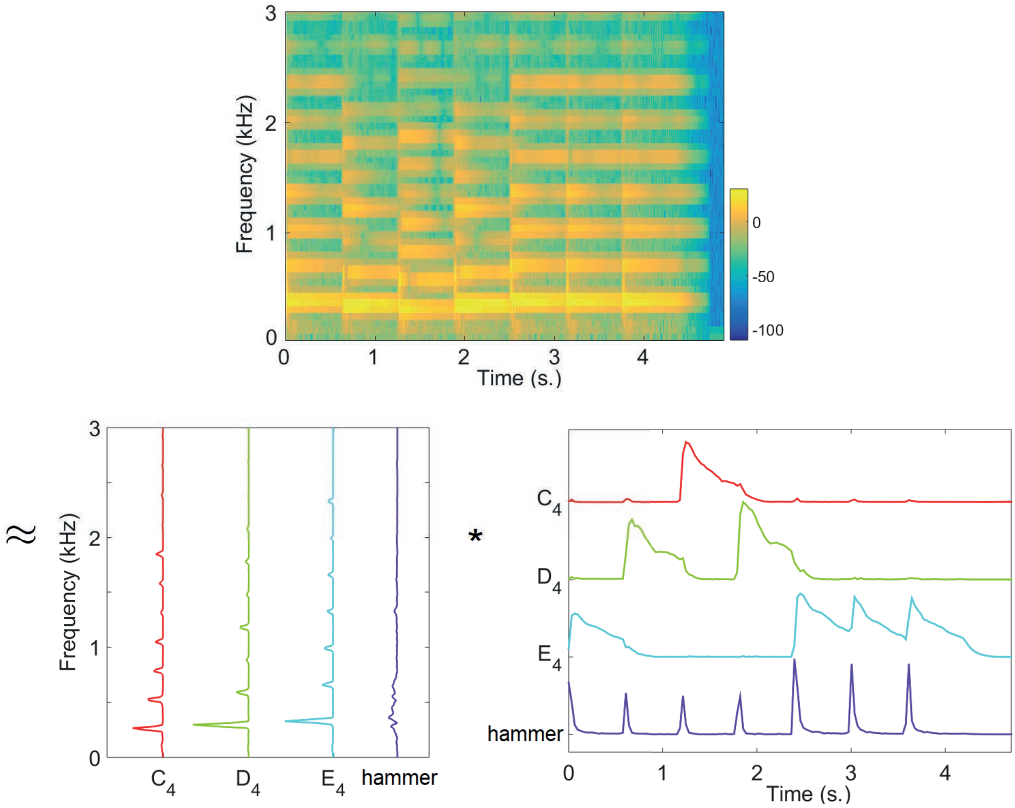


Figure 1.8. *Decomposition of the piano recording "Mary Had a Little Lamb" using NMF: (top) amplitude spectrogram X in dB; (bottom left) basis matrix W corresponding to the three notes C_4, D_4, and E_4, and the hammer noise; (bottom right) activation matrix H that indicates when each note is active. Image adapted from [191].* `[Matlab file: Mary_piano.m]`.

have rank one: each column of W is the signature of each note in the frequency domain, while the entries of H indicate when a note is active. However, there is a fourth source in this data set: it captures the common mechanism that triggers a note; in particular the hammer within the piano. Figure 1.8 shows the NMF decomposition of the magnitude spectrogram using $r = 4$. As expected, the three notes and the hammer noise are extracted as the columns of W, while the rows of H provide the activation of each note in the time domain. NMF is able to blindly separate the different sources and identify which source is active at which moment in time. NMF has been used, for example, for automatic music transcription; see the survey [34].

NMF shows its full potential for polyphonic music analysis when several notes, and even several instruments, are played at once. However, for such complicated scenarios, refined NMF models should be used, such as sparse NMF [471] or convolutive NMF [424]; see Chapter 5. Moreover sources usually have rank higher than one (for example, the voice of a person), and a postprocessing step is necessary to assign each rank-one factor to its corresponding source. Note that the phase information is missing when reconstructing the sound signal from the spectrogram of the sources. This is an important issue, and in practice one often uses the phase of the input signal; see [337, 468, 338] for more information on this topic.

1.4 ▪ History

The first use of the NMF model can be traced back to the fields of analytical chemistry and of geoscience and remote sensing. In both these fields, NMF corresponds to a meaningful physical model. In both cases,

- the columns of the matrix X correspond to nonnegative spectra of samples (also known as the spectral signature),
- the columns of W correspond to the pure component spectra, and
- the columns of matrix H provide the concentration of the pure components within each sample.

This linear mixing model makes sense physically as the spectrum of a sample is, in ideal conditions, proportional to the spectra of the pure components it contains; this is the so-called Lambert–Beer law [297, 30]; see Figure 1.5 (page 8). This model, which is equivalent to NMF, was discovered and used independently in the early 1960s in these two fields.

1.4.1 ▪ Analytical chemistry

The columns of $X \in \mathbb{R}^{m\times n}_+$ are the spectra of a chemical reaction measured over time, so that m is the number of measured spectral bands and n is the number of time steps for which the reaction is measured. These spectra can be obtained in different ways, for example using Raman spectroscopy; see Section 9.3 for a numerical example. Given these nonnegative spectra, the goal is to recover the pure spectra of the chemical compounds present in the reaction (the columns of W) along with their proportions in each sample (the rows of H). This is an NMF problem which is referred to as self-modeling curve resolution (SMCR); see Section 9.3 for more details.

To the best of our knowledge, Wallace in 1960 [473] was the first to describe the model. He then discussed a way to estimate the number of sources (that is, r). Later in 1971, Lawton and Sylvestre [301] focused on the case $r = 2$ which can be solved easily; see Sections 2.1.3 and 4.1. In 1985, Borgen and Kowalski focused on the case $r = 3$, and, in 1986, Borgen et al. studied the general case [53]. The literature on the topic has grown rapidly since then, and we refer the reader to [263, 390, 366] and the references therein for more information on SMCR. Note that the problem of multivariate curve resolution (MCR) is more general than SMCR as it does not necessarily assume nonnegativity [119, 403].

Interestingly, in the SMCR literature, most works have analyzed the noiseless case, that is, $X = WH$, with the additional assumption that $\mathrm{rank}(X) = \mathrm{rank}(W) = r$. Under these assumptions, Exact NMF is equivalent to finding a transformation of an unconstrained factorization (such as the SVD) to make it nonnegative; see Section 5.5.1. A unique feature within the SMCR literature is that, in most works, the goal is to recover all possible factorizations, that is, all possible nonnegative (W, H) such that $X = WH$, referred to as the set of feasible solutions. The task of choosing the “right” factorization is left to the expert analyzing such chemical reactions. This is a particularly challenging problem, which may explain why an important part of the literature has focused on the exact case, as pointed out in [366].

1.4.2 ▪ Geoscience and remote sensing

The columns of X are the spectra of pixels within a hyperspectral image. The spectrum of a pixel records the fraction of light reflected by that pixel for many wavelengths. The goal is to recover the pure materials present in the image (the columns of W) and the abundance of the materials in each pixel (the columns of H). This is referred to as blind HU; see Section 1.3.2. This model was first used in 1964 by Imbrie and Van Andel for analyzing the mixture of heavy mineral data [254]. Early findings in this field include the works by Craig in the early 1990s [108, 109], by Boardman [48] (1993), and by Winter [482] (1999). The main contribution of these authors is they have shed light on the geometric interpretation of NMF (Section 2.1) and devised algorithms based on this intuition; see Chapters 4 and 7.

The literature on blind HU has grown considerably since the 1990s, motivated by the development of hyperspectral cameras that are becoming higher performing and more affordable as the years go by. We refer the reader to [276, 377, 45, 334] and the references therein for more information on blind HU.

1.4.3 ▪ Stochastic sequential machines

Another very early account of the NMF model appears in the study of stochastic finite state systems, also known as stochastic sequential machines (SSMs). An important problem in this context is to obtain a minimal state representation of the given system. The SSM can be represented with a nonnegative matrix that contains the transition probabilities between the different states. To the best of our knowledge, Ott [369] (1966) was the first to show that computing an Exact NMF of this matrix is equivalent to finding the minimal state representation of the SSM. Moreover, Ott discovered the connection between Exact NMF and the nested polytope problem (NPP), an important problem in computational geometry. Recall that a polytope is a bounded set defined via affine inequalities, that is, a bounded polyhedron. In two dimensions, polytopes are convex polygons. The NPP requires finding a polytope with the minimum number of vertices nested between two given nested polytopes. As we will discuss in length in Chapter 2, the Exact NMF problem with $r = \mathrm{rank}(X)$ is equivalent to the NPP where the sought solution is required to have r vertices. Follow-up works investigating this connection and providing new insights include the papers of Paz [378] (1968) and Bancilhon [22] (1974); see also the first chapter of the book of Paz [379] (1971). The problem of minimal state representation of an SSM is equivalent to the minimal covering of a labeled Markov chain. We refer the reader to [88] for more details and for the proof of the equivalence between Exact NMF and minimal covering of a labeled Markov chain.

1.4.4 ▪ Computational geometry

As explained in the previous section, Exact NMF is equivalent to the NPP. In two dimensions, the NPP requires finding a convex polygon with a minimum number of vertices nested between two given convex polygons. Motivated by its applicability for stochastic sequential machines, Silio [420] (1979) solved this problem by proposing a practical polynomial-time algorithm. However, his paper seems to have been overlooked in the computational geometry literature. The problem was later solved independently in a very similar way by Aggarwal et al. [4] (1989). However, the algorithm of Aggarwal et al. has a lower computational cost; see Section 2.3.1.1. In dimension higher than two, the NPP was shown to be NP-hard by Das and Joseph [114] (1990).

1.4.5 ▪ Linear algebra

The Exact NMF problem, with $X = WH$, is closely related to the notion of nonnegative rank. It started to draw attention after a question of Berman and Plemmons [38] in *SIAM Review* in 1973 (Problem 73-14):

> It is well known that an $m \times n$ matrix A of rank r can be factored (in a variety of ways) in the form $A = BG$ where B is of order $m \times r$ and G is of order $r \times n$. Show by counterexample, that when A is nonnegative there need not exist such a "rank factorization" with both B and G nonnegative. If possible, find a simple characterization of the class of nonnegative matrices A for which a nonnegative rank factorization exists.

In other words, this question asks us to characterize when the rank and the nonnegative rank of a matrix coincide, that is, when $\operatorname{rank}(X) = \operatorname{rank}_+(X)$.

Thomas [450] answered the first part of the question in *SIAM Review* in 1974: he showed that $\operatorname{rank}(X) = \operatorname{rank}_+(X)$ always holds when $\operatorname{rank}(X) \leq 2$ and gave a counterexample to show that this is not necessarily true when $\operatorname{rank}(X) \geq 3$:

$$X = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \tag{1.2}$$

for which $\operatorname{rank}_+(X) = 4$ while $\operatorname{rank}(X) = 3$; see Section 2.1 for the proofs and more details. It turns out that it is NP-hard to check whether $\operatorname{rank}(X) = \operatorname{rank}_+(X)$ [465]; see Section 2.3, which discusses the computational complexity of Exact NMF.

Early works on the nonnegative rank include the papers of Wall [472] (1979), Jeter and Pye [261] (1981), Campbell and Poole [72] (1981), and Chen [84] (1984). The first comprehensive account of the properties of the nonnegative rank was written by Cohen and Rothblum [100] in 1993; see Section 3.1 for more details.

1.4.6 ▪ Probability

NMF can be used to unravel a particular probabilistic model. Let $Y^{(k)} \in \{1, \dots, m\}$ and $Z^{(k)} \in \{1, \dots, n\}$ be two independent random variables for $1 \leq k \leq r$, and let $P^{(k)}$ be the joint distribution with

$$P_{ij}^{(k)} \;=\; \mathbb{P}\left(Y^{(k)} = i, Z^{(k)} = j\right) \;=\; \mathbb{P}\left(Y^{(k)} = i\right)\mathbb{P}\left(Z^{(k)} = j\right)$$

for $1 \leq i \leq m$ and $1 \leq j \leq n$. Each distribution $P^{(k)}$ corresponds to a nonnegative rank-one matrix. Let us define the joint distribution of two random variables Y and Z as follows:

- Choose the distribution $P^{(k)}$ with probability α_k, where $\sum_{k=1}^r \alpha_k = 1$.
- Draw Y and Z from the distribution $P^{(k)}$.

Equivalently, (Y, Z) has the following probability distribution: for $1 \leq i \leq m$ and $1 \leq j \leq n$,

$$\mathbb{P}(Y = i, Z = j) \;=\; \sum_{k=1}^{r} \alpha_k P_{i,j}^{(k)} \;=\; P_{i,j},$$

where the matrix P is the sum of r rank-one nonnegative matrices. In other words, P is the mixture of r independent distributions. In practice, only P is observed and is referred to as a contingency table, and computing its nonnegative rank and a corresponding factorization amounts to explaining the distribution P with as few independent variables as possible. Early work using this connection includes De Leeuw and Van der Heijden [120] (1991) and Ritov and Gilula [398] (1993); see Cohen and Rothblum [100] (1993) and Kubjas, Robeva, and Sturmfels [292] (2015) for more details. However, the first to discuss the above decomposition were Suppes and Zanotti [443] (1981), although without linking it explicitly with the nonnegative rank. In their terms, the nonnegative rank of P is the smallest support of a hidden random variable, which explains the correlation of the two-valued random variable whose joint distribution is represented by P.

Motivated by this application, Mond, Smith, and Van Straten [353] (2003) also discovered the link between Exact NMF and the NPP (which they call the sandwiched simplices problem) and studied the set of feasible solutions of Exact NMF.

1.4.7 ▪ Extended formulations

A standard approach in combinatorial optimization is to model the convex hull of the set of feasible solutions using affine inequalities, and then solve the problem using linear optimization. These linear formulations are referred to as extended formulations, and their size is defined as the number of inequalities; see Section 3.6 for more details. In the 1980s, some researchers were trying to prove P=NP by constructing such formulations of polynomial size for NP-complete combinatorial optimization problems, such as the traveling salesman problem (TSP).[7] If such formulations have polynomial size, then linear optimization can be used to solve them in polynomial time, which would imply P=NP.

In 1988, Yannakakis proved that this was not possible for the matching and TSP polytopes using extended formulations that are symmetric (for the TSP, this means that they are invariant under permutations of the cities in the input) [492, 493]; see also the discussion by Yannakakis in [494]. To do this, Yannakakis unraveled a key result: the minimum-size extended formulation of a polytope, referred to as its extension complexity, is equal to the nonnegative rank of its slack matrix. Given a polytope

$$\mathcal{P} \;=\; \left\{x \in \mathbb{R}^d \mid a_i^\top x \le b_i \text{ for } i = 1, 2, \dots, m\right\},$$

whose vertices are v_j for $j = 1, 2, \dots, n$, its slack matrix $S \in \mathbb{R}^{m\times n}_+$ is an inequality-by-vertex matrix where

$$S(i, j) = b_i - a_i^\top v_j \ge 0$$

is the slack of the jth vertex for the ith inequality.

Many results were obtained 20 years later (starting around 2010) to provide bounds on the extended formulations of combinatorial problems using bounds for the nonnegative rank. Several long-standing open questions were addressed via the nonnegative rank. For example, Fiorini et al. [163, 164] proved that the extension complexity of the TSP polytope is exponential in the number of cities (the difference with Yannakakis' result is that here asymmetric extended formulations are allowed, and asymmetry may reduce the size of extended formulations [270]). This is not surprising if you believe that $P \neq NP$. Rothvoss proved that the perfect matching polytope[8] has exponential extension complexity so that any extended formulation for the perfect matching polytope must have exponential size [400, 401]. This is somewhat surprising since optimizing a linear function over the perfect matching polytope can be performed in polynomial time [142]. Moreover, Braun and Pokutta [60] later established that for all fixed $0 < \epsilon < 1$, even every linear program approximating the matching polytope by a factor $(1 + \epsilon/n)$ must have exponential size, where n is the number of nodes in the graph. We refer the reader to Section 3.6 for more details and examples.

1.4.8 ▪ The first appearance of NMF in its modern form

As far as we know, the first time the NMF problem was explicitly stated as in (1.1) is in the paper by Paatero and Tapper in 1994 [371]. As discussed above, the models previously studied in the literature either considered exact factorizations, assumed $\operatorname{rank}(X) = \operatorname{rank}(W) = r$, or were only based on geometric representations. In their paper, Paatero and Tapper referred to this problem as positive matrix factorization (PMF), proposed an algorithm based on alternatively

[7]Given a set of cities, the TSP requires finding the shortest possible route that visits each city and returns to the origin city.

[8]The perfect matching polytope is the convex hull of the set of all perfect matchings of a complete graph (a perfect matching decomposes the set of vertices into pairs of vertices).

updating W and H (see Section 8.3.1), and explained how it can be used to analyze environmental data, for example, for air emission control. However, until 1999, PMF remained a specialized physical/chemical model confined within the field of chemometrics.

1.4.9 ▪ The "big bang" of NMF: data analysis and machine learning

NMF gained momentum with the seminal paper "Learning the Parts of Objects by Non-negative Matrix Factorization" by Lee and Seung published in *Nature* in 1999 [303]. It explained why NMF is a powerful tool for the analysis of nonnegative data sets. They illustrate their findings on two examples: the extraction of facial features in a set of facial images (see Figure 1.2, page 7) and the identification of topics within a set of documents (see Figure 1.7, page 10). Note that Lee and Seung also proposed algorithms based on multiplicative updates (MU) that became the workhorse in the NMF literature [304]; see Section 8.2.

Let us point out the difference in spirit of Lee and Seung compared to the previous literature by quoting Pentti Paatero:[9]

> The original concept of NMF, as presented in the *Nature* paper, was essentially different from our PMF: they did not search for the (hopefully unique) model of a data set that describes a physical/chemical situation. Instead, their goal could be described as "data compression." Such compressed version of data is normally not unique, it is not "THE solution."

In fact, prior to the paper of Lee and Seung, most works using NMF for data analysis focused on the physical model behind NMF and were hoping that NMF would produce the true underlying sources (such as pure spectra; see Sections 1.4.1 and 1.4.2). In their paper, Lee and Seung did not discuss this issue, and their goal was rather to compute one possible NMF decomposition that compresses the data and can be meaningfully interpreted. We will discuss this key identifiability question for NMF in Chapter 4.

1.5 ▪ Take-home messages

NMF is a linear dimensionality reduction technique with nonnegativity constraints on the factors and is able to extract meaningful components in various applications. From our account of the early literature on the NMF model, we observe that, before the paper of Lee and Seung, the study of NMF was motivated by either specific applications or theoretical questions. Lee and Seung were able to popularize NMF for the analysis of nonnegative data sets via the extraction of sparse and part-based components. They showed that NMF is very versatile and can be used in many different settings. This has been confirmed since then as NMF has been used successfully in many applications; see Chapter 9. In summary, the paper of Lee and Seung set a spark on NMF that has ignited a fire that has been growing steadily since then.

[9] Private communication.

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