The Why and How of Nonnegative Matrix Factorization

Topic Presentation

Group 02

LINMA2380 — Matrix computations

December 10, 2020

Summary

1 Introduction

2 Applications

3 Connections to other problems

Agenda

Use : Analysis of high-dimensional data by automatically extracts sparse and meaningful features from a set of nonnegative data vectors

1. What : Definitions and properties
2. Why : Applications
3. How : Algorithms
4. What next : Connections with Problems in Mathematics and Computer Science
5. Conclusion

What : Definitions and properties

Nonnegative matrix factorization (NMF) is a Linear dimensionality reduction (LDR)

LDR :

- From a set of data points $x_j \in R^p$ for $1 \leq j \leq n$
- To a set of dimension $r < min(p, n)$
- Thanks to $w_k \in R^p$ for $1 \leq k \leq r$
- Such that : $\forall j, x_j \approx \sum_{k=1}^{r} w_k h_j(k)$, for some weights $h_j \in R^r$

Equivalent to **low-rank matrix approximation** : $X \approx WH$

- $X \in R^{p \times n}$: $X(:, j) = x_j$ for $1 \leq j \leq n$
- $W \in R^{p \times r}$: $W(:, k) = w_k$ for $1 \leq k \leq r$
- $H \in R^{r \times n}$: $H(:, j) = h_j$ for $1 \leq j \leq n$

NMF : decomposing a given nonnegative data matrix X as $X \approx WH$ where $W \geq 0$ and $H \geq 0$

Applications - Image processing

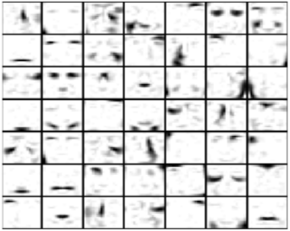
Goal : Facial Feature Extraction

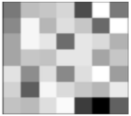
Data matrix : $X \in \mathbb{R}_{+}^{p \times n}$

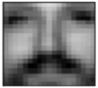
- p : total number of pixels
- n : number of faces
- $X(i,j)$: the gray-level of the i-th pixel in the j-th face

Applications - Image processing

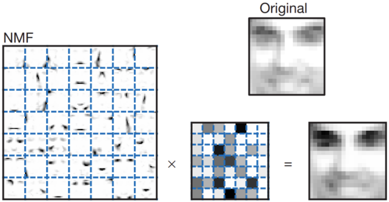
$$\underbrace{X(:,j)}_{j\text{th facial image}} \approx \sum_{k=1}^{r} \underbrace{W(:,k)}_{\text{facial features}} \underbrace{H(k,j)}_{\text{importance of features in } j\text{th image}} = \underbrace{WH(:,j)}_{\text{approximation of } j\text{th image}}$$



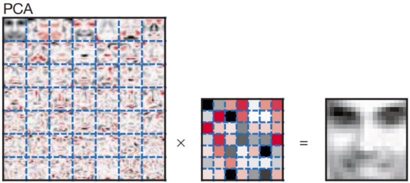




Applications - Image processing



NMF decomposition



PCA decompostion

Applications - Text Mining

Goal : Topic Recovery and Document Classification

Data matrix : $X \in \mathbb{R}_+^{n \times m}$

- each column : a document
- each line : a word
- $X(i,j)$: number of times the i-th word appears in the j-th document

$$\underbrace{X(:,j)}_{j\text{th document}} \approx \sum_{k=1}^{r} \underbrace{W(:,k)}_{k\text{th topic}} \quad \underbrace{H(k,j)}_{\substack{\text{importance of } k\text{th topic} \\ \text{in } j\text{th document}}} \quad , \quad \text{with } W \geq 0 \text{ and } H \geq 0.$$

Applications - Hyperspectral Unmixing

Goal :

1. Identify the constitutive materials present in an image
2. Classify the pixels according to their constitutive materials

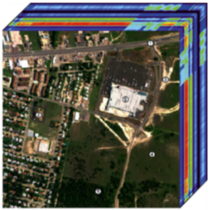
Spectral signature of a pixel: fraction of incident light being reflected by that pixel at different wavelengths

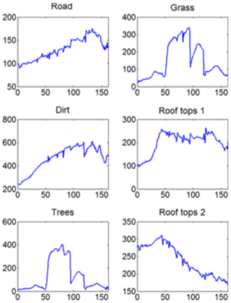
Applications - Hyperspectral Unmixing

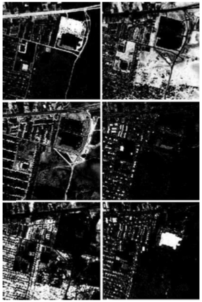
Data matrix : $X \in \mathbb{R}^{n \times m}$

- each column : spectral signature of a pixel

$$\underbrace{X(:,j)}_{\substack{\text{spectral signature}\\ \text{of } j\text{th pixel}}} \approx \sum_{k=1}^{r} \underbrace{W(:,k)}_{\substack{\text{spectral signature}\\ \text{of } k\text{th endmember}}} \underbrace{H(k,j)}_{\substack{\text{abundance of } k\text{th endmember}\\ \text{in } j\text{th pixel}}} .$$



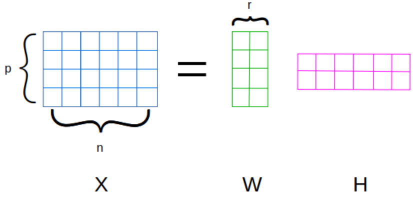


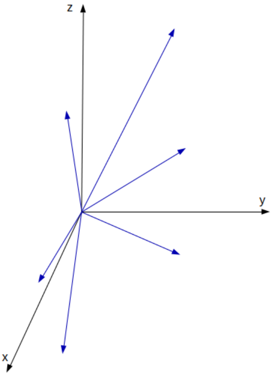


Nonnegative rank

Definition (Nonnegative rank)

Given $X \in \mathbb{R}_+^{p\times n}$, the nonnegative rank of X, denoted rank$_+(X)$ is the minimum r s.t. $\exists W \in \mathbb{R}_+^{p\times r}, H \in \mathbb{R}_+^{r\times n}$ with $X = WH$.





Computational Geometry : Nested polytopes problem

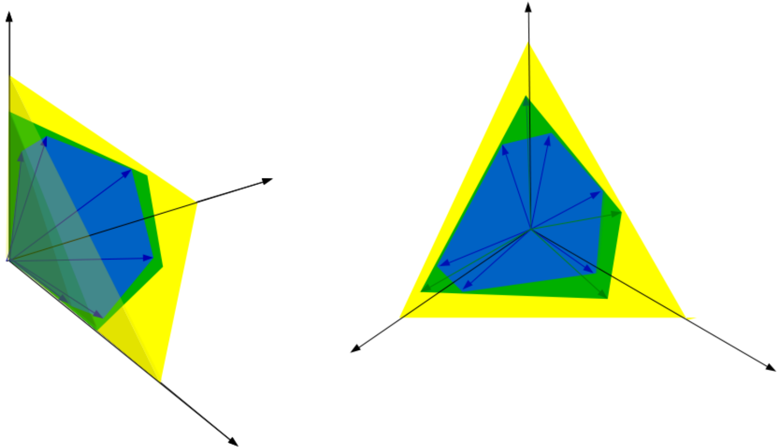


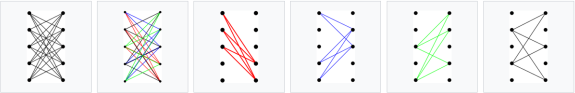
Figure: Finding a polytope with minimum nb of vertices nested between 2 polytopes

Graph Theory : Bipartite dimension

Let $G(X) = (V_1 \cup V_2, E)$ be a bipartite graph induced by X (i.e. $(i, j) \in E \Leftrightarrow X_{ij} \neq 0$).

Definition (Biclique and bipartite dimension)

- *A biclique (or a complete bipartite graph) is a bipartite graph s.t. every vertex in V_1 is connected to every vertex in V_2.*
- *The bipartite dimension (or the minimum biclique cover) bc$(G(X))$ is the minimum number of bicliques needed to cover all edges in E.*



A bipartite graph... | ...and a covering with four bicliques | the red biclique from the cover | the blue biclique from the cover | the green biclique from the cover | the black biclique from the cover

Figure: Example for biclique edge cover **[biclique]**

For any $(W,H) \geq 0$ s.t. $X = WH = \sum_{k=1}^{r} W_{:k} H_{k:}$, we have

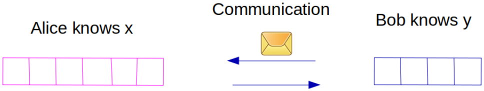
$$G(X) = \cup_{k=1}^{r} G(W_{:k} H_{k:})$$

where $G(W_{:k} H_{k:})$ are complete bipartite subgraphs (bc$(G(W_{:k} H_{k:} = 1 \forall k)$.

Theorem (Rectangle covering bound)

$$\mathit{bc}(G(X)) \leq \mathit{rank}_{+}(X)$$

Communication complexity



Alice and Bob want to compute :

$$f : \{0,1\}^m \times \{0,1\}^n \to \{0,1\} : (x,y) \to f(x,y)$$

While minimizing the nb of bits exchanged (i.e. communication complexity (CC)).
Nondeterministic comm. complex. of f (NCC): CC of f with oracle/ message before starting the communication.
The communication matrix $X \in \{0,1\}^{2^n \times 2^m}$ is equal to the function f for all possible combinations of inputs.

Theorem (Yannakis)

$$\textit{NCC of } f \leq \log_2(\textit{rank}_+(X))$$

Linear Optimization : Extended formulation

$$
\begin{aligned}
\text{(LP)}\max \quad & c^T x \\
s.t. \quad & Ax \leq b \\
& x \in \mathbb{R}^n \geq 0
\end{aligned}
$$

Definition (Extended formulation)

The extended formulation of a polytope P is a higher dimensional polytope Q and a linear projection π s.t. $\pi(Q) = P$.

In our LP problem, an extended formulation of the polytope $P \subset \mathbb{R}^n$ defined by the constraints $Ax \leq b$, is a polytope $Q \subset \mathbb{R}^{n+r}$ defined by $Cx + Dy \leq d$ with $y \in \mathbb{R}^r$, s.t. $\pi(Q) = P$.

The slack matrix $X(i,j) = b_i - A_i v_j$.
With v_j, the j^{th} vertex of P and $\{x \in \mathbb{R}^n | b_i - A_i x \geq 0\}$ its i^{th} facet.
The (i,j) entry measures the slack of the i^{th} inequality for the vertex j.

Theorem (Yannakis)

The minimum size of an extended formulation Q of P is equal to rank$_+(X)$.