The Why and How of Nonnegative Matrix Factorization

Group 2

In a few words

NMF is a powerful tool for the analysis of **high-dimensional** data as it automatically extracts **sparse** and **meaningful** features from a set of **nonnegative** vectors. NMF was introduced by Paatero and Tapper in 1994 and further developped by Lee and Seung in 1999.

Nonnegative Matrix Factorization : definition and properties

Nonnegative matrix factorization (NMF) is a Linear dimensionality reduction (LDR). As a reminder, a LDR computes a set of $r < min(p, n)$ basis elements $w_k \in R^p$ for $1 \leq k \leq r$ to approximate a set of data points $x_j \in R^p$ for $1 \leq j \leq n$ such that $\forall j, x_j \approx \sum_{k=1}^{r} w_k h_j(k)$, for some weights $h_j \in R^r$.
LDR is equivalent to low-rank matrix approximation where: $X \approx WH$ where

- $X \in R^{p \times n}$: $X(:, j) = x_j$ for $1 \leq j \leq n$. Each column of the matrix X is a data point.
- $W \in R^{p \times r}$: $W(:, k) = w_k$ for $1 \leq k \leq r$. Each column of the matrix W is a basis element.
- $H \in R^{r \times n}$: $H(:, j) = h_j$ for $1 \leq j \leq n$. Each column of the matrix H gives the coordinates of a data point X(:,j) in the basis W.

NMF : decomposing a given nonnegative data matrix X as $X \approx WH$ where $W \geq 0$ and $H \geq 0$. W and H are thus component-wise nonnegative.

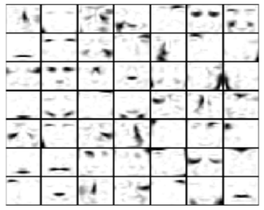
Applications

Image processing

Goal: facial feature extraction
The **data matrix** $X \in_{+}^{p \times n}$ carries information about n face images. Each image has q pixels and therefore each column of X represents an image of a face.
$\rightarrow$ The (i, j)th entry of X represents the gray-level of the ith pixel in the jth face.
The **nonnegative matrix factorization** can be interpreted as follows:

- Each column of the matrix W represents a facial feature
- The (k, j)th entry of H represents the importance of the kth feature in the jth face

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

Text Mining

Goal: topic recovery and document classification
The **data matrix** $X \in_{+}^{n \times n}$ encodes the frequency of some words in a list of documents.
$\rightarrow$ The (i, j)th entry of X represents the number of times the ith word appears in the jth document.
The **nonnegative matrix factorization** can be interpreted as follows:

- Each colum of the matrix W represents a topic
- The (k, j)th entry of H represents the importance of the kth topic in the jth document

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

Algorithms and Difficulties

Optimization Problem

We want to solve $\min_{W \in \mathbb{R}^{p \times r}, H \in \mathbb{R}^{r \times n}} \|X - WH\|_F^2$, such that $W \geqslant 0$, $H \geqslant 0$. Our use of the Frobenius norm implies the assumption that the noise is Gaussian. This is not always the best choice; in practice, depending on the application, other choices are possible too, such as:

- Kullback–Leibler divergence used in text mining;
- Itakura–Saito distance used in music analysis;
- ℓ_1 norm used to improve robustness against outliers;
- etc.

Difficulties

NMF is not a trivial task:

- NMF is **NP-hard**, but in practice, this is rarely problematic.
- NMF is **ill-posed**: if (W, H) is an NMF of X, then so is $(W', H') = (WQ, Q^{-1}H)$, where $WQ \geqslant 0$, $Q^{-1}H \geqslant 0$. This can be solved by
  - using **priors** for W and H, such as sparsity;
  - adding **regularization** terms.

Finding application-specific solutions is an active area of research.

Connections to other problems

In this section, we will present several connections between the NMF and other mathematical problems. But first, let us introduce the 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 $X = WH$.

Intuitively, the columns of X can be seen as vectors that we want to generate from a basis formed by the columns of W. We want our basis to have as few vectors as possible.

Graph theory : Bipartite dimension

finding the bipartite dimension of a graph gives a lower bound for the nonnegative rank. Indeed, let $G(X) = (V_1 \cup V_2, E)$ be a bipartite graph induced by X (i.e. $(i, j) \in E \Leftrightarrow X_{ij} \neq 0$).
The **bipartite dimension** (or the minimum biclique cover) $bc(G(X))$ is the minimum number of bicliques needed to cover all edges in E.
The rectangle covering bound :

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

Communication complexity

We talk about communication complexity when Alice knows only $x \in \{0,1\}^m$, Bob knows only $y \in \{0,1\}^n$ and both want to compute a common function

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

While minimizing their number of bits exchanged (i.e. communication complexity).
For the nondeterministic communication complexity of f (NCC), it is also the minimum number of communications required but Alice and Bob receive a message (oracle) before they start communicating.
We define the communication matrix $X \in \{0,1\}^{2^m \times 2^m}$ as a matrix containing the values of the function f for all possible combinations of inputs.
We, then, obtain a higher bound on the NCC of f

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

Linear Optimization : Extended Formulation

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

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

Finding the minimum size of an extended formulation of the polytope defined by the constrains amounts to calculating the nonnegative rank of 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 reason why it is interesting to find an extended formulation is that it allows to solve the (LP) in polynomial time.

Computational Geometry : Nested polytopes

In computational geometry, the nested polytopes problem is closely linked to the nonnegative rank.

Conclusion

TO DO

References