Non-negative Matrix Factorization and its Applications

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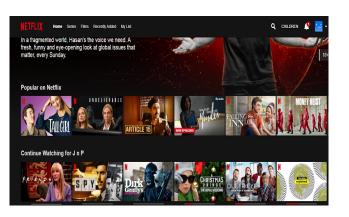
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- How?
- Linear Algebra.
 That's how!

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Toy Example

Let's construct a toy example which would help us understand *NMF* better.

Suppose we have the following data of ratings by certain users for certain TV shows. The ratings are on a scale of 1-5. A '0' entry denotes that the rating is not available.

Х	F.R.I.E.N.D.S	TBBT	Black Mirror	Modern Family	Sacred Games	GoT	Quantico
Jai	4.8	4.7	0	4.6	0	0	2.1
PB	4	4.1	4.8	0	4.9	4.7	1.5
Arnab	0	3.5	4	0	0	4.6	2.5
Abhi	4.9	4	0	0	0	4.4	0
Diya	2.1	4.4	4.7	0	0	4.9	0

Question: Based on this data, for a given TV show, can we predict the rating of a user who hasn't rated it yet? Thereby, create a scheme of recommending shows to users which they haven't watched yet.

Toy Example

Let X be a matrix whose rows correspond to the TV shows and columns correspond to the users in the given data.

$$X = \begin{bmatrix} 4.8 & 4 & 0 & 4.9 & 2.1 \\ 4.7 & 4.1 & 3.5 & 4 & 4.4 \\ 0 & 4.8 & 4 & 0 & 4.7 \\ 4.6 & 0 & 0 & 0 & 0 \\ 0 & 4.9 & 0 & 0 & 0 \\ 0 & 4.7 & 4.6 & 4.4 & 4.9 \\ 2.1 & 1.5 & 2.5 & 0 & 0 \end{bmatrix}$$

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- Let $A \in \mathbb{R}^{m \times n}$. Then it 'might' admit various decompositions such as LU, Cholesky, QR, Spectral, SVD etc...
- NMF is one such factorization with some caveats.
- As the name suggests, both A and its factors must be non-negative i.e. each of their entries must be non-negative.

Formal Definition

Definition

Let $X \in \mathbb{R}^{m \times n}$ and $X \ge 0$ (i.e. $\forall i, j; x_{ij} \ge 0$). It is said to admit *NMF* if $\exists \ 0 \le W \in \mathbb{R}^{m \times r}, 0 \le H \in \mathbb{R}^{r \times n}$, for some $r < \min(m, n)$, such that

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- The smallest r for which it is possible is called as the non-negative rank, say r^+ .
- r^+ is the smallest number such that the matrix can decomposed into a sum of non-negative rank-1 matrices.
- For our purpose, we interpret *X* to be a data matrix whose rows represent features, and columns represent observations.

Low Rank Approximation

- Given a choice of r, finding the exact NMF for a non-negative matrix has been shown to be infeasible.
- Therefore, we try to find the nearest factorization, in some sense, by numerically solving the following optimization problem.

$$(W^*, H^*) = \arg \min_{W \ge 0, H \ge 0} \|X - WH\|$$

- The minimization could be w.r.t. any norm that is appropriate for the particular application.
- Note that *NMF* is posed as a *constrained low rank approximation* problem. This indicates that it could be used for dimensionality reduction in data with non-negative values.

Closer look at NMF

- Suppose $V = [v_1, v_2, \dots, v_n] = WH$ where $W = [w_1, w_2, \dots, w_r]$ and $H = [h_1, h_2, \dots, h_n]$.
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- Then, it's clear that $v_i = Wh_i$ for $i = 1, 2, \dots, n$.
- Thus, in NMF the columns of the transformed matrix (the approximation) is the non-negative linear combinations of the columns of W.
- Therefore, the columns of W represent a set of basis functions for the transformed data, and H contains some sort of encoding.

Geometric View

- Since each of our observations x_i , the i^{th} column of X, is non-negative, it follows that our data lies in the non-negative orthant of \mathbb{R}^m which is a cone.
- Through *NMF* we essentially say that these data points actually lies in lower dimensional cone generated by $\{w_1, \dots, w_r\}$.
- However, the factors obtained in NMF is not unique, in general.
 Thus, every time we run the algorithm, we might end up with a different lower dimensional cone. Nevertheless, a unique solution for NMF does exist under certain regularity conditions.

NMF for the Toy Example

- Although, we have 7 TV shows (features) in our data, they seem to belong to two categories viz. thrillers and sitcoms. Therefore, we can choose r to be 2.
- On running an NMF algorithm, we obtained the following factors.

$$W = \begin{bmatrix} 0.971 & 1.929 \\ 1.699 & 1.626 \\ 1.872 & 0. \\ 0. & 1.317 \\ 0.77 & 0. \\ 2.219 & 0.232 \\ 0.452 & 0.543 \end{bmatrix} \qquad H = \begin{bmatrix} 0. & 2.53 & 1.898 & 1.09 & 2.217 \\ 2.853 & 0.312 & 0. & 1.314 & 0.045 \end{bmatrix}$$

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- On the other hand, looking from the perspective of columns (the new basis vectors), each entry corresponds to the contribution of the corresponding show to the respective column.
- Black Mirror and Sacred Games contribute nothing, based on this data, to the sitcom category. Good job, NMF!

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- Through this natural interpretation of the results, Linear Algebra, and hence math itself, has established its supremacy again.
- The interpretation made in this TV show-users setting can be naturally extended to any other setting where NMF can be employed.

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- In the dense matrix W each of the features are essentially points in \mathbb{R}^r .
- If the rating of user j for the item i is not available, it's estimated as the weighted average of the ratings of some number of nearest neighbors by the user i.

The similarity matrix for the shows in our example is as below:

$$S = \begin{bmatrix} 1. & 0.942 & 0.45 & 0.893 & 0.45 & 0.54 & 0.9747 \\ 0.942 & 1. & 0.722 & 0.691 & 0.722 & 0.79 & 0.994 \\ 0.45 & 0.722 & 1. & 0. & 1. & 0.995 & 0.64 \\ 0.893 & 0.691 & 0. & 1. & 0. & 0.104 & 0.769 \\ 0.45 & 0.722 & 1. & 0. & 1. & 0.995 & 0.64 \\ 0.54 & 0.79 & 0.995 & 0.104 & 0.995 & 1. & 0.716 \\ 0.974 & 0.994 & 0.64 & 0.769 & 0.64 & 0.716 & 1. \end{bmatrix}$$

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- The estimated rating is then 1.175. Thus, Black Mirror wouldn't be recommended to me. Right on point!

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- For instance, we didn't normalize each row of X in which case the average rating would be 0. Had we done that, how do we represent an unavailable rating?
- If we leave that cell empty, then NMF algorithm would crash!
- Non-uniqueness of this approximation might also cause some troubles.
 However, in most cases, the local optima obtained has proved to be effective in applications.
- Nevertheless, NMF was formerly used by big names like Netflix, Amazon etc... The present technology involves a low rank matrix completion problem.

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- Question: Given a large unstructured collection of documents, can we identify the hidden patterns in them and there-by group them?
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- Applications involve spam filtering, sentiment analysis, tagging content/genre classification etc...

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- We know that the entries of H indicate the extent to which a document belongs to a category.
- Therefore, a document j will be classified as the category-k if $h_k j$ is the largest entry in column h_j .

- As an example we shall look at the topic extraction example of a dataset in sklearn.datatsets of documents from 20 different news groups. The code can be found at the website of scikit_learn.
- This data has 2000 documents with 1000 features. We try to group them into 10 clusters based on the topics they deal with.

Application 3: Image Processing

- Image processing typically entails dimensionality reduction (decomposition into components), object classification, facial recognition etc...
- The data matrix X is typically a pixel by image matrix. Each column has the pixes values of the corresponding image.
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- Yes! We know that NMF is capable of doing this!

Application 4: Bioinformatics

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- X would be an expression level by gene matrix. Then H would be a metagene (the representative genes of various classes or sub-classes of cancer) by gene matrix.
- In a way similar to document classification, we can identify the correspondence of a particular gene with a particular class/subclass of cancer.