Nonnegative Matrix Factorization

Be Positive!

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NMF

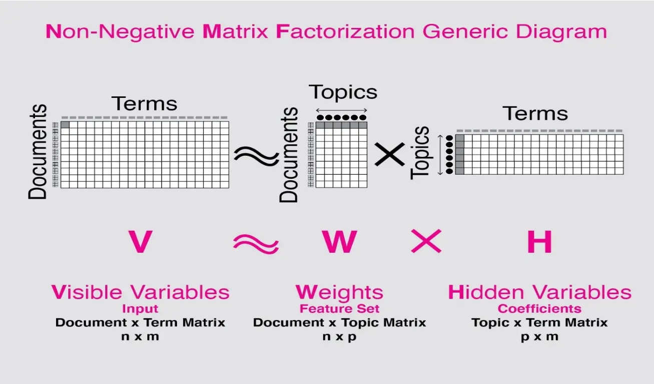
Problem

Given $A \in \mathbb{R}_{+}^{m \times n}$ non-negative and *rank* $r \leq \min(m, n)$.
Find $W \in \mathbb{R}_{+}^{m \times r}$ and $H \in \mathbb{R}_{+}^{r \times n}$ both non-negative s.t.:

$$A \approx WH$$

Text Mining

"Words which are similar in meaning occur in similar contexts"



Source: "NMF — A visual explainer and Python Implementation", Anupama Garla

Image Processing

Given vectorized gray-levels $X \in \mathbb{R}_+^{p \times n}$ of n facial images.

Problem: Facial Feature Extraction

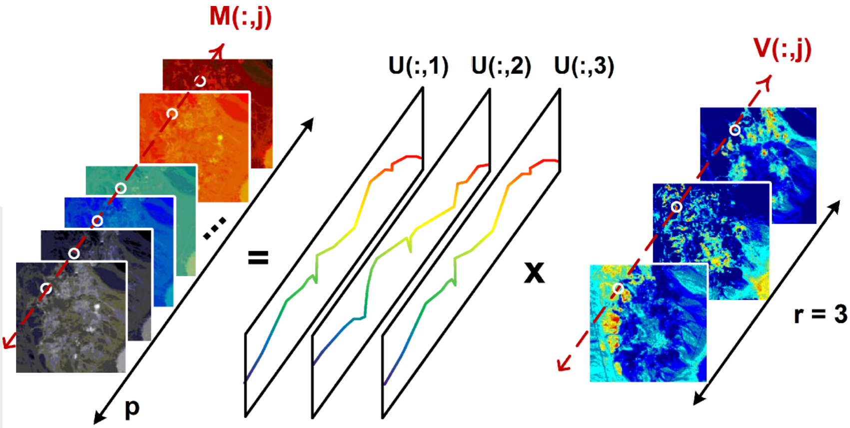
$X(:,j) \approx$	$\sum_{k=1}^{r} W(:,k)$	$H(k,j)$
j-th facial image	facial features	importance of feature in j-th image

Hyperspectral Unmixing

Given vectorized spectral signature $X \in \mathbb{R}_+^{p \times n}$ of an image.
Problem: Identify Endmembers (Grass, Stone,...)

$X(:,j) \approx$	$\sum_{k=1}^{r} W(:,k)$	$H(k,j)$
spectral signature	spectral signature of k-th endmember	abundance of k-th endmember

Hyperspectral Unmixing



Source: "Introduction to Nonnegative Matrix Factorization", Nicolas Gillis

Problem Reformulation

Optimization Problem

Given $A \in \mathbb{R}_+^{m\times n}$ non-negative and *rank* $r \leq \min(m, n)$.

$$\min_{W\in\mathbb{R}_+^{m\times r},\, H\in\mathbb{R}_+^{r\times n}} \quad \|A - WH\|_F^2$$

Note that $F(W, H) = \|A - WH\|_F^2$ is convex in U and convex in V, but not in both!

Stationary Points & KKT-Conditions

Checking the KKT-Conditions for $F(W, H)$ yields the following:

$$W \geq 0,\ \nabla_W F = WHH^T - AH^T \geq 0,\ \nabla_W F * W = 0$$

$$H \geq 0,\ \nabla_W F = W^T WH - W^T A \geq 0,\ \nabla_H F * H = 0$$

Stationary Points

A pair (U, V) is called a *stationary Point*, if and only if U and V satisfy the KKT-Conditions.

Stationary Points & KKT-Conditions

From the KKT-Conditions simple characteristics of the solutions can be derived:

Theorem

Suppose (W, H) be a stationary point of the problem, then it holds:

$$\frac{1}{2}\|A - WH\|^2 = \frac{1}{2}(\|A\|^2 - \|WH\|^2)$$

This furthermore implies that $\|A\|^2 \geq \|WH\|^2$, with equality attained only at the exact factoriztion.

Coordinate Descent

For Ω (pointwise) convex

$$\textit{solve} \ \min_{x \in \Omega} f(x)$$

Initialization: $x \in \mathbb{R}^n$

for $t \leftarrow 1, 2, ..., n$ **do**

$\quad \textit{solve} \ x_i = \arg\min_{\zeta \in \Omega_i} f(x_1, ..., x_{i-1}, \zeta, x_{i+1}, ..., x_n)$

end

Algorithm 1: General Coordinate Descent

"Convergence" Theorem

"Convergence" to stationary Points

Suppose f is continuously differentiable and furthermore that

$$\forall i \, \forall x : \min_{\zeta \in \Omega_i} f(x_1, \ldots, x_{i-1}, \zeta, x_{i+1}, \ldots, x_n)$$

is uniquely attained. Let $\{x^k\}$ be the sequence generated by the *Coordinate Descent*, then every limit point is a stationary point.

Exact Factorization

Now consider the case where A is exactly factorized by WH.

minimal rank

The smallest r such that exist $W \in \mathbb{R}_{+}^{m \times r}$ *and* $H \in \mathbb{R}_{+}^{r \times n}$ such that $A = WH$, is called the *inner rank* and denoted by $rank_{WH}^{+}(A)$.

Determining the inner rank

One algorithm to determine if A can be factorized with *inner rank* r would be the Renegar algorithm, which scales $(6mn)^{\mathcal{O}(mn)}$.
Since $rank^{+}_{WH}(A) \leq \min(m, n)$ this can be done in finite time.

Vavasis, 2008

- exact *NMF* is *NP-hard*
- $\exists$ polynomial time local search heuristics

Algorithms for NMF

The Multiplicative Update Rule

$$\min_{W,H>0} f(W,H) = \min_{W,H>0} \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{m} (A_{ij} - (WH)_{ij})^2 \tag{1}$$

The most used approach to minimize (1) is a simple multiplicative update method proposed by Lee and Seung (2001):
This algorithm is just a special case of Gradient Descent with a step size

$$\epsilon(W^t) = \frac{W^t}{W^t H^t (H^t)^T}$$

$$\epsilon(H^t) = \frac{H^t}{(W^t)^T W^t H^t}$$

The Multiplicative Update Rule

Initialization: $W^1, H^1 > 0$;

for $t \leftarrow 1, 2.. \ldots$ **do**

$$W^{t+1} = W^t \frac{A(H^t)^T}{W^t H^t (H^t)^T};$$

$$H^{t+1} = H^t \frac{(W^{t+1})^T A}{(W^{t+1})^T W^{t+1} H^t};$$

end

Algorithm 2: MUR Algorithm

The Multiplicative Update Rule

This algorithm is a type of fixed-point method, meaning that if $(H^t)^T H^t W^t \neq 0$ and $W^{t+1} = W^t$, then $A(H^t)^T = W^t H^t (H^t)^T$ implies $\nabla_W f(W^t, H^t) = 0$, which is part of the KKT condition.

"Convergence" Theorem

Theorem Lee and Seung

-The Euclidean distance $||A - WH||$ is non-increasing under the update rules

$$W \leftarrow W \frac{AH^T}{WHH^T}, \qquad H \leftarrow H \frac{W^T A}{W^T WH}$$

-The Euclidean distance is invariant under these updates if and only if W and H are at a stationary point of the distance.

Weaknesses

- Lee and Seung claim that this algorithm "converges" to a stationary point. However, it has been shown in 2005 that this claim is wrong, as having the cost function non-increasing may not imply convergence.

- Therefore, the algorithm still lacks optimization properties.

Weaknesses

- We can only make the following statement about the convergence of these algorithms: "When the algorithm has converged to a limit point, this point is a stationary point."

- Also it has been repeatedly shown that the convergence is notoriously slow.

Modifications: Convergence vs. speed trade-off

- Lin in 2007 proposed a modification that is guaranteed to converge to a stationary point. However, it requires more work per iteration so it is even slower.

- The Fast Multiplicative Update Rule Algorithm from 2014 is faster than the two algorithms in the case of convergence.

Comparison of the the three Algorithms

	MU Algorithm	Updated MU	Fast MU
initial values in case I			
CPUTime(s)	110.14	129.80	**106.60**
Iteration	2730.37	2978.53	**776.80**
OBJ.ave	149450.1	149354.3	**148681.0**
OBJ.std	35.39	43.57	**27.79**
initial values in case II			
CPUTime(s)	91.66	130.12	**88.18**
Iteration	2518.97	3330.40	**741.97**
OBJ.ave	149914.2	149290.5	**148639.6**
OBJ.std	34.86	48.45	**22.33**

Source: "A Fast Algorithm for Non-negative Matrix Factorization and Its Convergence", Li, Wu, and Zhang

Alternating Non-negative Least Squares (ANLS)

- In this algorithms, a least squares step is followed by another least squares step in an alternating fashion, thus giving rise to the ALS name.
- The Alternating Least Squares - ALS algorithms were first introduced by Paatero 1994 , who initially invented the whole NMF Theory.

Initialization: $W > 0$;

for $t \leftarrow 1, 2 \ldots$ **do**

Solve for H the LS equation $W^T WH = W^T A$;

Set all negative elements in H to 0;

Solve for W the LS equation $WHH^T = AH^T$;

Set all negative elements in W to 0;

end

Algorithm 3: Basic ALS for NMF

Convergence Theorem

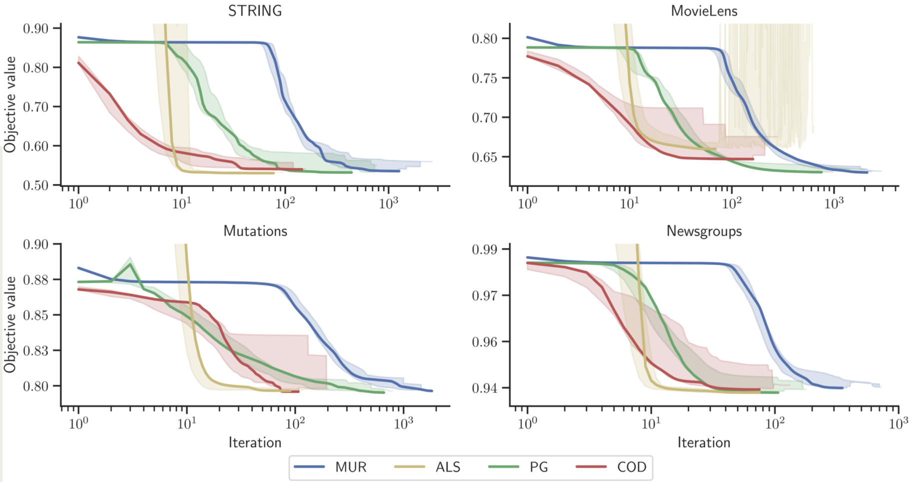
Theorem

Any limit point of the sequence $\{W^t, H^t\}$ *generated by ALS Algorithm is a stationary point.*

Comparison between ANLS and MU

ANLS	MU
+ Can be very fast depending on the implementation + Aids sparsity	+ Easy to use
- Once an element in W or H becomes 0, it must remain 0.	- Notoriously slow - Lacks optimization properties.

Comparison between ANLS and MU



Source: "Fast optimization of non-negative matrix tri-factorization", Zupan, Zitnik

References I

- Michael W. Berry, Murray Browne, Amy N. Langville, V. Paul Pauca, and Robert J. Plemmons.
  Algorithms and applications for approximate nonnegative matrix factorization.
  Computational Statistics Data Analysis, 52(1):155–173, 2007.
- Nicolas Gillis.
  The why and how of nonnegative matrix factorization.
  Regularization, Optimization, Kernels, and Support Vector Machines, 12, 01 2014.
- Nicolas Gillis.
  Introduction to nonnegative matrix factorization.
  03 2017.

References II

- Ngoc-Diep Ho.
  Nonnegative matrix factorization algorithms and applications.
  PhD thesis, 06 2008.
- Li-Xin Li, Lin Wu, Hui-Sheng Zhang, and Fang-Xiang Wu.
  A fast algorithm for nonnegative matrix factorization and its convergence.
  IEEE Transactions on Neural Networks and Learning Systems, 25(10):1855–1863, 2014.
- Stephen A. Vavasis.
  On the complexity of nonnegative matrix factorization.
  SIAM Journal on Optimization, 20(3):1364–1377, 2010.