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"

CHATGPT

picture

Visible Variables = Weights * Hidden Variables

Image Processing

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

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

Problem v2

Optimization Problem

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

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

Note that $F(W, H) = \|A - WH\|$ 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 $\|A\|^2 \geq \|WH\|^2$, which is only fulfilled at the exact factorization.

Coordinate Descent

For Ω (pointwise) convex

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

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

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

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

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^T.

minimal rank

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

Exact Factorization

Lemma

$$rank(A) \leq rank^{+}_{WH}(A) \leq \min(m, n)$$

existence of exact factorization of A of rank $r \iff$ determining $rank^{+}_{WH}(A)$

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 the 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 fixed-point type 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

$$W \leftarrow W \frac{(AH^t)}{[WH(H)^T]}, \qquad H \leftarrow H \frac{(W^T A)}{[(W)^T WH]}$$

-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 showed in 2005 that this claim is wrong as having the cost function non increasing may not imply the convergence.

- Therefore, the Algorithm still lacks optimization properties.

Weaknesses

- We can only make the following statement about the convergence of this 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 than the already slow one.

- The Fast Multiplicative Update Rule Algorithm in 2014. Which is faster then 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

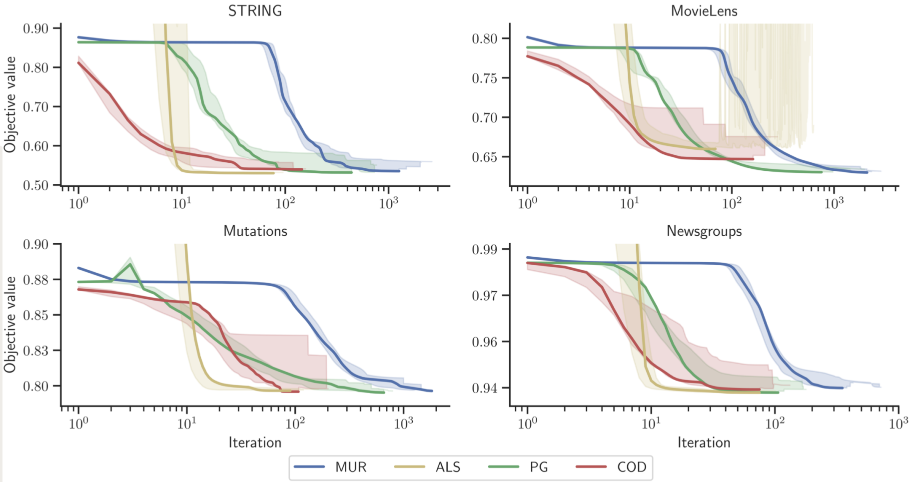
Theorem

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