# SIMPLICIAL CONE SHRINKING ALGORITHM FOR UNMIXING NONNEGATIVE SOURCES

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**ABSTRACT**

We consider a geometrical approach for solving the Nonnegative Blind Source Separation (N-BSS) problem in the case of noiseless linear instantaneous mixture model. When the sources are nonnegative, the scatter plot of the mixed data is contained in the simplicial cone generated by the mixing matrix. The proposed method, called Simplicial Cone Shrinking Algorithm for Unmixing Nonnegative Sources (SCSA-UNS), estimates the mixing matrix and the sources by finding the Minimum Volume (MV) simplicial cone containing all the mixed data. Simulations on synthetic data shows the efficiency of the proposed method.

***Index Terms*—** Blind Source Separation, Nonnegativity, Simplicial Cone, Minimum Volume, Facet

## 1. INTRODUCTION

Nonnegative Blind Source Separation (N-BSS) receives a great attention this last decade because it applies to many problems in signal and image processing. This paper considers the task of solving the N-BSS problem in the case of the noiseless linear intantaneous mixture model. Let $S$, $A$ and $X$ be respectively the sources, mixing and observations matrices. If $n$, $m$ and $p$ are the number of sources, observations and samples, the batch mixture model is given by:

$$\underset{m\times p}{X} = \underset{m\times n}{A}\,\underset{n\times p}{S} \tag{1}$$

The task of N-BSS is retrieving the hidden nonnegative sources $S$ and the unknown mixing matrix $A$ given only the observations $X$ without any prior knowledge on $S$ and $A$ except the nonnegativity of $S$.

Many methods were proposed for solving problem (1). The most popular approach is Nonnegative Matrix Factorization (NMF)[1] where the sources $S$ and the mixing matrix $A$ are estimated by minimizing a divergence measure between the left and right parts of equation (1) under nonnegativity constraints on both $A$ and $S$. But NMF techniques still suffer of non-uniqueness of the solution. For solving problem (1), Plumbley proposes Nonnegative Independent Component Analysis (N-ICA), this method however requires the nonnegative sources to be "independent" and "well-grounded" [2].

By adopting a statistical framework, another approach uses a Bayesian inference for solving N-BSS problem [3]. This kind of methods can unfortunately be computationally complex and time-consuming especially for large scale data.

Geometrical methods have also been proposed for solving problem (1). In this case, the mixing matrix is estimated by looking for the vertices of the convex hull of the mixed data [4][5] or by looking for the Minimum Volume (MV) simplicial cone containing the cloud of mixed data [6][7].

This paper proposes a new geometrical method for solving N-BSS problem. The proposed method, called Simplicial Cone Shrinking Algorithm for Unmixing Nonnegative Sources (SCSA-UNS), estimates the mixing matrix and the sources by finding the MV simplicial cone containing all the mixed data. In the next section we summarize the main idea of MV like methods for N-BSS problem. Section 3 describes the proposed SCSA-UNS method. In section 4, we show simulations on synthetic data to illustrate the efficiency of the proposed method. Finaly section 5 presents the conclusions and future works.

## 2. MINIMUM VOLUME LIKE METHODS FOR NONNEGATIVE BLIND SOURCE SEPARATION

We restrict this study to the case where $S$ and $A$ are all nonnegative. We also assume that $m = n$ and that the mixing matrix is full column rank. For a given nonnegative matrix $W = [w_1, w_2, \cdots, w_n]$, we define:

The ***simplicial cone*** $Span^+(W)$ generated by a given matrix $W$ by:

$$Span^+(W) = \left\{ z \,\middle|\, z = Wy \text{ with } y \in \mathbb{R}_+^n \right\} \tag{2}$$

One may note that the ***positive orthant*** $\mathbb{R}_+^n$, is the simplicial cone generated by the identity matrix:

$$\mathbb{R}_+^n = Span^+(I_n) \tag{3}$$

Considering each column $x_i$ of $X$ ($1 \leq i \leq p$) as a point in the $n$ dimension data space, it comes that when the sources are nonnegative, the scatter plot of the mixed data is contained in the simplicial cone generated by the mixing matrix.

$$\{x_i, x_i \in X, 1 \leq i \leq p\} \subseteq Span^+(A) \tag{4}$$

If the mixing matrix is also nonnegative, the cloud of mixed data points is located in the positive orthant.

$$\{x_i, x_i \in X, 1 \leq i \leq p\} \subseteq Span^+(A) \subseteq Span^+(I_n) \tag{5}$$

Fig 1. illustrates the scatter plot of the mixed data included in $Span^+(A)$ for $n = 3$.

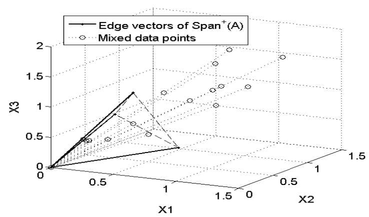


**Fig. 1**. Mixed data included in $Span^+(A)$ for $n = 3$

Assuming that $\{x_i, x_i \in X, 1 \leq i \leq p\}$ "***fill enough***" $Span^+(A)$, the MV like methods aim at estimating the mixing matrix (up to positive scaling and permutation indetermities) by fitting a simplicial cone to the cloud of mixed data points [6][7]. Filling enough mean that $Span^+(A)$ must be well recognizable from the cloud of mixed data (i.e. there should be at least $n-1$ observation points on each ***facet*** of $Span^+(A)$ [8]). On the one hand, we may note that the ***local dominance of the sources*** (i.e. for every source there is at least one instance where the underlined source is active and all the others are not), generally needed in certain geometrical methods [4][5] is not required for MV like methods. This strength condition is replaced by the weaker one "filling enough". On the other hand, it's necessary to specify that beside the nonnegativity, some minimum volume like methods [6][7] require the ***full additivity of the sources*** (i.e. the sum on every column of the sources matrix is equal to one) when SCSA-UNS does not.

## 3. SIMPLICIAL CONE SHRINKING ALGORITHM FOR UNMIXING NON-NEGATIVE SOURCES

### 3.1. Principle of the proposed method

The proposed SCSA-UNS method aims at recovering the mixing matrix by finding the minimum volume simplicial cone containing all the mixed data. In this objective, we define the volume of a given simplicial cone $Span^+(W)$ (generated by a given square matrix $W = [w_1, w_2, \cdots, w_n]$) by :

$$V(W) = \frac{|\det(W)|}{\|w_1\|_2 \times \|w_2\|_2 \times \cdots \times \|w_n\|_2} \tag{6}$$

$0 \leq V(W) \leq 1$ for any square matrix $W$ (Hadamard's inequality) and for nonnegative $W$, $V(W) = 1$ iff $W$ is a monomial matrix. $V(W)$ strictly represents the "aperture" of the simplicial cone generated by $\left[\frac{w_1}{\|w_1\|_2}, \frac{w_2}{\|w_2\|_2}, \cdots, \frac{w_n}{\|w_n\|_2}\right]$. The problem of finding the minimum volume simplicial cone containing the observations and contained in the positive orthant can be written as the following optimization:

$$W^* = \underset{W \geq 0,\ W^{-1}X \geq 0}{\arg\min} \quad V(W) \tag{7}$$

**NB**: For a given matrix $M$, $M \geq 0 \Longleftrightarrow M_{ij} \geq 0 \; \forall \, i, j$.
For solving (7), we define the $R_k$ like matrix (size $n \times n$) by:

$$R_k = \begin{pmatrix} 1 & 0 & \cdots & 0 & r_{1k} & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & r_{2k} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & \cdots & 1 & r_{k-1k} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & r_{k+1k} & 1 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & r_{nk} & 0 & \cdots & 1 \end{pmatrix} \tag{8}$$

where $r_{kk} = 1$ and $r_{ik} \geq 0, \; \forall \, 1 \leq i \leq n, i \neq k$.

**Proposition 1.** *For a given nonnegative matrix $W$, $V(W)$ decreases when $W$ is multiplied to the right by $R_k$ like matrix.*

The proof of Proposition 1. is omitted due to lack of space.

For estimating the mixing matrix (i.e. solving (7)), SCSA-UNS starts with the initial matrix $W = I_n$ and iteratively decreases $V(W)$ by multiplying to the right $W$ by several sets of $R_k$ matrices ($1 \leq k \leq n$) until $Span^+(W)$ fits the simplicial cone generated by the scatter plot of the mixed data. The obtained solution $W^*$ is the estimated mixing matrix $A = W^*$ and the sources are then estimated by $S = A^{-1}X$.

### 3.2. Computing the $R_k$ matrices for SCSA-UNS

Let $W \geq 0$ and $Y = W^{-1}X \geq 0$ the current estimations of $A$ and $S$ ($X = WY$). For fixed $k$ between 1 and $n$, we look for $R_k$ so that $U = WR_k$ verify:

1. $U \geq 0$
2. $V(U) \leq V(W)$
3. $Z = U^{-1}X \geq 0$

Conditions 1. and 2. are automatically satisfied because $W$ and $R_k$ are all nonnegative and due to Proposition 1.
The expression of $Z$ leads to $Z = R_k^{-1}W^{-1}X = R_k^{-1}Y$.

Now according to the definition of $R_k$ given by (8), we get:

$$R_k^{-1} = \begin{pmatrix} 1 & \cdots & 0 & -r_{1k} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & \cdots & 1 & -r_{k-1k} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & -r_{k+1k} & 1 & \cdots & 0 \\ \vdots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & -r_{nk} & 0 & \cdots & 1 \end{pmatrix} \quad (9)$$

so $[Z]_{ij} = [Y]_{ij} - r_{ik}[Y]_{kj}, \forall\, 1 \leq i \leq n, \forall\, 1 \leq j \leq p$.
For fixed $i$, $[Z]_{ij} \geq 0 \Longleftrightarrow r_{ik} \leq \frac{[Y]_{ij}}{[Y]_{kj}}$, $\forall\, 1 \leq j \leq p$.
Therefore, a matrix $R_k$ also verifying condition 3., can be computed by taking $r_{kk} = 1$ and for $i \neq k$

$$r_{ik} = \min_{1 \leq j \leq p} \frac{[Y]_{ij}}{[Y]_{kj}}, [Y]_{kj} \neq 0 \quad (10)$$

### 3.3. Freezing situation and proposed unfreezing method

The SCSA-UNS algorithm stops when $V(W)$ does not decrease anymore during the iterations. This often corresponds to the convergence of $W$ to the truth mixing matrix $A$. However it may happen that $V(W)$ does not decrease anymore during the iterations while $W$ has not converged yet to $A$. In fact, given $W \geq 0$ and $Y = W^{-1}X \geq 0$, lets $U = WR_k$. $V(U) = V(W) \Leftrightarrow R_k = I_n \Leftrightarrow r_{ik} = \delta_{ik}$.
According to (10), for $i \neq k$, $r_{ik} = 0 \Rightarrow \exists\, 1 \leq j \leq p$ so that $[Y]_{ij} = 0$. The freezing arises when the SCSA-UNS algorithm finds $R_k = I_n$, $\forall\, 1 \leq k \leq n$. This situation meets when $\forall\, 1 \leq i \leq n, \exists\, 1 \leq j \leq p, [Y]_{ij} = 0$.
To overcome this problem, we introduce the unfreezing matrix $Q$ as follows: $X = WQ^{-1}QY = HT$ where $H = WQ^{-1}$ and $T = QY$. We compute an orthogonal matrix $Q$ to eliminate the zeros values of $Y$ without modifying $|\det(W)|$.

1. $T > 0$ (i.e. $T_{ij} > 0, \forall\, 1 \leq i \leq n, \forall\, 1 \leq j \leq p$)
2. $Q^TQ = I_n \;\Rightarrow |\det(H)| = |\det(W)|$

For doing so, we define the criterion $J(Q)$ by (11):

$$J(Q) = \sum_{i=1}^{n}\sum_{j=1}^{p} 1_{T_{ij}} \text{ where } 1_{T_{ij}} = \begin{cases} 1 & \text{if } T_{ij} = 0 \\ 0 & \text{elsewhere} \end{cases} \quad (11)$$

The unfreezing procedure can then be reduced to solving the following optimization problem:

$$Q^* = \arg\min_{Q^TQ = I_n} J(Q) \quad (12)$$

To deal with problem (12) in one step by gradient like method, we slightly modify the original problem by :

- Regularizing the criterion $J$ by $J_\sigma$ to avoid Dirac distributions when computing the gradient.

$$J_\sigma(Q) = \sum_{i=1}^{n}\sum_{j=1}^{p} \exp(-\frac{T_{ij}}{\sigma}),\ \sigma > 0$$

- Adding a penalty term $J_{orth}(Q) = \left\|Q^TQ - I_n\right\|_F^2$ to $J_\sigma(Q)$ to penalyze the deviation to orthogonality.

The optimization problem becomes :

$$Q^* = \arg\min_{Q} J_\sigma(Q) + \gamma J_{orth}(Q), \text{with } \gamma \geq 0 \quad (13)$$

and can be solved by the iterative gradient algorithm (14):

$$Q_{l+1} = Q_l - \mu\left[-\frac{T^{null}Y^T}{\sigma} + 4\gamma Q_l\left(Q_l^TQ_l - I_n\right)\right] \quad (14)$$

where $T_{ij}^{null} = \exp(-\frac{T_{ij}}{\sigma}) = \exp(-\frac{\sum_{t=1}^{n} Q_{it}Y_{tj}}{\sigma})$.

### 3.4. SCSA-UNS algorithm framework

**Algorithm 1** summarizes the proposed SCSA-UNS method.

**Algorithm 1** : SCSA-UNS
**Require:** $X$
1: Initialization : $W = I_n, Y = X$
2: **for** $k = 1 \rightarrow n$ **do**
3: Compute $R_k$ as describe in section 3.2
4: $W \leftarrow WR_k$ and $Y \leftarrow R_k^{-1}Y$
5: **end for**
6: **if** Freezing **then**
7: Compute $Q$ as describe in section 3.3
8: $W \leftarrow WQ^{-1}$ and $Y \leftarrow QY$
9: **end if**
10: **if** $V(W)$ minimum **then**
11: $A \leftarrow W$ and $S \leftarrow Y$
12: **return** $A$ and $S$
13: **else**
14: Back to 2
15: **end if**

## 4. SIMULATION RESULTS

Experiments are performed on synthetic data to evaluate the efficiency of the proposed method. SCSA-UNS is compared to MVSA [6] and MVES [7], others MV like methods.
Two performance measures are used for evaluation, the CPU time to convergence $T$ (using Intel(R) Core(TM) 2 Duo CPU P8400 computer) and the separation index $E_{sep}$ defined by:

$$E_{sep} = \frac{1}{n(n-1)}\left[\sum_i\left(\sum_j \frac{\left|(W^{-1}A)_{ij}\right|}{\max_l|(W^{-1}A)_{il}|} - 1\right)\right] + \frac{1}{n(n-1)}\left[\sum_j\left(\sum_i \frac{\left|(W^{-1}A)_{ij}\right|}{\max_l|(W^{-1}A)_{lj}|} - 1\right)\right]$$

$E_{sep}$ is similar to an inter-symbol interference ratio, the smaller is $E_{sep}$ the better is the separation.
The nonnegative sources matrix $S$ has been generated by the *Matlab* "sparse uniformly distributed random matrix generator" (*sprand* function). Different number of sources were considered (from 3 to 10). We set the number of samples to

$p = 5000$ and the sparsity degree to $spar = 1$ corresponding to 64% of non-zero elements in the sources matrices. The mixing matrix entries are independent and uniformly distributed between 0 and 1. In all the simulations, the parameters are fixed to $\sigma = 10^{-3}$, $\gamma = \frac{1}{4}$ and $\mu = 10^{-1}$. The unfreezing procedure is initialized by $Q_0 = I_n$.
Fig. 2. and Fig. 3. show the variation of the average perfomance index (obtained with 20 independent Monte Carlo runs) versus the number of sources in the case where the sources are full additive and where there are not. One may note (Fig. 2.) that when the sources are full additive all the three methods perform a perfect separation $\left(E_{sep} \leq 10^{-2}\right)$ but SCSA-UNS method is faster than MVSA and MVES. We may also note (Fig. 3.) that when the sources are not full additive, the SCSA-UNS method still performs a perfect separation while MVSA and MVES do not.

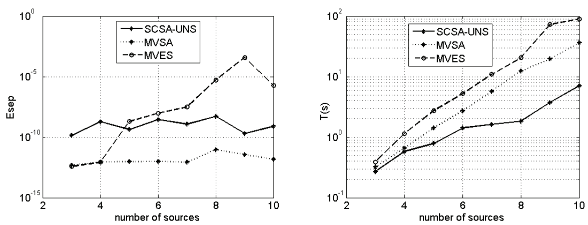


**Fig. 2**. Variation of $E_{sep}$ and $T$ for full additive sources

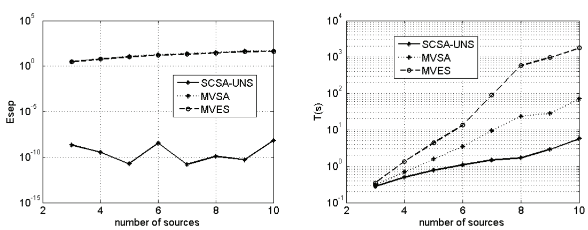


**Fig. 3**. Variation of $E_{sep}$ and $T$ for not full additive sources

Fig 4. illustrates $V(W)$ decreasing towards $V(A)$ during the iterations of SCSA-UNS for $n = 5$. This confirms that the estimated mixing matrix converges towards the real one during the iterations. The same results (not shown) are observed when varying $n$.

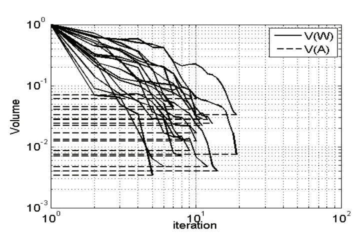


**Fig. 4**. $V(W)$ decreasing towards $V(A)$ for $n = 5$

## 5. CONCLUSIONS AND FUTURE WORKS

In this paper we propose a geometrical method for solving the Nonnegative Blind Source Separation (N-BSS) problem. Given the observations, the proposed algorithm SCSA-UNS estimates the mixing matrix and the sources by finding the minimum volume simplicial cone containing all the mixed data. SCSA-UNS does not require independence of sources, neither their local dominance, nor even their full additivity. Simulations on synthetic data shows that proposed method outperform existing Minimum Volume like methods, specially when the sources are not full additive.
As a future works, we will investigate how to relax the non-negativity constraint on the mixing matrix. Considering noisy mixtures and the case $m \neq n$ will also be a good challenge.

## 6. REFERENCES


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