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An alternating projected gradient algorithm for nonnegative matrix factorization

Lu Lin [a,*], Zhong-Yun Liu [b]

[a] School of Mathematical Sciences, Xiamen University, Xiamen 361005, PR China
[b] School of Mathematics, Changsha University of Science and Technology, Hunan 410076, PR China

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ABSTRACT

Due to the extensive applications of nonnegative matrix factorizations (NMFs) of nonnegative matrices, such as in image processing, text mining, spectral data analysis, speech processing, etc., algorithms for NMF have been studied for years. In this paper, we propose a new algorithm for NMF, which is based on an alternating projected gradient (APG) approach. In particular, no zero entries appear in denominators in our algorithm which implies no breakdown occurs, and even if some zero entries appear in numerators new updates can always be improved in our algorithm. It is shown that the effect of our algorithm is better than that of Lee and Seung's algorithm when we do numerical experiments on two known facial databases and one iris database.

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1. Introduction

For a given $n \times m$ nonnegative matrix V and a fixed integer r, the so-called nonnegative matrix factorization (NMF) of V is to find a nonnegative matrix pair (W,H) with $W \in \mathbb{R}^{n\times r}$ and $H \in \mathbb{R}^{r\times m}$ such that

$$\min_{W \geqslant 0, H \geqslant 0} (W,H),$$

where $f(W,H)$ is a cost function of W and H.

Nonnegative matrix factorizations of a nonnegative matrix play an important role in many real applications, such as in image processing [11,12], text mining [18], spectral data analysis [17], speech processing, etc. Therefore the theory and algorithms of this topic have intrigued researchers for years [8,16].

There are various definitions on cost functions for different purposes. For example, Lee and Seung [12] defined a cost function based on Frobenius norm and Kullback–Leibler divergence. Hoyer [10], Shahnaz et al. [18], Berry et al. [7], and Pauca et al. [17] defined other cost functions with additional conditions on sparseness or smoothness.

The classical algorithm for NMF is the following multiplicative updating algorithm (MU), which was proposed by Lee and Seung [11,12].

* Corresponding author.
E-mail addresses: llin@xmu.edu.cn (L. Lin), liuzhongyun@263.net (Z.-Y. Liu).

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Algorithm 1. MU Algorithm

1. $W = rand(m,r)$; $H = rand(r,n)$;
2. for $iter = 1$: $maxiter$
   $H = H \cdot * (W^T V)./(W^T W\, H)$;
   $W = W \cdot * (V\, H^T)./(W\, H\, H^T)$;
   end

Here the operations $\cdot^*$ and ./ denote the component-wise multiplications and component-wise divisions respectively.

Recently, some variants of the MU algorithm have been developed, see for instance [9,14,15,18]. However, when a zero entry appears in a denominator or in a numerator, a breakdown will occur or the updates cannot be further improved in MU-like algorithms. In this case, a small scale, e.g., eps, is artificially added to zero entries so that breakdown can be avoided, or new updates can be improved. Anyway, the flexibility of the algorithms is seriously affected.

We remark here that such a class of algorithms is closely related to the alternating minimization technique for solving optimization problems. This idea is recently used to develop some effective alternating iterative methods for solving positive-definite linear systems, see [4–6].

In this paper, we propose an alternating projected gradient (APG) algorithm for NMF, for which the cost function is defined as the Frobenius norm of $V - WH$. Especially, no zero entries appear in denominators in our algorithm which implies no breakdown occurs, and even if some zero entries appear in numerators new updates can always be improved in our algorithm. Numerical experiments on known facial databases and iris database show that our algorithm is better than the MU algorithm.

This paper is organized as follows. After introducing an alternating projected gradient algorithm for NMF in Section 2, we then show some experiments on known facial databases and iris database in Section 3, and give some conclusions in the last section.

2. Alternating projected gradient algorithms

In this section we first introduce an alternating gradient (AG) algorithm and then develop an alternating projected gradient (APG) algorithm.

2.1. Alternating gradient algorithm (AG)

Let

$$f = \|V - WH\|_F,$$

then the NMF problem becomes a constrained least square problem with respect to H, when W is firstly fixed.

Therefore H can be updated with a stepsize in the weighted gradient direction of $f(W,H)$, that is

$$H_{i,j} \leftarrow H_{i,j} - \tilde{\varepsilon}_H \left(\frac{\partial f(W,H)}{\partial H}\right)_{i,j}, \quad i = 1,2,\ldots,r, \quad j = 1,2,\ldots,n. \tag{1}$$

where

$$\frac{\partial(f(W,H))}{\partial H} = W^T WH - W^T V, \quad \tilde{\varepsilon}_H \geqslant 0.$$

In order to ensure $H \geqslant 0, \tilde{\varepsilon}_H$ should be chosen such that

$$\tilde{\varepsilon}_H \leqslant H_{i,j} / \left(\frac{\partial f(W,H)}{\partial H}\right)_{i,j}, \quad \text{when} \quad \frac{\partial f(W,H)}{\partial H})_{i,j} > 0.$$

Setting

$$\varepsilon_H^* = arg \min_{\varepsilon} f\left(W, H - \varepsilon \frac{\partial f(W,H)}{\partial H}\right),$$

we then have

$$\varepsilon_H^* = \frac{\|W^T WH - W^T V\|_F^2}{\|W(W^T WH - W^T V)\|_F^2}, \tag{2}$$

$$\tilde{\varepsilon}_H = \min_{(\frac{\partial f(W,H)}{\partial H})_{i,j} > 0} \left(\varepsilon_H^*, H_{i,j} \Big/ \left(\frac{\partial f(W,H)}{\partial H}\right)_{i,j}\right), \tag{3}$$

and thus $H \geqslant 0$.

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