Anti-lopsided Algorithm forLarge-scale Non-negative Least Squares

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Abstract

Non-negative least squares (NNLS) problem is one of the most fundamental problems in numeric analysis. It has been widely used in scientific computation and data modeling. In big data, the limitations of algorithm speed and accuracy are typical challenges. In this paper, we propose fast and robust anti-lopsided algorithm with high accuracy that is totally based on the first order methods. The main idea of our algorithm is to transform the original NNLS into an equivalent non-negative quadratic programming, which significantly reduce the scaling problem of variables. The proposed algorithm can reach high accuracy and fast speed with linear convergence \((1 - \frac{1}{\sqrt{n}||Q||_2})^k\) where \(\sqrt{n} \leq ||Q||_2 \leq n\), and \(n\) is the dimension size of solutions. The experiments on large matrices clearly show the high performance of the proposed algorithm in comparison to the state-of-the-art algorithms.

1 Introduction

Non-negative least squares (NNLS) is one of the most fundamental problems in numeric analysis. It has been widely used in scientific computation and data mining. Various scientific problems use NNLS to optimize their objective functions \([4]\) such as image processing, computer vision, text mining, environmetrics, chemometrics, and speech recognition. Particularly, in these fields, we often need to estimate a large number of observations \(b \in \mathbb{R}^d\) by a set of measures or basis factors \(\{A_i\}\) contained in a matrix \(A \in \mathbb{R}^{d \times n}\). The popular task is to approximate \(b\) by by minimizing \(\frac{1}{2}||Ax - b||_2^2\).

Nonnegativity constraints enhance interpretability of approximate solutions, which makes NNLS pervasive throughout many applications \([4]\). One of the most popular problems in scientific computation is the approximation of observations. Non-negative coefficients of solutions can be interpreted as contributions of these measurements over the observations in additive models, while mixed sign coefficients are uninterpretable because they lead to overlapping and mutual elimination of these measurements. For example, in many applications of machine learning and physics, when observed instances or signals must be represented by the latent features or blind sources, the non-negative coefficients are the contribution of latent features or blind sources.

Since 1990s, the methods of nonnegative matrix or tensor factorizations widely use NNLS to achieve low-rank representations of nonnegative data \([11,17]\). The low-rank representation for data is meaningful and essential to applications in many disciplines such as statistics, signal and image processing, machine learning, and data mining \([4]\). The low-rank representation transfers data instances into lower-dimensional spaces of components or sources to obtain higher speed and accuracy, and more concise interpretability of data processing.

Although NNLS is a convex optimization problem, non-negativity constraints and high dimensional complexity lead to various difficulties. In our point of view, the performance of NNLS algorithms mainly depends on two main factors about using the second derivative and the active set. Using the second derivative \([2,12,10]\) discovered the more effective direction to reduce more effectively the objective function. However, these approaches have two main drawbacks: invertibility of \(A^TA\) and its heavy computation, especially for those methods recomputing \((A^TA)^{-1}\) several times for different passive sets. Hence, some other algorithms only using the first derivative \([6,15,10]\) can be more effective for large-scale least squares problems. Meanwhile, almost all effective algorithms remove several redundant variables based on the concept of active sets \([2,4]\) for each iteration, although they are different in the employed strategies \([4]\). Fundamentally, these algorithms are based on the observation that several variables can be ignored if they are negative when the problem is unconstrained \([2,12,10]\). In other words, NNLS can be considered as an unconstrained problem in a subspace of several variables \([10]\) that are positive in the optimal solution.

Therefore, in this paper, we propose a fast robust iterative algorithm called anti-lopsided algorithm. The main idea of this algorithm is to transfer the original problem into an equivalent problem, by which scaling problems in the first order methods are significantly reduced. The proposed algorithm has significant advantages:

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• **Fastness:** The proposed algorithm has an exponent convergence rate $O(1 - \frac{1}{2||Q||^2})^k$ in the subspace of passive variables [10], where $\sqrt{n} \leq ||Q|| \leq n$, and $n$ is the dimension size of solutions. In addition, it does not need to compute the inverse of matrices $(ATA)^{-1}$ because it is totally based on the first derivative.

• **Robustness:** It can stably work in ill-conditioned cases since it is totally based on the first derivative,

• **Effectiveness:** the experimental results are highly comparable with the state-the-art methods,

• **Simplicity:** Interestingly, the source code is actually simple to be implemented, paralleled and distributed since it is totally based on the first order derivative and gradient methods using exact line search.

The rest of paper is organized as follows: Section 2 discusses the background and related works of least square problems; then, Section 3 mentions the details of our proposed algorithm Anti-llopsided; subsequently, the theoretical analysis is discussed in Section 3; finally, Section 4 shows the experimental results, and Section 5 summarizes the main contributions of this paper.

2 Background and Related Works

In this section, we introduce the non-negative least square (NNLS) problem, its equivalent solutions as well as non-negative quadratic problem (NQP), and significant milestones of the algorithmic development for NNLS.

2.1 Background

Non-negative least square (NNLS) can be considered one of the most central problems in data modeling to estimate the parameters of models for describing the data [4]. It comes from scientific applications where we need to estimate a large number of vector observations $b \in R^d$ by a set of measures or basis factors $\{A_i\}$ contained in a matrix $A \in R^{d \times n}$. The common task is to approximate an observation $b$ by the measures by minimizing $\frac{1}{2}||Ax - b||_2^2$. Hence, we can define NNLS as follows:

**Definition 2.1.** Given $n$ measurement vectors $A = [A_1, A_2, ..., A_n] \in R^{d \times n}$ and an observed vector $b \in R^d$, we need to find an optimal solution $x$ of the optimization problem:

\[
\begin{align*}
& \text{minimize} & & \frac{1}{2}||Ax - b||_2^2 \\
& \text{subject to} & & x \geq 0 \\
& \text{where} & & A \in R^{d \times n}, b \in R^d
\end{align*}
\] (2.1)

Obviously, it can be equivalently turned into a non-negative quadratic programming (NQP) problem:

\[
\begin{align*}
& \text{minimize} & & f(x) = \frac{1}{2}x^THx + h^Tx \\
& \text{subject to} & & x \geq 0. \\
& & H = A^TA, h = -A^Tb
\end{align*}
\] (2.2)

From this NQP formulation, these problems are convex since $Q$ is positive semidefinite and the non-negativity constraints form a convex feasible set. In this paper, we will solve Problem 2.2 instead of Problem 2.1.

2.2 Related Works

For more several decades of developments, many different approaches have been employed to tackle the NNLS problem that aims to optimize the objective function. Based on features of methods, algorithms for solving NNLS can be divided into two main groups: active-set methods and iterative methods [1].

The active-set methods are based on the observation that variables can be divided into subsets: active and passive variables [7]. Particularly, the active set contains variables being zero or negative when solving the least square problem without concerning non-negative constraints, otherwise the other variables belong to the passive set. The active-set algorithms employ the fact that if the active set is identified, the values of the passive variables in NNLS are their values in the unconstrained least squares solution when removing active variables, which will be set to zero. Unfortunately, these sets are unknown in advance. Hence, a number of iterations is employed to find out the passive set, each of which needs to solve a unconstrained least squares problem on the passive set to update the passive set and the active set. Concerning the significant milestones of the active-set methods, Lawson and Hanson [12] proposed a standard algorithm for active-set methods. Subsequently, Bro and Jong [2] avoided unnecessary recomputations on multiple right-hand sides to speed up the basic algorithm [12]. Finally, Dax [5] proposed selecting a good starting point by Gauss-Seidel iterations and moving away from a “dead point” to reduce the number of iterations.

Moreover, iterative methods use the first order gradient on the active set to handle multiple active constraints in each iteration, while the active-set methods only handle one active constraint [4]. Hence, iterative methods can deal with more large-scale problems [9] [10] than the active-set methods. However, they are still not guaranteed about the convergence rate. More recently, accelerated methods [13] and proximal methods [14] having a fast convergence $O(1/k^2)$ [8] only require the
first order derivative. However, one major disadvantage of these methods is that the accelerated methods require a large number of iterations, if the solution requires high accuracy since the step size is limited by a large number of iterations, if the solution requires high accuracy since the step size is limited by $\frac{1}{M}$, where $M$ is Lipschitz constant that may be very large for large-scale problems with big matrices.

In summary, active-set methods and iterative methods are two major approaches in solving NNLS. The active-set methods are classical to accurately solve non-negative least square problem. However, they require a huge computation of solving unconstrained least squares problems and unstable when $A^TA$ is ill-conditioned. The iterative methods are more potential for solving large-scale NNLS because they can handle multiple active constraints per each iteration. In our point of views, the iterative methods are still ineffective due to the scaling problem on variables that seriously affects finding out the appropriate gradient direction to guarantee the convergence rate. Therefore, we propose Anti-lopsided algorithm iterative methods, which re-scales variables to achieve an exponent convergence rate.

3 Anti-lopsided Algorithm

In this section, we discuss our new idea to develop a fast robust iterative algorithm for large-scale non-negative least squares (NNLS) problem. For more readability, we separate the proposed algorithm into two module algorithms: Algorithm 1 for solving NNLS problem by transforming NNLS problem into NQP problem and re-scaling variables, by which the scaling problem of variables is significantly reduced; then, calling Algorithm 2 for solving NQP problem by a first-order gradient method using exact line search.

Based on the literature review, iterative methods using the first order derivative can be suitable for designing large-scale algorithms for NNLS. However, this method heavily depends on the scaling of variables [1]. For example, if we employ iterative exact line search method using the first order derivative to optimize the function $f(x) = \frac{1}{2}x^T[A1 0.1 9]x + [-4 - 5]x$ starting at $x_0 = [30 2]^T$, we need to 40 iterations to reach the optimal solution, see Figure 1:

**Algorithm 1: Anti-lopsided Algorithms for NNLS**

**Input:** $A \in \mathbb{R}^{n \times m}; b \in \mathbb{R}^{n}$

**Output:** $x$ minimizing $\frac{1}{2}\|Ax - b\|_2^2$

subject to: $x \geq 0$

\[
\begin{align*}
1 & \text{ begin } \\
2 & H = A^TA; \\
3 & Q = \frac{H}{\sqrt{\text{diag}(H)\text{diag}(H)^T}}; \\
4 & q = \frac{-A^Tb}{\sqrt{\text{diag}(H)}}; \\
5 & y = \text{solveNQP}(Q, q)/*by Algorithm 2*/; \\
6 & x = \frac{y}{\sqrt{\text{diag}(H)} }; \\
7 & \text{return } x
\end{align*}
\]

(3.3) \quad f(x) = \frac{1}{2}x^T[A1 0.1 9]x + [-4 - 5]x

Hence, we re-scale variables into a new space, in which new variables have more balanced roles for the reason that we call our algorithm as anti-lopsided algorithm. Particularly, we re-scale:

\[(3.4) \quad x = \frac{y}{\sqrt{\text{diag}(H)}} \quad \text{or} \quad x_i = \frac{y_i}{\sqrt{H_{ii}}} \quad \forall i
\]

It is noticeable that $H_{ii} = A_i^TA_i = ||A_i||^2 \geq 0$. For the special case $H_{ii} = 0$, we give $x_i = y_i$. After re-scaling variables, the original Problem 2.2 is equivalently transformed into NQP Problem 3.5:

\[(3.5) \quad \begin{align*}
\text{minimize} & \quad f(y) = \frac{1}{2}y^TQy + q^Ty \\
\text{subject to} & \quad y \geq 0
\end{align*}
\]

where $Q_{ij} = \frac{H_{ij}}{\sqrt{H_{ii}H_{jj}}}; q_i = \frac{h_i}{\sqrt{H_{ii}}}$

**Remark 3.1.** Consider the values of matrix $Q$, we have:

- $Q_{ii} = \frac{H_{ii}}{\sqrt{H_{ii}}} = \cos(A_i, A_i) = 1 \quad \forall \quad i = 1...n$

- $Q_{ij} = \frac{H_{ij}}{\sqrt{H_{ii}H_{jj}}} = \cos(A_i, A_j) \quad \forall \quad 1 \leq i \neq j \leq n$

Obviously, the scaling problem of variables is reduced significantly. The shape of function is transformed from ellipse-shaped, see Figure 1 to ball-shaped, see Figure 2. Hence, the first order methods can work...
much more effectively. For example, we need 3 iterations instead of 40 iterations to reach the optimal solution for the function $3.3$ with the same initial point $y_0$ where $y_0 = x_0, H_{ii} \forall i$.

Subsequently, we discuss Algorithm 2 for solving NQP with input $Q$ and $q$. For each iteration, the objective function is optimized on the passive set:

$$P(x) = \{ x_i | x_i > 0 \text{ or } \nabla f_i(x) < 0 \}$$

Hence, the first order gradient will be projected into the sub-space of the passive set $\nabla f = \nabla f_{P(x)}$ $(\nabla f_i = \nabla f_i$ for $i \in P(x)$, otherwise $\nabla f_i = 0)$. Noticeably, the passive set can change through iterations. Algorithm 2 is converged when $P(x) = \emptyset$ or $\|\nabla f\|^2 < \epsilon$. In addition, the orthogonal projection on the sub-space of passive variables $x = [x_0 + \alpha \nabla f_i^+]$ is trivial [10] since NQP Problem 3.5 is a strongly convex problem on a convex set.

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Algorithm 2: Gradient Method with Exact Line Search for NQP

1. \textbf{Input}: $Q \in R^{n \times n}; q \in R^n$
2. \textbf{Output}: $x$ minimizing $f(x) = \frac{1}{2} x^T Q x + q^T x$
3. begin
4. $x^0 = 0$
5. $\nabla f = q$
6. repeat
7. $\nabla f = \nabla f[x > 0 \text{ or } \nabla f < 0]$; \[\alpha = \arg \min \alpha f(x_k - \alpha \nabla f) = \frac{\| \nabla f \|^2}{\nabla f^T Q \nabla f};\] \[x_{k+1} = [x_k - \alpha \nabla f^+] ;\]
8. $\nabla f = \nabla f + Q(x_{k+1} - x_k)$;
9. until $A(x) = 0 \text{ or } ||\nabla f||^2 < \epsilon$
10. return $x_k$
11.

Regarding computing $a$ of Algorithm 2 we have:

$$f(x - \alpha \nabla f) = -\alpha \nabla f^T[Qx + q] + \frac{\alpha^2}{2} \nabla f^T Q \nabla f + C$$

$$\nabla f^a = 0 \iff a = \frac{\nabla f^T Q x + q}{\nabla f^T Q \nabla f} = \frac{||\nabla f||^2}{\nabla f^T Q \nabla f}$$

where $C$ is constant.

4 Theoretical Analysis

In this section, we investigate the convergence and complexity of the proposed algorithm.

Figure 2: 3 optimizing steps in iterative exact line search method using the first order derivative after applying anti-lopsided steps starting at $y_0 = \frac{x_0}{\sqrt{\text{diag}(H_i)}}$

4.1 Convergence Considering the the convergence rate, our method argues Barzilai and Borwein’s note that NNLS is an unconstrained optimization on the passive set of variables [2].

In this section, we consider the convergence rate of the Algorithm 2 without concerning active variables satisfied KKT conditions.

Let $f(x) = \frac{1}{2} x^T Q x + q^T x$, where $Q_{ij} = \cos(A_i, A_j) = \cos(a_i, a_j)$, where $a_k = \frac{A_k}{\|A_k\|}$ is the unit vector $A_k \forall k$.

Since $f(x)$ is strongly convex, we have:

- $\exists m, M > 0$ satisfy $m I \leq \nabla^2 f \leq M I$
- $\forall x, y : f(y) \geq f(x) + \nabla f(x)^T(y - x) + \frac{m}{2}||y - x||^2$
- $\forall x, y : f(y) \leq f(x) + \nabla f(x)^T(y - x) + \frac{M}{2}||y - x||^2$

Based on [3], we have:

Theorem 4.1. After $(k+1)$ iterations, $f(x^{k+1}) - f^* \leq (1 - \frac{\alpha M}{2})^k(f(x^0) - f^*)$, where $f^*$ is the minimum value of $f(x)$.

Proof. Since $f(y) \leq f(x) + \nabla f(x - y) + \frac{M}{2}||y - x||^2 \forall x, y$ selecting $y = x - \frac{1}{M} \nabla f$ and $x^+$ is the updated value of $x$ after an iteration by the first order gradient using exact line search, we have:

$$f(x^+) \leq f(x - \frac{1}{M} \nabla f)$$

$$\leq f(x) - \frac{1}{M} ||\nabla f||^2 + \frac{M}{2} (\frac{1}{M})^2 ||\nabla f||^2$$

$$\leq f(x) - \frac{1}{2M} ||\nabla f||^2$$

Hence, for $f^*$ is the minimum value of the objective function, we have:

$$f(x_{k+1}) - f^* \leq (f(x_k) - f^*) - \frac{1}{2M} ||\nabla f||^2$$

Consider $f(y) = f(x) + \langle \nabla f, y - x \rangle + \frac{M}{2}||y - x||^2$

(fixing $x$) is a convex quadratic function of $y$. Hence,
From 4.7 and 4.9, we have the necessary result:

\[ f(y) \text{ minimizes when } \nabla f(y) = 0 \Leftrightarrow y = \hat{y} = x - \frac{1}{m} \nabla f. \]

In addition, since \( f(y) \geq f(x) + \langle \nabla f, y - x \rangle + \frac{m}{2} \| y - x \|^2 \) \( \forall x, y, \), we have:

\[
\begin{align*}
    f(y) & \geq f(x) + \langle \nabla f, y - x \rangle + \frac{m}{2} \| y - x \| \\
    (4.9) & \geq f(x) + \langle \nabla f, \hat{y} - x \rangle + \frac{m}{2} \| \hat{y} - y \| \\
    & = f(x) - \frac{1}{2m} \| \nabla f \|_2^2 \forall x, y
\end{align*}
\]

Selecting \( y = x^* \) and \( z = x_k \) where \( x^* \) is the optimal solution, we have:

\[
(4.10) - \| \nabla f \|_2^2 \leq 2m(f^* - f(x_k))
\]

From 4.7 and 4.9, we have the necessary result:

\[
f_{k+1} - f^* \leq (1 - \frac{m}{M})(f(x_k) - f^*) \leq (1 - \frac{m}{M})^k(f(x_0) - f^*)
\]

**Lemma 4.1.** For \( f(x) = \frac{1}{2}x^TQx + q^Tx \), where \( Q_{ij} = \cos(a_i, a_j) \) and \( a_i, a_j \) are unit vectors, \( \hat{I} \equiv \nabla^2 f \leq \|Q\|_2I \), where \( \|Q\|_2 \leq n \), and \( \|Q\|_2 = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij}} \).

Proof. We have: \( \nabla^2 f = Q \), and

\[
\begin{align*}
\frac{1}{2}x^TQx & \leq \frac{1}{2}(\sum_{i=1}^{n} x_i^2) + \frac{1}{2} \sum_{i=1}^{n} x_i a_i^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j = x^TQx \forall x \Rightarrow \frac{1}{2}I \leq \nabla^2 f.
\end{align*}
\]

Moreover, based on Cauchy-Schwarz inequality, we have:

\[
(\sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j)^2 \leq (\sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij}^2)(\sum_{i=1}^{n} x_i x_j)^2
\]

\[
\Rightarrow \sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij} x_i x_j \leq \sqrt{\sum_{i=1}^{n} Q_{ij}^2} \sqrt{\sum_{i=1}^{n} x_i^2}^2 = \sqrt{\sum_{i=1}^{n} Q_{ij}^2} \sqrt{\sum_{i=1}^{n} x_i^2} \leq \|Q\|_2 \sqrt{\sum_{i=1}^{n} x_i^2}
\]

\[
\Leftrightarrow x^TQx \leq \|Q\|_2 x^TI \forall x \Rightarrow Q \leq \|Q\|_2I
\]

Finally, \( \sqrt{n} \leq \sum_{i=1}^{n} Q_{ij}^2 \leq \|Q\|_2 = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} Q_{ij}^2} \leq \sqrt{n^2} = n \) since \( -1 \leq Q_{ij} = \cos(a_i, a_j) \leq 1 \).

From Theorem 4.1 and Lemma 4.1, setting \( m = \frac{1}{2} \) and \( M = \|Q\|_2 \), we have:

**Theorem 4.2.** After \( k+1 \) iterations, \( f(x^{k+1}) - f(x^*) \leq (1 - \frac{2}{\|Q\|_2^2})^k(f(\bar{x}) - f(x^*)) \), where \( \sqrt{n} \leq \|Q\|_2 \leq n \) and \( n \) is the dimension of \( x \).

### 4.2 Complexity

Concerning the average complexity of Algorithm [2], we consider the important operators:

- **Line 7:** The complexity of computing \( \|\nabla f\|^2 \) is \( O(n) \), and \( \nabla f^T \nabla f \) is \( O(nS(n)) \).

- **Line 10:** The complexity of computing \( Q(x_{k+1} - x_k) \) is \( O(nS(n)) \).

Therefore, based on Lemma 4.2 if we consider computing \( A^TA \) and \( A^Tb \) in \( O(dn + dn^2) \), we have:

**Theorem 4.3.** The average complexity of Algorithm [7] is \( O(dn+dn^2+knS(n)) \), where \( k \) is the average number of iterations.

#### 5 Experimental Evaluation

In this section, we investigate the convergence speed, running time and optimality of the proposed algorithm in comparison to state-of-the-art algorithms for active-set methods, iterative methods and accelerated methods. Particularly, we compare our algorithm Antilop with the following algorithms:

- **Fast:** This is a modified effective version of active-set methods according to Bro R., de Jong S., Journal of Chemometrics, 1997 [2], which is developed by S. Gunn [3]. This algorithm can be considered as one of the fastest algorithms of active-set methods.

- **Nm:** This is a non-monotonic fast method for large-scale nonnegative least squares based on iterative methods [10]. The source code is downloaded from [4].

- **Accer:** This is a Nesterov accelerated method with convergence rate \( O(1/k^2) \) [8]. The source code is extracted from a module in the paper [8]. The source code is downloaded from [4].

- **Anti+Acc:** This is a Nesterov accelerated method with convergence rate \( O(1/k^2) \) after using the anti-lopsided steps (from Line 2 to Line 4 in Algorithm [1]). This algorithm investigates the effectiveness of the anti-lopsided steps for iterative algorithms only using the first derivative.

To be a fair comparison, we test these algorithms on various test-cases which are generated randomly.

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1. http://web.mit.edu/mkgray/matlab/svm/fnnls.m
2. http://suvrit.de/work/progs/nl1s.html
3. https://sites.google.com/site/nmfsolvers/
Particularly, we use a set of test cases with \( n = 4000 \) and \( d = 1.5n = 6000 \) since often \( d > n \). Furthermore, we design 6 test-cases \( \{T_1, ..., T_6\} \), which have high potential to happen in practice. In the test-cases, the sign of values in \( A, b \) can be non-negative(+) or mixed-sign(±); and measure vectors \( \{A_i\}_{i=1}^{d} \) have the same (SAM), randomized (RAN), or various (VAR) lengths as enumerated in Table 1. Test cases containing \( A, b \) negative are ignored because they are equivalent to test-cases that \( A \) and \( b \) are nonnegative.

For each test-case, we randomize 5 sub-tests having different sparsity of optimal solutions from 0% to 40% in order to create the objective functions having different values of Lipschitz constant.

| \( T \) | Length | \( A, b \) | \( f^* \) | \( ||f||_2^2 \) | \( ||Q||_2^2 \) |
|---|---|---|---|---|---|
| T1 | SAM | + | 1.8e-03 - 4.7e+06 | 1.1e+05 - 1.4e+13 |
| T2 | RAN | ± | 1.7e-03 - 3.5e+06 | 9.4e+04 - 3.9e+11 |
| T3 | VAR | + | 2.4e-03 - 3.1e+06 | 5.6e+05 - 6.0e+12 |
| T4 | SAM | ± | 2.3e-03 - 3.9e+06 | 1.6e+05 - 7.5e+12 |
| T5 | RAN | + | 2.6e-03 - 2.9e+06 | 2.1e+05 - 5.1e+12 |
| T6 | VAR | ± | 9.9e+02 - 5.0e+06 | 3.1e+04 - 1.5e+13 |

Table 2: Range of \( ||A||_2^2 \) and \( ||Q||_2^2 \) in test cases

5.1 Convergence Concerning the optimal values, \( f^* \) is 0 for nonnegative test cases; and it is the best minimum value found by all the methods for mixed-sign test cases because we do not know it for these test-cases in advance. Since algorithms can run for a long time, we must stop our algorithm and other algorithms when new solutions with a smaller value of \( ||\nabla f||^2 \) are not found, reaching the maximum number of iterations is \( 5n = 2.10^4 \), or the maximum of running time is 1600 (s) that is the necessary running time for the traditional accurate method Fast [2] for all the tests.

In addition, we develop Algorithm [1] and Algorithm [2] in Matlab to easily compare with other algorithms. Furthermore, we set system parameters to use only 1 CPU for Matlab and the IO time is excluded. All source codes of our algorithm and generating test-cases, and 30 used tests are published [1] for free.

In this section, we investigate the convergence speed of the square of derivatives \( ||f||_2^2 \to 0 \) in Figure 3 and the difference between the values of objective function and the optimal values \( (f(x_k) - f^* + 1) \to 0 \) during the running time in Figure 4. The results clearly show that our algorithm and algorithm Fast [2] converge to the optimal values in all 30 test-cases. Remarkably, our algorithm converges to the optimal values much faster than the other methods. Moreover, interestingly, algorithm Anti+Acc works more effectively than algorithm Accer. This proves that the anti-llopsided transformation makes iterative methods using the first derivative more effective because it significantly reduces scaling problems of variables.

| \( T \) | Antilop | Fast | Nm | Accer | Anti+Acc |
|---|---|---|---|---|---|
| T1 | 146.8 | 1384.2 | 205.2 | 1600.0 | 1600.0 |
| T2 | 11.9 | 160.6 | 2.7 | 253.4 | 166.7 |
| T3 | 71.5 | 1471.9 | 917.6 | 1600.0 | 1600.0 |
| T4 | 12.5 | 255.6 | 906.4 | 1600.0 | 138.5 |
| T5 | 154.7 | 1455.3 | 905.3 | 1600.0 | 1600.0 |
| T6 | 12.3 | 265.7 | 906.9 | 1600.0 | 276.2 |

Table 3: Average of running time in seconds for test-cases \( T_1, ..., T_6 \)

5.2 Running Time In the final comparison, we compare the algorithms in the average of running time on 5 sub-tests of test-cases as shown in Table 3. Clearly, our proposed algorithm has the best averages of running time in most of test-cases, excepted for test-case T2. Remarkably, the non-monotonic algorithm (Nm) [10] is unstable in other kinds of test-cases. Furthermore, the difference between our proposed algorithm and the non-monotonic algorithm for test-case T2 is not considerable. In comparison to the another stable algorithm Fast [2], our algorithm has the similar accuracy of optimal values, but it runs faster from 9 times to 21 times faster than algorithm Fast [2].

| \( T \) | Antilop | Fast | Nm | Accer | Anti+Acc |
|---|---|---|---|---|---|
| T1 | 7E-15 | 2E-15 | 2E+03 | 2E-03 | 2E-03 |
| T2 | 6E-08 | 7E-08 | 6E-08 | 7E-08 | 1E-07 |
| T3 | 6E-16 | 2E-16 | 2E-01 | 1E-01 | 2E-04 |
| T4 | 9E-09 | 8E-09 | 6E+03 | 2E+03 | 1E-10 |
| T5 | 3E-09 | 9E-10 | 5E+05 | 5E+05 | 1E+03 |
| T6 | 6E-03 | 4E-03 | 7E+09 | 1E+09 | 6E-04 |

Table 4: Average of \( |f(x_k) - f^*| \) in testcases \( T_1, ..., T_6 \)

5.3 Optimality This section is dedicated to investigate the optimal effectiveness among our algorithm

*https://bitbucket.org/xxx/yyy
Figure 3: $\|\bar{f}\|_2^2$ during running time

Figure 4: $(f(x_k) - f^* + 1)$ during running time
and four other algorithms. The results shown in Table 4 are the average values of $|f(x_k) - f^*|$ in 5 sub-test cases. Obviously, our algorithm and Fast [2] achieved the best values that are highly distinguished from the other methods. All the methods have errors $|f(x_k) - f^*|$ that can be raised by approximately computing float numbers in computers and characteristics of methods. Hence, this can be acceptable for the large matrix size $d \times n$, and the values of Lipschitz constant related to $||Q||_2$ and $||A||_2$.

6 Conclusion and Discussion

In the paper, we proposed a fast robust anti-lopsided algorithm to solve the nonnegative least squares problem that is one of the most fundamental problems in data modeling. We theoretically proved that our algorithm has a linear convergence $(1 - \frac{1}{2||Q||_2})^k$ on the sub-space of passive variables, where $\sqrt{n} \leq ||Q||_2 \leq n$, and $n$ is the dimension of solutions.

In addition, we carefully compare the proposed algorithm with state-of-the-art algorithms in different research directions on large matrices in three aspects: convergence rate, running time and optimality of solutions on 30 randomized tests among 6 different test cases which often occur in the reality. On convergence rate and running time, the proposed algorithm’s results are highly distinct from other ones’ results. On the optimality of solutions, the results of our algorithm are very close to the most accurate results. These differences are not significant and inevitable because they are raised by computing approximately float numbers in computers and the characteristics of iterative methods needing more float operators. In our opinion, these differences can be acceptable because of the large-scale matrices. Therefore, our proposed algorithm has all of three significant aspects on convergence speed, running time and accuracy.

Finally, the convergence speed of the Nesterov accelerated method [5] using the anti-lopsided steps is much more faster than Nesterov accelerated method directly applied. Hence, we strongly believe that the anti-lopsided steps can have a significant impact on iterative methods using the first derivative for least squares problems and quadratic programming problems.

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