A Randomized Kaczmarz Algorithm for Total Least Square Problem

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1. Introduction

The Total Least Squares (TLS) problem is a well known technique for solving the following over-determined linear systems of equations

$$Ax \approx b \quad A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}, \quad m > n$$

in which both the matrix A and the right hand side b are affected by errors. We consider the following classical definition of TLS problem, see [1]

Definition 1.1: (TLS problem).

The Total Least Squares problem with data $A \in \mathbb{R}^{m\times n}$ and $b \in \mathbb{R}^m, m > n$ is given by

$$\min \ \|E \mid f\|_F \quad \text{subject to} \quad b + f \in \mathrm{Im}(A + E) \tag{1}$$

where $E \in \mathbb{R}^{m\times n}$ and $f \in \mathbb{R}^m$. Here, $\|E \mid f\|_F$ denotes the Frobenius matrix norm and $(E \mid f)$ denotes the $m \times (n + 1)$ matrix whose first n columns are the columns of E, and the last column is the vector f. In various engineering and statistics applications where a mathematical model reduces to the solution of an over-determined, possibly inconsistent linear equation $Ax \approx b$, solving that equation in the TLS sense yields a more convenient approach than the ordinary least squares approach, in which the data matrix is assumed constant and errors are considered right-hand side b

The TLS problem was firstly introduced by Golub and Van Loan in [1],[2] motivated by the idea of statistical literature on orthogonal regression, errors-in-variables, and 'measurement error' methods and models. Their numerical algorithm for solving the TLS problem was based on the singular value decomposition of the matrix $(A \mid b)$. That algorithm, which requires about $2mn^2 + 12n^3$ arithmetic operations [4] and can also solve problems with multiple right hand sides, is still today one of the reference methods for the solution of general TLS problems. Van Huffel and Vandewalle [3], [4] extended the algorithm of Golub and Van Loan in order to deal with TLS problems having non-unique solutions, the so called non-generic problems.

Since then, many variants and solution methods have been introduced on the basic TLS problem because of its occurrence in many different fields [5].In [6] authors developed a Gauss-Newton algorithm for solving the TLS problem.

2. Main Result

Let us make some assumptions before deriving the update formula of Total Least Square problem using Randomized Kaczmarz algorithm.

Let $\sigma_j(A)$ denote singular value j of A, organized in decreasing order so that

$$\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_{\min\{m,n\}}$$

In their analysis [7],[8] Strohmer and Vershynin use the extra assumption that $\sigma_n(A) > 0$. This implies that $m \geq n$, that A has n independent columns, and that there can be at most one solution x.

Update formula Using Randomized Kaczmarz

We will use another characterization of the the solution of the total least squares problem with data A and b for our formulation. The other definition of TLS problem is given in terms of the minimization of the function $\eta(x)$,

$$\eta(x) = \min \frac{\|Ax - b\|^2}{1 + x^T x} \tag{2}$$

Indeed, it was shown in [3] that, under well posedness hypotheses, the solution x_{TLS} can be characterized as the global minimum of $\eta(x)$, by means of arguments based on the SVD of the matrix $(A|b)$, and $\eta(x_{TLS}) = \sigma_{n+1}$.

In their analysis of Total Least Square problem [2] Golub proved the equivalence definition for solving the Total Least Square problem in terms of Linear system as

$$(A^T A - \eta(x)I)x = A^T b \tag{3}$$

Now component wise we can write the above linear system as

$$c_i^T x - \eta(x) e_i^T x = a_i^T x$$

where a_i is the ith column of A and $c_i^T = [\langle a_i, a_1 \rangle, \langle a_i, a_2 \rangle, \ldots, \langle a_i, a_n \rangle]$

Now we rewrite the iteration formula as follows

$$x_{k+1} = \arg\min_x \frac{1}{2}\|x - x_k\|^2 \quad \text{s.t} \quad c_i^T x - \eta(x) e_i^T x = a_i^T x \tag{4}$$

which is strongly convex (the solution is unique). For deriving the solution of the above problem let us derive the Lagrangian as

$$L(x, \lambda) = \frac{1}{2}\|x - x_k\|^2 + \lambda\left(c_i^T x - \eta(x) e_i^T x - a_i^T x\right)$$

Now taking the gradient with respect to x and λ we get

$$\begin{aligned} x_{k+1} - x_k + \lambda c_i - \lambda \eta(x_k) e_i = 0 \\ c_i^T x_{k+1} - \eta(x_k) e_i^T x_{k+1} - a_i^T x_{k+1} = 0 \end{aligned} \tag{5}$$

Now solving the equation (5) for λ we have

$$x_{k+1} = x_k - \frac{c_i^T x_k - \eta(x_k) e_i^T x_k - a_i^T b}{\|c_i - \eta(x_k) e_i\|^2} \left(c_i - \eta(x_k) e_i\right) \tag{6}$$

Now by letting $d_i = c_i - \eta(x_k) e_i$ we van simplify the above update formula as

$$x_{k+1} = x_k - \frac{d_i^T x_k - a_i^T b}{\|d_i\|^2} \, d_i \tag{7}$$

which is the required update formula for Total Least Square problem. Using the update formula we get the following iterative algorithm for TLS problem:

Algorithm 1 TLS Algorithm: $x_{k+1} = \mathbf{TLS}(A, b, x_0, K)$

Initialize $k \leftarrow 0$;
while $k \leq K$ **do**
  Choose $i = i(k)$ from $1, 2, 3, ..., m$ with equal probability
  Update $x_{k+1} = x_k - \frac{d_{i(k)}^T x_k - a_{i(k)}^T b}{\|d_{i(k)}\|^2} \, d_{i(k)}$
  $k \leftarrow k + 1$;
end while
return x

Convergence analysis of Algorithm 1 with uniform sampling:

Let us take x^* to be the optimal solution then we have

$$\begin{aligned} \|x_k - x^*\|^2 &= \|x_k - x_{k+1} + x_{k+1} - x^*\|^2 \\ &= \|x_k - x_{k+1}\|^2 + \|x_{k+1} - x^*\|^2 - 2\langle x_k - x_{k+1}, x_{k+1} - x^* \rangle \end{aligned} \tag{8}$$

Now for this algorithm the last term is 0 because $x_k - x_{k+1}$ and $x_{k+1} - x^*$ are orthogonal, this means

$$\langle x_k - x_{k+1}, x_{k+1} - x^* \rangle$$

Using this (8) is simplified as

$$\|x_{k+1} - x^*\|^2 = \|x_k - x^*\|^2 - \|x_{k+1} - x_k\|^2 \tag{9}$$

The simplest randomized scheme for selecting i is to choose each possible column i with probability $1/n$. With this choice by taking expectation of equation (9) we have

$$\begin{aligned}\mathbb{E}\left[\|x_{k+1} - x^*\|^2\right] &= \|x_k - x^*\|^2 - \mathbb{E}\left[\|x_{k+1} - x_k\|^2\right] \\ &= \|x_k - x^*\|^2 - \mathbb{E}\left[\|\frac{d_i^T x_k - a_i^T b}{\|d_i\|^2}\ d_i\|^2\right] \\ &= \|x_k - x^*\|^2 - \mathbb{E}\left[\frac{\left(d_i^T x_k - d_i^T x^*\right)^2}{\|d_i\|^2}\right]\end{aligned} \tag{10}$$

Here we used $a_i^T b = d_i^T x^*$. Now by using the definition of expectation we have

$$\mathbb{E}\left[\|x_{k+1} - x^*\|^2\right] = \|x_k - x^*\|^2 - \sum_{i=1}^{n} \frac{1}{n} \frac{\left(d_i^T x_k - d_i^T x^*\right)^2}{\|d_i\|^2} \tag{11}$$

Now let us define a norm for matrix B

$$\|B\|_{\infty,2}^2 = \max_i \|f_i\|^2$$

with f_i denotes the i th row of B. For our case the matrix $B = A^T A - \eta(x)I$ is a $n \times n$ symmetric matrix, so the corresponding rows and columns are same for our case. And also the i th row/column of $B = A^T A - \eta(x)I$ is given by d_i. So

$$\|B\|_{\infty,2}^2 = \|A^T A - \eta(x)I\|_{\infty,2}^2 = \max_i \|d_i\|^2$$

Using the fact $\|A^T A - \eta(x)I\|_{\infty,2}^2 \geq \|d_i\|^2$ for all $1 \leq i \leq n$ in equation (11) we have

$$\mathbb{E}\left[\|x_{k+1} - x^*\|^2\right] \leq \|x_k - x^*\|^2 - \sum_{i=1}^{n} \frac{1}{n} \frac{\left(d_i^T x_k - d_i^T x^*\right)^2}{\|A^T A - \eta(x_k)I\|_{\infty,2}^2} \tag{12}$$

Now For any vector $z \in \mathbb{R}^n$ we have

$$\|\left(A^T A - \eta(x_k)I\right) z\|^2 = \sum_{i=1}^{n} \left(d_i^T z\right)^2$$

Using this in equation (12) we have

$$
\begin{aligned}
\mathbb{E}\left[\|x_{k+1}-x^*\|^2\right] &\le \|x_k-x^*\|^2 - \frac{\|\left(A^TA-\eta(x_k)I\right)(x_k-x^*)\|^2}{n\|A^TA-\eta(x_k)I\|_{\infty,2}^2} \\
&= \left(1-\frac{\|\left(A^TA-\eta(x_k)I\right)(x_k-x^*)\|^2}{n\|A^TA-\eta(x_k)I\|_{\infty,2}^2\|x_k-x^*\|^2}\right)\|x_k-x^*\|^2 \\
&= \left(1-\frac{\|B(x_k-x^*)\|^2}{n\|B\|_{\infty,2}^2\|x_k-x^*\|^2}\right)\|x_k-x^*\|^2 \qquad (13)
\end{aligned}
$$

In the last line we denoted $A^TA-\eta(x_k)I=B$ for simplification. Now if we denote

$$
\gamma_k = 1-\frac{\|B(x_k-x^*)\|^2}{n\|B\|_{\infty,2}^2\|x_k-x^*\|^2}
$$

at each iteration, then using successive iteration we have from (13)

$$
\begin{aligned}
\mathbb{E}\left[\|x_{k+1}-x^*\|^2\right] &\le \gamma_k\|x_k-x^*\|^2 \\
&\le \gamma_k\gamma_{k-1}\|x_{k-1}-x^*\|^2 \\
&\vdots \\
&\le \gamma_k\gamma_{k-1}\ldots,\gamma_0\|x_0-x^*\|^2 \\
&= \prod_{i=1}^{k}\gamma_i\ \|x_0-x^*\|^2 = \gamma\|x_0-x^*\|^2 \qquad (14)
\end{aligned}
$$

Now for the algorithm to converge we need $0\leqslant\gamma=\prod_{i=1}^{k}\gamma_i<1$. If we can prove $0\leqslant\gamma_i<1$ for each $1\leqslant i\leqslant k$, then we are done. Now for any $z\in\mathbb{R}^n$ we have

$$
\frac{\|z\|}{\|Bz\|}\leqslant \sup_{Bx\neq 0}\frac{\|x\|}{\|Bx\|}\leqslant\frac{1}{\sigma_n(B)}
$$

Thus for $z\neq 0$ we have

$$
\frac{\|Bz\|}{\|z\|}\geqslant\sigma_n(B)
$$

Now for our case $x_k-x^*\neq 0$ is trivially true. As if $x_k-x^*=0, Bx_k=Bx^*$ the x_k solves the problem, we don't need to proceed to the next iteration. By using above result we have

$$
\gamma_k\leqslant 1-\frac{\sigma_n^2(B)}{n\|B\|_{\infty,2}^2}
$$

For $0\leqslant\gamma_k<1$ we need to prove that

$$
0<\sigma_n^2(B)\leqslant n\|B\|_{\infty,2}^2
$$

Now the lower bound holds as our assumption $\sigma_n(B) > 0$. Now by using the definition of Frobenious norm we have

$$\|B\|_F \triangleq \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} b_{ij}^2} = \sqrt{\mathbf{Tr}(B^T B)} = \sqrt{\sum_{i=1}^{\min\{m,n\}} \sigma_i^2}$$

As our matrix B is symmetric $n \times n$ we have $m = n$. Then we have

$$\begin{aligned} \sigma_n(B) \leqslant \sigma_1(B) \leqslant \sqrt{\sum_{i=1}^{n} \sigma_i^2} &= \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n} b_{ij}^2} \\ &\leqslant \sqrt{n \, \max_i \sum_{j=1}^{n} b_{ij}^2} \\ &\leqslant \sqrt{n \, \max_i \|d_i\|^2} = \sqrt{n}\|B\|_{\infty,2} \end{aligned} \tag{15}$$

This implies $0 \leqslant \gamma_k < 1$ irrespective of k and x_k. As a consequence $0 \leqslant \gamma < 1$. Therefore using (14) we can say this algorithm converges.

3. Conclusion

In this short report we have developed and analyzed the convergence of Randomized Kaczmarz algorithm for solving the Total Least Square problem. We have calculated the expected error bound for uniform sampling data. We can also consider non-uniform sampling and calculate the bound same way.

4. References

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