A Total Least Squares Approach for the Solution of the Perturbation Equation *

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Abstract

This paper presents a new algorithm for solving the perturbation equation of the form $\mathbf{W}\Delta\mathbf{x} = \Delta\mathbf{I}$ encountered in optical tomographic image reconstruction. The methods we developed previously are all based on the least squares formulation, which finds a solution that best fits the measurement $\Delta\mathbf{x}$ while assuming the weight matrix $\mathbf{W}$ is accurate. In imaging problems, usually errors also occur in the weight matrix $\mathbf{W}$. In this paper, we propose an iterative total least squares (ITLS) method which minimizes the errors in both weights and detector readings. Theoretically the total least squares (TLS) solution is given by the singular vector of the matrix $[\mathbf{W}|\Delta\mathbf{I}]$ associated with the minimal singular value. The proposed ITLS method obtains this solution using a conjugate gradient method which is particularly suitable for very large matrices. Experimental results have shown that the TLS method can yield a significantly more accurate result than the LS method when the perturbation equation is overdetermined.

1 Introduction

Research on medical optical imaging, which uses near infrared light emitted into human tissue to determine the interior structure, has made rapid progress recently. For imaging methods such as X-ray CT, in which the path of the detected signal is a straight line, the inverse problem can be accurately formulated by a system of linear equation of the form $\mathbf{y} = \mathbf{A}\mathbf{x}$, where $\mathbf{y}$ is the measured

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data, $\mathbf{A}$ is the imaging operator and $\mathbf{x}$ is the unknown [1]. With optical imaging, the relation between the unknown and the measured data is much more complicated and highly non-linear. This is because in this frequency range, photons propagate through the tissue in a random path. There is generally no direct method for solving the inverse problem.

In the past few years, for modeling light propagation in tissue, our group has developed an iterative perturbation approach for both CW and TR data [1, 3-5]. This requires the solution of a linear perturbation equation at each iteration of the form:

$$\mathbf{W}\boldsymbol{\Delta}\mathbf{x} = \boldsymbol{\Delta}\mathbf{I}, \tag{1}$$

where $\boldsymbol{\Delta}\mathbf{x}$ is a vector of differences in the optical property (absorption or scattering) between a reference and test medium, $\boldsymbol{\Delta}\mathbf{I}$ is a vector of changes in detector readings between the two media, and $\mathbf{W}$ a matrix of weights describing the influence of each volume element (voxel) on the detector readings, which are essentially the derivatives of the detector readings with respect to the absorption or scattering coefficient in the reference medium. In practice, the perturbation equation is often both underdetermined and ill-conditioned. The underdeterminedness results from the number of detector readings, m, being less than the number of unknowns n. Even if $m \geq n$, the matrix $\mathbf{W}$ can be rank deficient, which also leads to an underdetermined system. The cause of the ill–conditioning is that $\mathbf{W}$ contains many nearly zero columns. Very small variations in $\boldsymbol{\Delta}\mathbf{I}$ can result in very large deviations in $\boldsymbol{\Delta}\mathbf{x}$. To solve the linear perturbation equation, several iterative algorithms have been developed, including projection onto convex sets (POCS) [2], a conjugate gradient descent (CGD) method [2], a multigrid method [2], and a layer stripping scheme [4],[5]. These methods are all based on the least squares formulation, which finds a solution that best fits the measurement $\boldsymbol{\Delta}\mathbf{x}$ while assuming the weight matrix $\mathbf{W}$ is accurate. In general, both the weight matrix $\mathbf{W}$ and the data $\boldsymbol{\Delta}\mathbf{x}$ are subject to errors. One type of error in $\mathbf{W}$ is a modeling error which can arise when the reference and test media differ strongly. Another type can arise from the numerical errors in calculating the forward solution. In this paper, we propose an ITLS method which minimizes the errors in both weights and detector readings.

2 Total Least Squares

In general, when $m > n$, the perturbation equation, which is linear, is incompatible due to errors in both $\mathbf{W}$ and $\boldsymbol{\Delta}\mathbf{I}$. In the conventional least squares solution, we assume the measurement $\boldsymbol{\Delta}\mathbf{I}$ is noisy but the weight matrix $\mathbf{W}$ is exact and we seek a correction vector $\mathbf{E}_{\boldsymbol{\Delta}\mathbf{I}}$ to $\boldsymbol{\Delta}\mathbf{I}$ such that

$$\text{minimize } \| \mathbf{E}_{\boldsymbol{\Delta}\mathbf{I}} \|_2, \tag{2}$$

$$\text{subject to } \boldsymbol{\Delta}\mathbf{I} + \mathbf{E}_{\boldsymbol{\Delta}\mathbf{I}} \in \textbf{ Range}(\mathbf{W}). \tag{3}$$

Here$\| \cdot \|_2$ denotes the Euclidean norm. Once $\mathbf{E}_{\boldsymbol{\Delta}\mathbf{I}}$ is found, $\boldsymbol{\Delta}\mathbf{x}$ is easily determined by solving the compatible equation:

$$\boldsymbol{\Delta}\mathbf{I} + \mathbf{E}_{\boldsymbol{\Delta}\mathbf{I}} = \mathbf{W}\boldsymbol{\Delta}\mathbf{x}. \tag{4}$$

It is known that the solution of the above least squares problem satisfies the normal equation

$$\mathbf{W}^{\mathbf{T}}\mathbf{W}\boldsymbol{\Delta}\mathbf{x} = \mathbf{W}^{\mathbf{T}}\boldsymbol{\Delta}\mathbf{I}. \tag{5}$$

In reality, as descibed in Sec.1. the weight matrix $\mathbf{W}$ may also be erroneous and should be corrected. In TLS approach, we try to find a correct matrix $\mathbf{E_W}$ to $\mathbf{W}$, in addition to $\mathbf{E_{\Delta I}}$, so that

$$\text{minimize } \| \mathbf{E_W} | \mathbf{E_{\Delta I}} \|_F, \tag{6}$$

$$\textbf{subject to } \mathbf{\Delta I} + \mathbf{E_{\Delta I}} \in \textbf{Range}(\mathbf{W} + \mathbf{E_W}). \tag{7}$$

Here $\| \cdot \|_F$ denotes the Frobenius norm, which is defined as $\| \mathbf{E} \|_F = \left(\sum_m \sum_n (E_{mn})^2\right)^{1/2}$. After $\mathbf{E_W}$ to $\mathbf{W}$ and $\mathbf{E_{\Delta I}}$ are found, then any $\mathbf{\Delta I}$ satisfying

$$(\mathbf{W} + \mathbf{E_W})\mathbf{\Delta x} = \mathbf{\Delta I} + \mathbf{E_{\Delta I}} \tag{8}$$

is said to solve the TLS solution.

The TLS solution to an incompatible linear quation was first described by Golub and Van Loan [6]. The problem in Eq. (6-7) can be restated as:

$$\text{minimize } \| \mathbf{E} \|_F, \tag{9}$$

$$\text{subject to } (\mathbf{A} + \mathbf{E})\mathbf{q} = \mathbf{0}, \tag{10}$$

where

$$\mathbf{A} = [\mathbf{W} | \mathbf{\Delta I}] \qquad \mathbf{E} = [\mathbf{E_W} | \mathbf{E_{\Delta I}}] \tag{11}$$

and

$$\mathbf{q} = \begin{pmatrix} \mathbf{\Delta x} \\ -1 \end{pmatrix}.$$

Golub and Van Loan showed that the TLS solution is the right singular vector of $\mathbf{A}$ associated with the smallest singular value, under the condition that the singular value $\sigma_n > \sigma_{n+1}$ and $v_{n+1,n+1} \neq 0$, where σ_n represents the nth largest singular value, and $v_{n+1,n+1}$ is the last component of the singular vector v_{n+1} associated with σ_{n+1}. One way to obtain the TLS solution is by singular value decomposition (SVD) of $\mathbf{A}$ [6]. However, the SVD based TLS algorithm can become computationally intensive for large scale systems [7], [8]. In this paper, we adopt an iterative scheme that is more suitable for large scale problems. It has been shown [9] that constrained minimization problem in Eq. (9-10) is equivalent to the following minimization problem:

$$\text{minimize } F(\mathbf{q}) = \frac{\mathbf{q^T A^T A q}}{\mathbf{q^T q}}, \tag{12}$$

which in turn is equivalent to finding the eigenvector $\mathbf{q}$ associated with smallest eigenvalue of $\mathbf{A^T A}$ [9]. The function $F(\mathbf{q})$ is called the Rayleigh quotient. The minimal value of $F(\mathbf{q})$ is in fact equal to the minimal perturbation that satisfies Eq.(9), which in turn equals the minimal singular value, *i.e.*, $\min \| \mathbf{E} \|_F^2 = \min F(\mathbf{q}) = \sigma_{n+1}$. In the following, we describe a conjugate gradient (CG) method for the minimization of $F(\mathbf{q})$.

3 Conjugate Gradient Method

In most reported studies, the TLS problem is solved by SVD [7], [8], [10], for which the SVD method needs $O(L^3)$ multiplications, where L is the length of vector $\mathbf{q}$. Therefore the SVD based method is not suitable for large-scale systems. A recursive TLS algorithm was first used by Davila [11]. There the generalized eigenvector **q** was updated with a correction vector chosen as a Kalman filter gain vector, and the scalar (step size) was determined by minimizing the Rayleigh quotient (Eq.(12)). When the underlying linear equation originates for a 1-D linear convolution operation, this algorithm requires only on the order of L multiplications per iteration [11]. Bose et al. [12] applied this algorithm to reconstruct high resolution images from undersampled low resolution noisy multiframes. In this case, the convolution operator corresponds to a 2-D convolution operation and this algorithm requires $O(L^2)$ multiplications per iteration. In ther perturbation equation considered here, the matrix **W** does not correspond to a convolution operation. Our goal is to find an algorithm that is suitable for very large matrices of arbitrary structure. Toward this goal, the CG method [13], [14] has been applied. Although the CG method requires $O(L^2)$ multiplication per iteration, it is well-known that the CG method converges very fast and is particularly suitable for large matrices.

As stated above, the TLS solution can be obtained by minimizing the Rayleigh quotient in Eq.(12). Let $\mathbf{q}(k)$ represent the solution at kth iteration, the CG algorithm updates **q** by successive approximation as below:

$$\mathbf{q}(k+1) = \mathbf{q}(k) \; + \; \alpha(k)\mathbf{p}(k), \tag{13}$$

where $\alpha(k)$ is chosen to reach the minimum of $F(\mathbf{q})$ in the direction $\mathbf{p}(k)$. Following Hsavitt et al. [15], it can been shown that $\alpha(k)$ is always real and given by

$$\alpha(k) = [-B + \sqrt{B^2 - 4CD}\,]/(2D), \tag{14}$$

where

$$D = P_b(k)P_c(k) \; - \; P_a(k)P_d(k), \tag{15}$$

$$B = P_b(k) \; - \; \lambda(k)P_d(k), \tag{16}$$

$$C = P_a(k) \; - \lambda(k)P_c(k), \tag{17}$$

$$\lambda(k) = < \mathbf{Aq}(k), \mathbf{Aq}(k) >, \tag{18}$$

$$P_a(k) = < \mathbf{Aq}(k), \mathbf{Ap}(k) >, \tag{19}$$

$$P_b(k) = < \mathbf{Ap}(k), \mathbf{Ap}(k) >, \tag{20}$$

$$P_c(k) = < \mathbf{p}(k), \mathbf{q}(k) >, \tag{21}$$

$$P_d(k) = < \mathbf{p}(k), \mathbf{p}(k) > . \tag{22}$$

In the above equations, $< \cdot >$ represents the inner product. At time (k+1), the new search direction is chosen as

$$\mathbf{p}(k+1) = \mathbf{r}(k+1) \; + \; \beta(k)\mathbf{p}(k), \tag{23}$$

and the residue $\mathbf{r}(K+1)$ is given by

$$\mathbf{r}(k+1) = \lambda(k)\mathbf{q}(k+1) \; - \; \mathbf{A}^T\mathbf{Aq}(k+1). \tag{24}$$

In our implementation, the method for choosing $\beta(k)$ is slightly different from that used in [13]. We use the method developed by Fletcher and Reeves [16], also described by Yang et al. [14]. The $\beta(k)$ is chosen as

$$\beta(k) = < \mathbf{r}(k+1)\mathbf{r}(k+1) > / < \mathbf{r}(k), \mathbf{r}(k) > \tag{25}$$

to make the direction vectors $\mathbf{p}(k)$ $\mathbf{A}^T\mathbf{A}-$conjugate, *i.e.*,

$$< \mathbf{A}^T\mathbf{A}\mathbf{p}(k), \mathbf{p}(k+1) > = 0. \tag{26}$$

The convergence criterion we used is $|(\lambda(k+1) - \lambda(k))/\lambda(k)| < 10^{-3} \sim 10^{-4}$. The initial solution $\mathbf{q}(0)$ is set to a vector in which all elemnets are zero, except the last element which is set to 1.

4 Simulation Results

To compare the LS and TLS approaches, reconstruction of two test media containing an absorption inhomogeneity are attempted. One is a three-layer medium; the other one is a cylindrical phantom. A steady state (CW) measurement is considered, although the ITLS can be equally applied to TR data. The LS solution is the CGD algorithm [2].

1. A Three-Layer Medium

We first present reconstruction results for the three-layer medium. The original medium is illustrated in Fig. 1, which is 10 mean free path (mfp) thick, and the three layers are located from 0-3, 3-7 and 7-10 mfp, respectively. The absorption coefficient of the first and the third layers is 1%, and that of the middle layer is 5%. The scattering property in the three layers is homogeneous. This medium is discretized to 10 slices, each 1 mfp thick. The goal is to reconstruct the absorption coefficient of each slice. The source and detector reading are positioned only on the top surface, so that only backscattered photons are measured. The source-detector configurations are given in [2]. There are 40 detector readings and 10 unknowns, so the problem is overdetermined.

The weight functions have been calculated for both a homogeneous 10 mfp slab as well as the actual three-layer medium. These two sets of weights will be referred to as half-space weights and the three-layer weights, respectively. Two sets of readings are used: One is calculated according to Eq.(1) using the three-layer weights, the other one is obtained from Monte-Carlo simulations. Four experiments have been conducted. The first experiment is to evaluate the TLS reconstruction algorithm in an ideal situation. The calculated data and three-layer weights are used. Gaussian white noise is added to both the data and weights. The noise levels tested are 1%, 2%, and 5%. Here the noise level is defined as the ratio of noise standard deviation to a datum or weight value, which is between the minimum and average. Each column in the weight matrix and the data column are then scaled by noise standard deviations, such that the noise added in each column has the identical variance. This is usually required by the TLS algorithm. The reconstruction results by LS and TLS are shown in Fig. 2. The displayed images (*i.e.*, the image of $\Delta\mathbf{x}$) are all normalized so that the maximum value in $\Delta\mathbf{x}$ in each case is represented by the same darkness level. It can be seen that the LS algorithm began to break down as the noise level increases beyond 1%, while the TLS yielded a quite consistent and accurate result under all noise levels. This result is as expected, because the noise in both the weights and data are truly identically and independently distributed (i.i.d.), which is required for the TLS algorithm to work well. The second experiment is implemented by using the same data set (*i.e.*, calculated data from three layer weights) but with half plane weights. LS and TLS are used to reconstruct the medium, the reconstruction results are illustrated in Fig. 3(c) and Fig. 3(b), respectively. In this case, the noise in the weight matrix is not white, rather with a certain structure. The weight for voxels in the upper slices are likely to be under-estimated, while those in the lower slice are over-estimated. Even in this case, the TLS algorithm gives a fairly accurate result, significantly better than the LS. The third experiment uses simulated detector readings and the three-layer weights. The reconstruction results are shown in Fig.4. Fig. 4(a) is the result using LS, and Fig. 4(b) is the reconstruction result using TLS. It is reasonable to assume that the error in weights and data by Monte Carlo calculation are approximately i.i.d. The noise level should be fairly low because Monte Carlo simulation was done with a very high precision. In this case, the LS algorithm gave a reasonably good result, but not as accurate as the TLS. Both correctly identify the transition from the first to the second layer. The last experiment is conducted using simulated detector readings and the half-plane weight. The reconstruction results by the LS and TLS approaches are illustrated in Fig. 5(a) and Fig. 5(b), respectively. In this case, as in Experiment 2, the noise in the weight matrix is not white. Although the result of LS is qualitatively similar to that in Experiment 3, they are quite different quantitatively. The absorption strength is over-estimated in this experiment by a large amount. With TLS, the absorption strength is over-estimated in the upper slices. This is as expected because the weights there are under-estimated. One interesting observation is that the TLS algorithm yielded a more smooth reconstruction than the LS algorithm in all four experiments, more clearly indicating the actual three-layer structure. The reconstructed image by LS algorithm on the other hand often contain spurious peaks and valleys.

2. A Cylindrical Phantom

The second test medium is a cylindrical phantom. The cylindrical axis is infinitely long, and its diameter is 20 mfp. The heterogeneity is a 2 mfp diameter rod whose axis is halfway between the cylinder axis and the boundary (see [17]). The rod is a black absorber with infinite absorption. Only a 2D reconstruction on a single cross section is attempted. This cross section is discretized to 400 pixels. The sources and detectors are positioned around this cross section. The light source is a pencil beam directed normally to the surface. The detectors were spaced at 10° intervals about the cylinder (see [17]). The detector readings are calculated using Monte Carlo simulations for four different locations of the source, separated by 90° [17]. In the simulation, each photon incident on a medium undergoes repeated scattering until it is either absorbed in the interior or it escapes. Detector readings were calculated by counting all photons emerging from the cylinder within a patch of surface whose area is $5\pi/9$ mfp^2. Similar methods are employed to compute the weight function for a homogeneous cylinder medium with the same structure. The total number of detector reading is 144. So the problem is underdetermined. To circumvent this problem, a positivity constraint is added during the CG iteration similar to the approach described before for the LS using CGD [2].

To compare LS and TLS algorithm, white Gaussian noise is added to both the weights and detector readings. Two experiments are conducted, with noise levels of 7% and 10%, respectively. The noise level is defined as the ratio of the noise standard derivation to the square-root of the signal power. Fig. 6(a) shows the cross-section of the original medium, Fig. 6(b) and 6(d) are the reconstructed results by LS with positivity constraint at the two noise levels. Figs.6(c) and 6(e) are the reconstructed results by TLS with positivity constraint at the two noise levels. It can be seen that the TLS yielded slightly better reconstruction results than LS, especially quantitatively. Note that here we did not obtain as a significant improvement as in the three-layer slab case. This may be because the system is underdetermined so both LS and TLS do not have a unique solution.

5 Concluding Remarks and Discussion

In this paper, an iterative TLS reconstruction algorithm using conjugate gradient method is proposed for the solution of the perturbation equation in optical tomography. It is more suitable for large scale system compared to SVD based TLS algorithm. Compared to the LS solution, when noise is present in both the weight and detector readings, TLS outperforms the LS significantly when the system is overdetermined. This is true not only when the noise in the weights are truly random, but also when the weight matrix is subject to a systematic error caused by the mismatch between the reference medium and the test medium. This bears important implications. It suggests that the use of TLS may reduce the number of iterations in the perturbation approach.

When the system is underdetermined, the performance of TLS with positivity constraint is not significantly better than LS. The use of the TLS for an underdetermined problem needs further study. Furthermore, because of the ill-posed nature of the inverse problem, the weight matrix is often rank deficient, so regularization may be needed. In SVD based TLS, this can be accomplished by suppressing or truncating very small singular values. With optimization based approaches, one needs to investigate how to suppress the effects of insignificant but numerically non-zero singular values.

Finally, if the weight matrix is only partially subject to errors, *i.e.*, some weights are accurate, while others are noisy, the constrained TLS can be used [18, 19].

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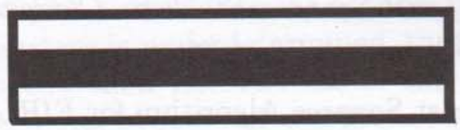

Figure 1: A cross section of the original three layer medium. The darkness gray level represents Δx_{max}, the maximum value of Δx, here Δx_{max} =5.0e-4

(a) (b) (c) (d) (e) (f)

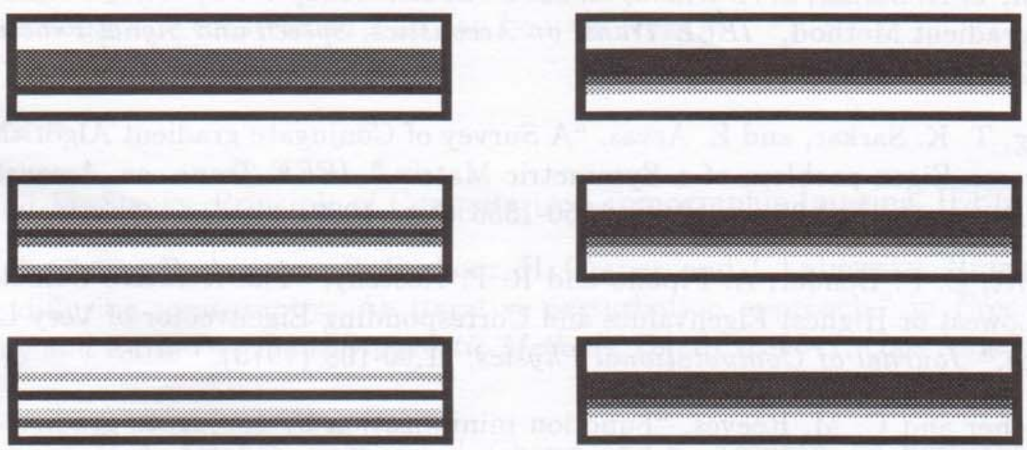

Figure 2: Reconstruction results using the three-layer weight and calculated data. Images in (a),(c) and (e) are the LS reconstruction results under the noise levels 1%, 2% and 5%, respectively, with Δx_{max} = 6.8e-4, 6.7e-4 and 1.9e-3. Images in (b),(d) and (f) are the ITLS reconstruction results under the corresponding noise levels, with Δx_{max} = 5.6e-4, 5.6e-4 and 5.8e-4, respectively.

(a)  (b)

Figure 3: Reconstruction for the three-layer medium using the half-plane weight and calculated data: (a) LS reconstruction result by CGD method, $\Delta \mathbf{x}_{max} = 8.7\text{e-}3$ (b) ITLS reconstruction result, $\Delta \mathbf{x}_{max} = 3.9\text{e-}4$.

(a)  (b)

Figure 4: Reconstruction for the three-layer medium using the three-layer weight simulated data: (a) LS reconstruction result by CGD method, $\Delta \mathbf{x}_{max} = 8.4\text{e-}3$ (b) ITLS reconstruction result, $\Delta \mathbf{x}_{max} = 8.4\text{e-}3$.

(a)  (b)

Figure 5: Reconstruction for the three-layer medium using the half-plane weight and simulated data: (a) LS reconstruction result by CGD method, $\Delta \mathbf{x}_{max} = 6.5\text{e-}1$ (b) ITLS reconstruction result, $\Delta \mathbf{x}_{max} = 1.7\text{e-}3$.

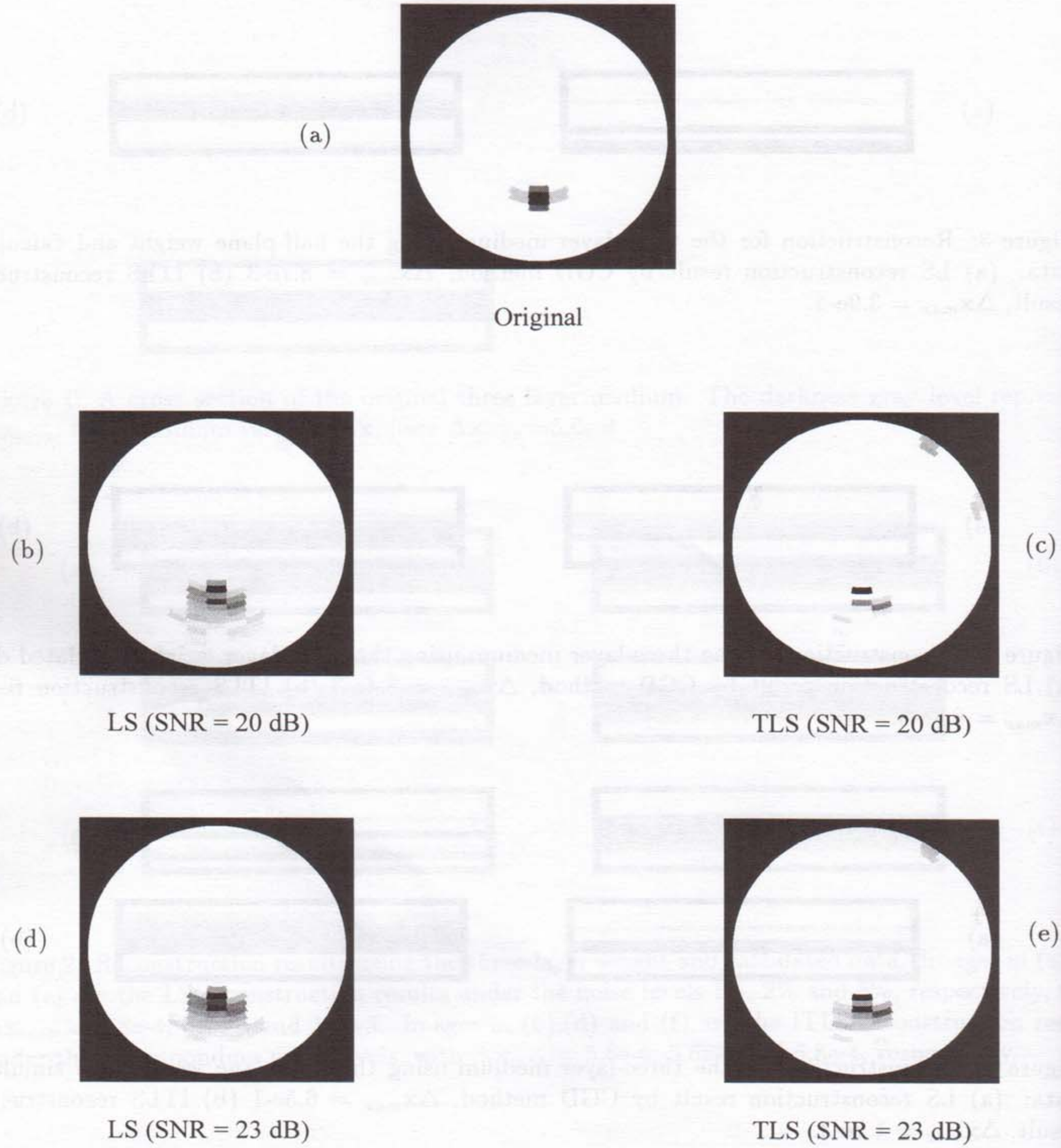

Figure 6: Reconstruction for the cylindrical phantom: (a) original; (b) and (c) reconstruction results by LS and ITLS with positivity constraint, respectively, under 10% (SNR=20 dB) noise. $\Delta \mathbf{x}_{max}$ = 5.0e-4 and 8.1e-3, respectively; (d) and (e) reconstruction results under 7% (SNR=23 dB) noise, $\Delta \mathbf{x}_{max}$ = 4.2e-4 and 7.6e-4, respectively.