A CONSTRAINED ITERATED TIKHONOV REGULARIZATION ALGORITHM FOR IMAGE RESTORATION

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Abstract. Many problems that arise in image processing applications require the solution of an ill-posed inverse problem, that is, one in which minor noise or perturbations in the data may result in major instabilities in the computed solution. Tikhonov regularization can be used to stabilize the inverse solution. However, it is well known that iterative schemes must be used to efficiently solve large-scale, sparse, or structured problems. Furthermore, due to physical properties of image processing, it is often desirable to compute nonnegative solutions. In this paper, we develop a constrained iterative Tikhonov scheme for image restoration (i.e. deblurring) that incorporates nonnegativity, and we use sophisticated state-of-the-art solvers for efficient implementation and automatic selection of regularization parameters.

Key words. Ill-posed problems, iterative methods, Lanczos bidiagonalization, regularization, Tikhonov, nonnegativity constraint

AMS Subject Classifications: 65F10, 65F22, 65F30

1. Introduction. Efficient implementation of accurate image reconstruction algorithms is advantageous to many fields. From astronomy to biomedical imaging, scientists require highly advanced techniques for computing clearer and more detailed images. Oftentimes, massive amounts of data and extensive computational power are needed for quality reconstructions, for example, in determining molecular structure from cryo-electron microscopy data [25]. Thus, the main challenge of image reconstruction is to develop algorithms that can reconstruct high-quality images in an efficient manner.

The basic image restoration or deblurring problem can be modeled as

$$\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}_{true} + \boldsymbol{n} \tag{1.1}$$

where $\boldsymbol{x}_{true}$ represents the true image, $\boldsymbol{A}$ models the blurring operation, often defined by a point spread function (PSF), and $\boldsymbol{n}$ is additive noise, that when added to the blurred image, results in the observed image, $\boldsymbol{b}$. The goal is to compute a faithful reconstruction of $\boldsymbol{x}_{true}$, given $\boldsymbol{b}$ and $\boldsymbol{A}$.

A common approach to solve the above problem is to solve the following optimization problem:

$$\min_{\boldsymbol{x}} \|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|, \tag{1.2}$$

where $\|\cdot\|$ denotes the 2-norm. However, the desired digital image consists of pixels representing light intensities, which are nonnegative values. We would like our computed image to satisfy this property, and thus our objective is to solve the nonnegatively constrained problem:

$$\min_{\boldsymbol{x}\geq 0} \|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|. \tag{1.3}$$

An important remark here is that problem (1.1) is ill-posed, meaning small noise in the observed image may result in large errors in the computed solution. This is

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a problem that has been studied extensively by many researchers, and some sort of regularization must be incorporated to stabilize the solution. We use the Tikhonov approach to dampen the least squares problem by solving the modified problem:

$$\min_{\boldsymbol{x}} \left\{ \|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|^2 + \lambda^2 \|\boldsymbol{x}\|^2 \right\} \tag{1.4}$$

where λ is a regularization parameter. It is easy to show that the solution can be found by solving the normal equations: $(\boldsymbol{A}^T\boldsymbol{A} + \lambda^2\boldsymbol{I})\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$, but a more stable approach is to solve the equivalent least squares problem:

$$\min_{\boldsymbol{x}} \left\| \begin{bmatrix} \boldsymbol{A} \\ \lambda\boldsymbol{I} \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ 0 \end{bmatrix} \right\| . \tag{1.5}$$

An inherent drawback of the Tikhonov regularization method is the limited accuracy of reconstruction that one can achieve when working with noisy data, which is often the case [7, 10]. The Iterated Tikhonov Regularization (ITR) method was developed to address this problem. Originally proposed by Riley in 1955 [23] and analyzed by Golub in 1965 [6], the iterated Tikhonov regularization method has the following basic form:

$$\begin{aligned} \boldsymbol{r}_k &= \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_k \\ (\boldsymbol{A}^T\boldsymbol{A} + \lambda^2\boldsymbol{I})\boldsymbol{e}_k &= \boldsymbol{A}^T\boldsymbol{r}_k \\ \boldsymbol{x}_{k+1} &= \boldsymbol{x}_k + \boldsymbol{e}_k \, . \end{aligned}$$

The great advantage of the ITR method is that if sufficiently enough iterations are made, we reach an accuracy that cannot be improved significantly with any other method, as noted in [10] and proved in [17].

In this paper, we develop an iterated Tikhonov regularization scheme which not only enforces nonnegativity, but also incorporates recently developed iterative methods, making this algorithm suitable for solving large-scale problems such as image restoration. The paper is organized as follows. Section 2 contains a description and development of the constrained iterated Tikhonov regularization algorithm, with special attention to using a conjugate gradient-type iterative algorithm for efficient implementation. Numerical results illustrating the favorable behavior of this algorithm are presented in Section 3, and conclusions are presented in Section 4.

2. Constrained Iterated Tikhonov Regularization.

Solving the nonnegatively constrained optimization problem (1.3) is surprisingly very difficult, and a variety of work has been done by many researchers [3, 11, 14, 16, 19]. Our approach to ensuring nonnegativity is motivated by the MRNSD algorithm presented in Nagy and Strakoš [19], originally suggested by Kaufman [13]. In this section, we develop a constrained ITR algorithm and describe an efficient conjugate gradient-type method based on the Lanczos bidiagonalization that makes the constrained ITR method robust and suitable for large-scale problems.

2.1. Incorporating Nonnegativity.

In order to maintain nonnegativity in the computed solution, we ensure nonnegativity at each iteration of the ITR algorithm. This is achieved in two ways. First, we scale the step direction with the current iterate, and secondly we use a bounded line search.

Let $\boldsymbol{r}_k = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_k$, and $\boldsymbol{X}_k = \mathrm{diag}(\boldsymbol{x}_k)$, then the solution update is given in the following form

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{s}_k$$

where $\boldsymbol{s}_k = \boldsymbol{X}_k \boldsymbol{p}_k$, and $\boldsymbol{p}_k$ solves the following least squares problem

$$\min_{\boldsymbol{p}} \|\boldsymbol{A}\boldsymbol{p} - \boldsymbol{r}_k\|. \tag{2.1}$$

The step length α_k is selected such that we minimize the current residual norm, $\|\boldsymbol{r}_{k+1}\|$, and maintain nonnegativity. We remark here that with simple algebraic manipulations, we can obtain formulas for the efficient update of the residual vector at each iteration. Furthermore, solving (2.1) efficiently is not trivial and will be addressed in Section 2.2. A summary of the constrained iterated Tikhonov regularization algorithm is provided in Algorithm 1.

Algorithm 1 Constrained ITR Algorithm

Choose $\boldsymbol{x}_0$
$\boldsymbol{r}_0 = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0$
$\boldsymbol{X}_0 = \mathrm{diag}(\boldsymbol{x}_0)$
for k = 0, 1, 2, ... **do**
  Solve equation (2.1) to get $\boldsymbol{p}_k$
  $\boldsymbol{s}_k = \boldsymbol{X}_k \boldsymbol{p}_k$
  $\boldsymbol{u}_k = A\boldsymbol{s}_k$
  $\gamma = \boldsymbol{r}_k^T \boldsymbol{u}_k$
  $\theta = \gamma / \boldsymbol{u}_k^T \boldsymbol{u}_k$
  $\alpha_k = \min(\theta, \min_{s_i<0}(\frac{-x_k}{s_i}))$
  $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{s}_k$
  $\boldsymbol{X}_{k+1} = \mathrm{diag}(\boldsymbol{x}_{k+1})$
  $\boldsymbol{r}_{k+1} = \boldsymbol{r}_k - \alpha_k \boldsymbol{u}_k$
end for

We remark here that by letting $\boldsymbol{p}_k = -\boldsymbol{g}_k$ where $\boldsymbol{g}_k = \boldsymbol{A}^T \boldsymbol{r}_k$ is the gradient at iteration k, we get the MRNSD algorithm. The MRNSD approach is essentially a scaled steepest descent approach in which the step direction is scaled by the distance of each variable to the nonnegativity constraint [16]. Thus, we allow variables further from the constraint to take larger steps than those near the constraint. A potential disadvantage of using this scaling factor is that variables that attain very small or zero values are highly unlikely to become large again. However, in experimental results we did not encounter such difficulties.

2.2. Efficient Implementation. In each iteration of the constrained ITR algorithm, we must solve a least squares problem (2.1) involving $\boldsymbol{A}$ and the current residual $\boldsymbol{r}_k$. Due to the ill-posed properties of the problem, we follow the framework of the iterated Tikhonov method and solve the augmented problem:

$$\min_{p} \left\| \begin{bmatrix} \boldsymbol{A} \\ \lambda \boldsymbol{I} \end{bmatrix} \boldsymbol{p} - \begin{bmatrix} \boldsymbol{r}_k \\ 0 \end{bmatrix} \right\|. \tag{2.2}$$

In the standard iterated Tikhonov method, λ is selected *a priori* and fixed. There are a variety of methods such as the Morozov discrepancy principle, Generalized

Cross-Validation(GCV), and L-curve that can guide one in selecting a regularization parameter, but many of these methods require a priori information about the noise or significant computation which is difficult for large-scale problems [12]. Other methods such as that proposed by Frommer and Mass [5] require the solution of multiple systems with different regularization parameters in order to find an optimal one. However, a fixed parameter is not necessarily the best option for the iterated Tikhonov method. Some advancements by Hanke, Groetsch [9] and Schock [24] illustrate that a non-stationary iterated Tikhonov method in which the the regularization parameter is allowed to change per iteration in a geometric manner can improve the convergence rate. However, an initial estimate of the noise level is required in their implementation, and they do not address an efficient solver to use, once the regularization parameter is determined.

We propose to solve the least squares problem using a recently developed conjugate gradient type method called HyBR [4]. HyBR is a hybrid bidiagonalization regularization method based on the well known iterative method LSQR [21]. Many researchers have studied hybrid methods which incorporate additional regularization at each iteration of the Krylov subspace method to stabilize the solution [1, 2, 8, 15, 20]. Some of the many advantages of using a hybrid method include fast convergence, stabilization of error amplification and efficient implementation for large-scale problems. A careful implementation which can reliably select regularization parameters and a stopping iteration is not trivial. Full details can be found in [4] and full MATLAB codes for HyBR are available at `www.mathcs.emory.edu/~nagy/WGCV`. This particular implementation uses a weighted GCV method to select the regularization parameters, and the stopping iteration is determined by monitoring the convergence behavior of the selected regularization parameters at each Lanczos iteration. More specifically, the GCV approach is used for both parameter estimation and choice of stopping criteria.

The iterated Tikhonov regularization method was developed in the 1950s as a simple update method for solving linear systems of equations, but in this paper, we have brought a new light to this old method. The novelty of our approach is that we incorporate a nonnegativity constraint with very little additional computational effort. Furthermore by using HyBR to solve (2.1) at each iteration of the constrained ITR algorithm, we can solve the Tikhonov problem efficiently and compute regularization parameters automatically.

3. Numerical Results. In this section, we illustrate the performance of the constrained ITR algorithm on some image reconstruction problems. First we try the algorithm on a smaller 1-D signal deblurring problem, and then we evaluate its performance on larger 2-D image reconstruction examples. In all experiments, the initial guess is a constant vector of the maximum value in the observed image. More specifically, it can be computed in MATLAB as

```
>> x_0 = max(b(:))*ones(size(b));
```

The iterative scheme is run for 50 outer iterations and a maximum of 50 inner HyBR iterations. We remark that not all 50 HyBR iterations are usually needed for the inner iterations, and HyBR is able to stop automatically based on its stopping criteria. We use 1% additive random noise, where the noise vector $\boldsymbol{n}$ consists of pseudo-random values drawn from a normal distribution with mean zero and standard deviation one. All computations were done in MATLAB , using IEEE double precision arithmetic.

Spectra Example: The 1-D spectra example is a small problem in which the goal is to reconstruct a pulse signal of dimension 64 which has been degraded by a

Gaussian blur. This example will allow us to see how the algorithm may perform when the desired solution contains many zero values. First, we compare the effect of using ITR with fixed regularization parameter to using ITR with HyBR (ignoring the nonnegativity constraint). By examining the first three curves on the relative error plots provided in Figure 3.1, we see that standard ITR may perform poorly (e.g. $\lambda = 0.01$) if the regularization parameter is inaccurate. HyBR allows the regularization parameter to change per iteration and selects these parameters automatically. We have thus illustrated the positive effects of using HyBR with the iterated Tikhonov method, even without including the nonnegativity constraint.

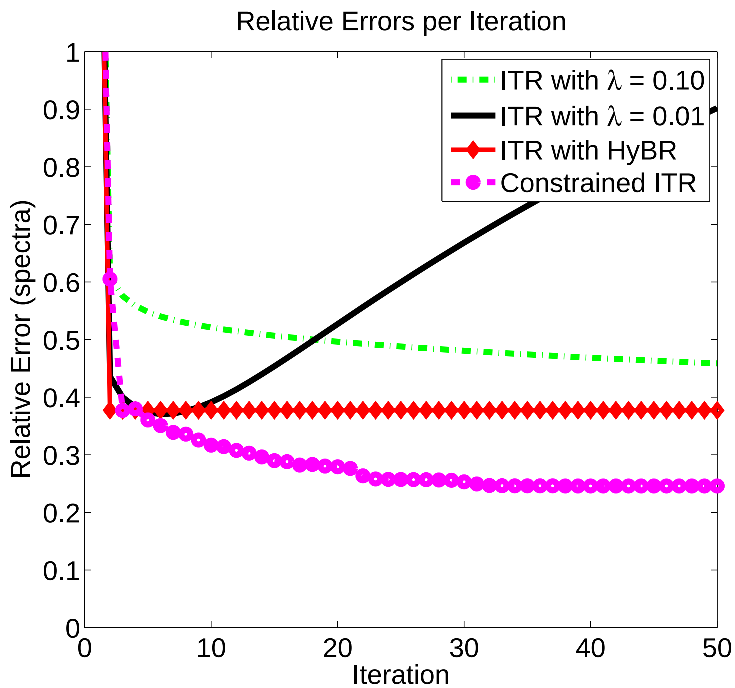

Fig. 3.1. *Relative error plots for 1-D spectra deblurring example.*

Then, comparing ITR with HyBR (no constraints) to the constrained ITR solution, we see that we can achieve significantly faster convergence accuracy by incorporating the constraint. Furthermore, the reconstructed solution has less oscillations and no negative values, as illustrated in Figure 3.2. This motivates our use of constrained ITR for larger 2-D image reconstruction problems, especially those where the solution contains many zeros.

Satellite Example: The satellite example comes from the iterative image deblurring package, 'RestoreTools' [18]. The true image, shown in Figure 3.4 (a), has 256×256 pixels and the blurring operator is defined by a Gaussian point spread function. The observed image is shown in Figure 3.4 (b), and the goal is to reconstruct an approximation of the true image. An object-oriented implementation that takes advantage of the special structure of the problem allows for efficient computation of matrix-vector multiplications. See [18] for further details.

The relative error plots for ITR with HyBR and constrained ITR are provided in Figure 3.3. The constrained ITR algorithm has slightly better convergence, which

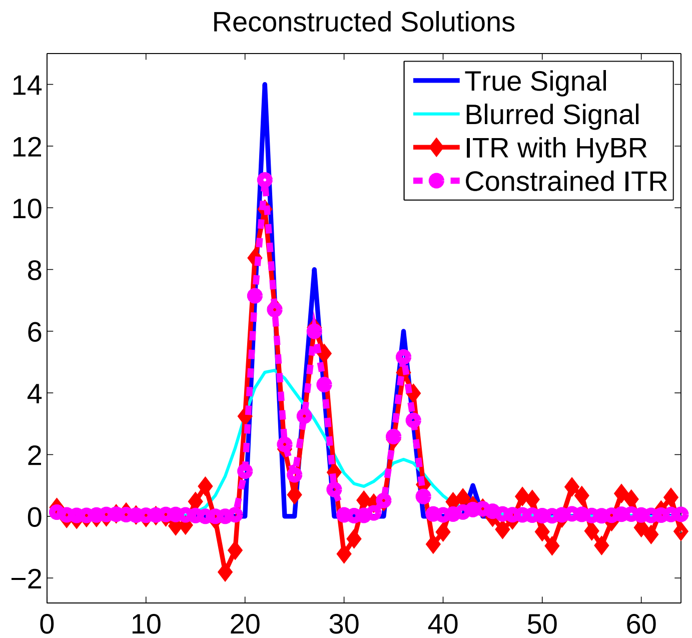

FIG. 3.2. *Reconstructed Solutions for 1-D spectra example.*

is illustrated in the reconstructed images displayed in Figure 3.4 (c-d). After 50 iterations, the solution from ITR with HyBR contained many negative values, thus we set all pixels with negative entries to zero before displaying.

Grain example: The constrained ITR with HyBR method performed well in deblurring Gaussian blur, but we also want to try it on other types of blur. Another image processing example is to recover a partial image of a piece of grain that was blurred by a cubic phase mask. The true and observed images shown in Figure 3.6 (a-b) are 256×256, and efficient matrix-vector multiplications are necessary for implementation, similar to the Satellite example.

The relative error plots for this example are shown in Figure 3.5, and as expected, the constrained ITR algorithm reflects faster convergence to a higher accuracy. This observation is further supported by the reconstructed images, which can be found in Figure 3.6 (c-d). The reconstructed image for ITR with HyBR after 50 iterations (with negative entries set to zero) contains image artifacts, whereas the constrained ITR reconstruction is significantly better.

4. Conclusions. In this paper, we have developed a novel method for solving nonnegatively constrained least squares problems and illustrated its positive performance on a variety of image deblurring examples. Using a scaled step direction and bounded line search, we were able to enforce nonnegativity at each iteration of the Iterated Tikhonov Regularization method. Furthermore, we used a sophisticated conjugate gradient-type iterative method at each ITR iteration for improved convergence and automatic selection of regularization parameters. Our results showed that the convergence behavior of the constrained ITR with HyBR was very good, and more importantly, the solution images were more visually appealing, with more clarity and

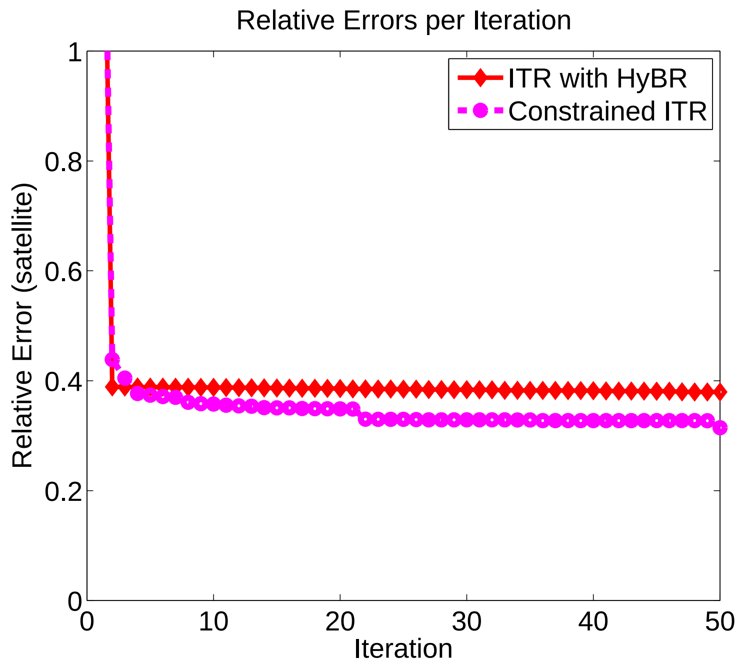

FIG. 3.3. *Relative error plot for Satellite example.*

details.

Future goals will be to gain a solid theoretical understanding of the algorithm. A variety of authors have studied the convergence behavior of the standard and non-stationary ITR algorithm [9, 17], but more work must be done to analyze the effects of including a line search parameter and scaling at each iteration for nonnegativity. Also, since the major computational effort required in the constrained ITR algorithm lies in solving the least squares problem (2.1) with a new residual vector, it may be possible to recycle some of the information from previous iterates to make the bidiagonalization process from the HyBR algorithm more efficient [22].

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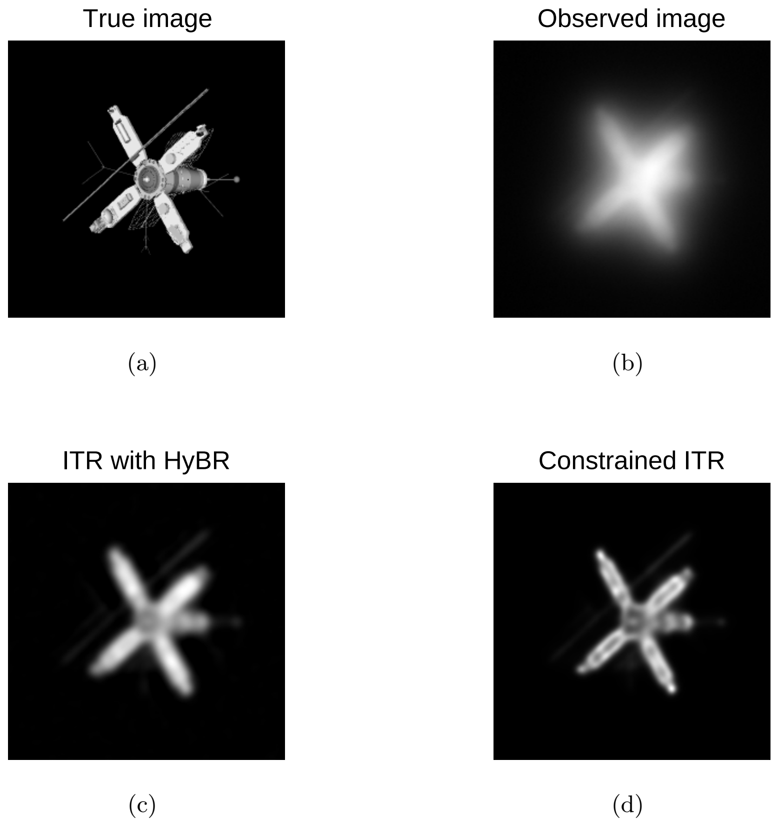

FIG. 3.4. *True, observed and reconstructed images for the satellite example after* 50 *iterations.*

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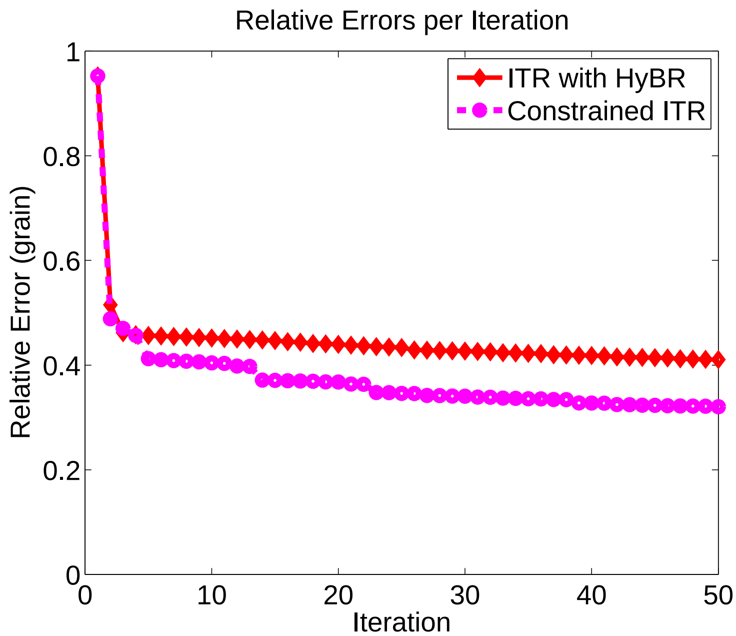

FIG. 3.5. *Relative error plot for Grain example.*

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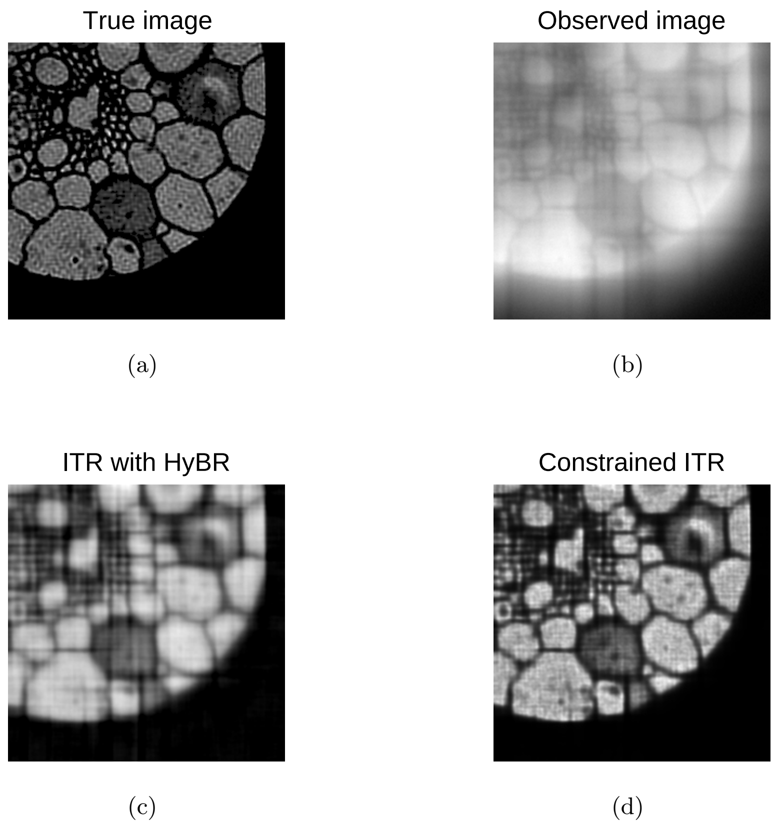

FIG. 3.6. *True, observed and reconstructed images for the Grain example after* 50 *iterations.*