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# A New Method for Linear Ill-posed Problems

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## Abstract

In this paper, we propose a new method for solving large-scale ill-posed problems based on the Karush-Kuhn-Tucker conditions and the discrepancy principle. We actually provide a framework for the solution of large-scale ill-posed problems. The big difference of our method from the existing methods for the solution of ill-posed problems is that, we do not need to choose regularization parameter in advance, but decide it iteratively. Experimental results show that the proposed method is effective and promising.

**Keywords.** Newton's method, ill-posed problems, Tikhonov regularization, L-curve, generalized cross validation.

## 1 Introduction

We consider the solution of linear systems that arise from large-scale inverse problems:

$$Ax = b, \quad b = b_{true} + N, \quad b_{true} = Ax_{true}, \quad (1.1)$$

where  $A \in R^{m \times n}$  ( $m \geq n$ ),  $b_{true} \in R^m$  and  $x_{true} \in R^n$ .  $N \in R^m$  represents unknown noise due to measurement interference and other errors in the recorded signal, as well as noise and inaccuracies in the measuring device.

Inverse problems of the form (1.1) arise in a variety of important applications in science and industry, including image reconstruction, image deblurring, geophysics, parameter identification and inverse scattering. See, for example, [4] [17] [22] and the references therein. In these applications the goal is to estimate some unknown attributes of interest, given measurements that are only indirectly related to these attributes. Typically these problems are ill-posed, meaning that noise in the data may give rise to significant errors in computed approximations of  $x_{true}$ . So regularization is necessary to deal with the ill-posedness.

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Many regularization methods have been developed. Probably the most well known is Tikhonov regularization [13], which is equivalent to solving the least squares problem

$$\min_x (\|Ax - b\|_2^2 + \lambda^2 \|Lx\|_2^2), \quad (1.2)$$

where  $L$  is a regularization operator, often chosen as the identity matrix or a discretization of a differentiation operator. The regularization parameter  $\lambda$  is a scalar, usually satisfying  $\sigma_n \leq \lambda \leq \sigma_1$ , where  $\sigma_n$  is the smallest singular value of  $A$  and  $\sigma_1$  is the largest singular value of  $A$ .

In Tikhonov regularization, parameter selection is very important. An optimal regularization parameter should fairly balance the perturbation error and the regularization error in the regularized solution. There are several possible strategies that depend on additional information referring to the analyzed problem and its solution, e.g., the discrepancy principle, the L-curve, and generalized cross validation (GCV) [4] [17] [22]. There are advantages and disadvantages to each of these approaches [4], especially for large-scale problems.

An alternative to Tikhonov regularization for large-scale problems is iterative regularization. In this case, an iterative method such as LSQR is applied to the least squares problem,

$$\min_x \|b - Ax\|_2. \quad (1.3)$$

However, when applied to ill-posed problems, these iterative methods exhibit an interesting “semi-convergence” behavior [14, 4], in that the quantity of the relative solution error first decreases and then increases.

The semiconvergence behavior of LSQR can be stabilized by using a hybrid method that combines an iterative Lanczos bidiagonalization algorithm with a direct regularization scheme, such as Tikhonov or truncated SVD [4]. The basic idea of this approach is to project the large-scale problem onto Krylov subspaces of small (but increasing) dimension. The projected problem can be solved cheaply using any direct regularization method. In [4], a very effective method called weighted-GCV (W-GCV) was developed.

In this paper, we develop a new method for solving large-scale ill-posed problems based on the Karush-Kuhn-Tucker conditions and the discrepancy principle, and actually provide a framework for the solution of large-scale ill-posed problems. The big difference of our method from the above mentioned methods is that, we do not need to choose regularization parameter in advance, but decide it iteratively. Experimental results show that the proposed method is effective and promising.

Our paper is organized as follows. In section 2, we review Tikhonov regularization and the GCV method. In section 3, we review Lanczos-hybrid method and W-GCV, which is very effective for large scale ill-posed problems. In section 4, we introduce a new regularization method, and provide some properties of the new regularization method. In section 5, we develop our proposed method. Experimental results are provided in section 6, and some concluding remarks are given in section 7.

## 2 Tikhonov regularization and GCV

In this section, we briefly review Tikhonov regularization and GCV.

Tikhonov regularization requires solving the minimization problem given in (1.2). For ease of notation, we take  $L$  to be the identity matrix throughout the paper.

Let  $A = U\Sigma V^T$  denote the SVD of  $A$ , where the columns  $u_i$  of  $U$  and  $v_i$  of  $V$  contain, respectively, the left and right singular vectors of  $A$ , and  $\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n)$  is a diagonal matrix containing the singular values of  $A$ , with  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$ . Replacing  $A$  by its SVD and performing a little algebraic manipulation, we obtain the Tikhonov regularized solution

$$x_\lambda = \sum_{i=1}^n \phi_i \frac{u_i^T b}{\sigma_i} v_i, \quad (2.1)$$

where  $\phi_i = \frac{\sigma_i^2}{\sigma_i^2 + \lambda^2} \in [0, 1]$  are the Tikhonov filter factors. As mentioned in the introduction, a variety of parameter choice methods can be used to determine  $\lambda$ . Here we just describe GCV, for the introduction of W-GCV in the next section. The basic idea of GCV is that a good choice of  $\lambda$  should predict missing values of the data. That is, if an arbitrary element of the observed data is left out, then the corresponding regularized solution should be able to predict the missing observation fairly well [4]. We leave out each data value  $b_j$  in turn and seek the value of  $\lambda$  that minimizes the prediction errors, measured by the GCV function

$$G_{A,b}(\lambda) = \frac{n \|(I - AA_\lambda^+)b\|_2^2}{(\text{trac}(I - AA_\lambda^+))^2}, \quad (2.2)$$

where  $A_\lambda^+ = (A^T A + \lambda^2 I)^{-1} A^T$ , and accordingly gives the regularized solution  $x_\lambda = A_\lambda^+ b$ . Replacing  $A$  with its SVD, (2.2) can be rewritten as

$$G_{A,b}(\lambda) = \frac{n \left( \sum_{i=1}^n \left( \frac{\lambda^2 u_i^T b}{\sigma_i^2 + \lambda^2} \right)^2 + \sum_{i=n+1}^m (u_i^T b)^2 \right)}{\left( (m-n) + \sum_{i=1}^n \frac{\lambda^2}{\sigma_i^2 + \lambda^2} \right)^2}, \quad (2.3)$$

which is a computationally convenient form to evaluate, thus making GCV easily used with standard minimization algorithms.

## 3 Lanczos-hybrid methods and W-GCV

Using GCV to determine the Tikhonov regularization parameter can be quite effective, but the minimization function (2.3) requires that the SVD of the matrix  $A$  be computed, and this is not feasible when  $A$  is too big. This leads us to Lanczos-hybrid

methods, which make computing the SVD of the operator feasible by projecting the problem onto a subspace of small dimension. Hybrid methods can be an effective way to stabilize the semiconvergent behavior that is characteristic of iterative methods like LSQR when applied to ill-posed problems. In this section, we review the Lanczos-hybrid methods and W-GCV proposed in [4].

Given a matrix  $A$  and a vector  $b$ , the  $k$ th-iteration of Lanczos bidiagonalization ( $k = 1, \dots, n$ ) computes an  $m \times (k+1)$  matrix  $W_k$ , an  $n \times k$  matrix  $Y_k$ , an  $n \times 1$  vector  $y_{k+1}$ , and a  $(k+1) \times k$  bidiagonal matrix  $B_k$  such that

$$A^T W_k = Y_k B_k^T + \alpha_{k+1} y_{k+1} e_{k+1}^T, \quad (3.1)$$

$$A Y_k = W_k B_k, \quad (3.2)$$

where  $e_{k+1}$  denotes the  $(k+1)$ st unit vector. Matrices  $W_k$  and  $Y_k$  have orthonormal columns, and the first column of  $W_k$  is  $b/\|b\|$ . We appropriate the problem (1.3) by the projected LS problem

$$\min_{x \in R(Y_k)} \|b - Ax\|_2 = \min_f \|W_k^T b - B_k f\|_2 = \min_f \|\beta e_1 - B_k f\|_2, \quad (3.3)$$

where  $\beta = \|b\|$ . Since the original problem is ill-posed,  $B_k$  may become very ill-conditioned. Regularization must be applied to solve the LS problem

$$\min_f \|B_k f - \beta_1 e_1\|_2. \quad (3.4)$$

This leads to Lanczos-hybrid method. The standard GCV method for parameter selection can be effective for most problems, however, the method may not perform well for the Lanczos-hybrid method as pointed in [4]. So weighted GCV for parameter selection was proposed in [4]. Instead of the GCV function defined in (2.2), the weighted-GCV function defined by

$$G_{A,b}(\omega, \lambda) = \frac{n\|(I - AA_\lambda^+)b\|_2^2}{(\text{trac}(I - \omega AA_\lambda^+))^2} \quad (3.5)$$

is proposed. This method has been proved to be very effective for large-scale ill-posed problem [4].

## 4 A new regularization method and its properties

There are some other regularization methods instead of Tikhonov's regularization. For example, in [17], P. C. Hansen suggested two methods that are formulated as the following least squares problems with a quadratic constraint:

$$\min \|Ax - b\|_2 \quad \text{subject to} \quad \|L(x - x^*)\|_2 \leq \alpha, \quad (4.1)$$

$$\min \|L(x - x^*)\|_2 \quad \text{subject to} \quad \|Ax - b\|_2 \leq \delta, \quad (4.2)$$

where  $x^*$  is an a priori estimate of the desired regularized solution, and  $\alpha$  and  $\delta$  are nonzero parameters each playing the role of the regularization parameter in (4.1) and (4.2), respectively.

These regularization methods may be not good, because in this way, the regularized solution may be biased towards the a priori estimate  $x^*$ . So in this section, we consider the following regularization methods:

$$\min \|x\|_2^2 \quad \text{subject to} \quad \|Ax - b\|_2^2 \leq \delta^2, \quad (4.3)$$

where  $\delta$  is a nonzero parameter playing the role of the regularization parameter. Now we consider some properties of the regularization method (4.3).

Let

$$\mathcal{L}(x, \lambda) = \|x\|_2^2 + \lambda(\|Ax - b\|_2^2 - \delta^2) \quad (4.4)$$

be the Lagrangian function related to (4.3),  $\partial_x \mathcal{L}(x, \lambda) = 0$  leads to

$$x + \lambda A^T(Ax - b) = 0. \quad (4.5)$$

From (4.5), we see that, regularization method (4.3) is closely related to Tikhonov regularization methods (1.2).

On the other hand, we can prove that, when  $\delta \rightarrow 0$ , the solution of (4.3) converges to the minimal solution of the least squares problem (1.3).

Let  $A = U\Sigma V^T$  be the SVD of  $A$ , then  $x^+ = \sum_{i=1}^{\text{rank}(A)} \frac{u_i^T b}{\sigma_i} v_i$  is the minimal-norm least squares solution of the problem (1.3). Since the solution of (4.3) satisfies  $\|Ax - b\|_2^2 \leq \delta^2$ , there exist  $\bar{\delta} = (\bar{\delta}_1, \bar{\delta}_2, \dots, \bar{\delta}_m)^T$ , such that  $x$  satisfies

$$Ax - b = \bar{\delta} \quad (4.6)$$

with  $\|\bar{\delta}\|_2 \leq \delta$ . Using the SVD of  $A$ , we can deduce from (4.6) that,

$$x = \sum_{i=1}^{\text{rank}(A)} \left( \frac{u_i^T b}{\sigma_i} v_i + \frac{u_i^T \bar{\delta}}{\sigma_i} v_i \right). \quad (4.7)$$

From (4.7), we have  $x \rightarrow x^+$  when  $\delta$  goes to zero. From the expression (4.7), we known also that the solution of (4.3) is continuous with  $\delta$ . So we have

**Lemma 4.1.** *The solution of (4.3) is continuous with  $\delta$ .*

**Lemma 4.2.** *If  $\delta$  goes to zero, then the solution  $x$  of (4.3) converges to the minimal solution of the least squares problem (1.3).*

## 5 Our proposed method

In this section, we present a new method for large-scale ill-posed problems, which is based on the Karush-Kuhn-Tucker conditions and the discrepancy principle. This method does not require any prior good estimate of the regularization parameter. In the proposed regularization method, the original linear system (1.1) is formulated as the following least squares problem with a quadratic constraint:

$$\min \|x\|_2^2 \quad \text{subject to} \quad \|Ax - b\|_2^2 \leq \delta^2, \quad (5.1)$$

see section 4.

By the Karush-Kuhn-Tucker conditions, there exist Lagrange multiplier  $\lambda \geq 0$ , such that

$$\begin{cases} x + \lambda A^T(Ax - b) = 0, \\ \lambda \geq 0, \quad \|Ax - b\|_2^2 \leq \delta^2. \end{cases} \quad (5.2)$$

It is well known that the Fisher-Burmeister function  $\phi : R^2 \rightarrow R$ , defined by

$$\phi(a, b) = \sqrt{a^2 + b^2} - a - b.$$

possesses the following characterization:

$$\phi(a, b) = 0 \iff a \geq 0, \quad b \geq 0 \quad \text{and} \quad ab = 0.$$

By using the above property, it is easy to deduce that solving the system (5.2) is equivalent to solving the system of nonlinear equations

$$F(z) = 0, \quad (5.3)$$

where  $F : R^{n+1} \rightarrow R^{n+1}$  is defined by

$$F(z) = \begin{pmatrix} x + \lambda A^T(Ax - b) \\ \phi(\lambda, \delta^2 - \|Ax - b\|_2^2) \end{pmatrix}, \quad (5.4)$$

and  $z = (x^T, \lambda)^T$ . The function  $F$  is not differentiable when  $\lambda^2 + (\delta^2 - \|Ax - b\|_2^2)^2 = 0$ . To overcome this drawback, we can set  $\phi(a, b) = \sqrt{a^2 + b^2 + \epsilon} - a - b$ , where  $\epsilon$  is a small positive number, usually chosen as *eps*, the machine precision. In this way, we can solve the large-scale ill-posed problem by solving the nonlinear equations (5.3).

Now we consider the solution of nonlinear equation (5.3). Newton's method is the first choice.

$$z_{k+1} = z_k + s_k, \quad k = 0, 1, 2, \dots, \quad (5.5)$$

where  $s_k$  satisfies

$$F'(z_k)s_k + F(z_k) = 0, \quad k = 0, 1, 2, \dots, \quad (5.6)$$

with  $z_0$  the initial chosen point.

In order to globalize this method, a line search technique is used to achieve a sufficient decrease of the natural merit function

$$M(z) = \frac{1}{2} \|F(z)\|_2^2.$$

**Algorithm 5.1.** (The global Newton method)

1. Given initial guess  $z_0 = (x_0^T, \lambda_0)^T \in R^{n+1}$ , a positive integer  $L$ . For  $k = 0, 1, \dots, K_{\max}$ , do the following steps.

2. Compute search direction using Newton's method. That is, find  $s_k$  satisfies

$$F'(z_k)s_k + F(z_k) = 0, \quad k = 0, 1, 2, \dots. \quad (5.7)$$

3. Line search.

Find the first number  $\lambda_k$  of the sequence  $\{1, \frac{1}{2}, \frac{1}{4}, \dots, \frac{1}{2^i}, \dots\}$  satisfying:

$$M(z_k + \lambda_k s_k) \leq \max_{0 \leq j \leq L} M(z_{k-j}) + \alpha \lambda_k \nabla M(z_k)^T s_k.$$

4. Updates. Set  $z_{k+1} = z_k + \lambda_k s_k$ .

**Remark 1.** It is generally difficult to solve the Newton equation (5.7) because of a large number of variables for large-scale ill-posed problems. In this case, inexact Newton's methods are useful candidates. Combining with Krylov subspace methods, the nonlinear equation can be solved efficiently. Based on (5.3) (5.4), any efficient method for solving nonlinear equations can be used to solve linear ill-posed problems, so we provide an alternative way for the solution of ill-posed problems.

**Remark 2.** As it is well-known, Newton's method is a local convergent method. That is, the convergence of the method depends on the initial point. To overcome this drawback, global convergence method like numerical continuation method can be used to solve the corresponding nonlinear equation. We will consider this in the future work.

## 6 Numerical Results

In this section, we present six numerical examples, which are taken from the "Regularization Tools" package [16]. In each case we generate a  $256 \times 256$  matrix  $A$ , the solution  $x_{true}$  and noise free observation vector  $b_{true} = Ax_{true}$ . The noise vector  $b$  was generated by  $b = b_{true} + N$ , where  $N$  is a noise vector whose entries are chosen from a normal distribution with mean 0 and variance 1, and scaled so that

$$\frac{\|N\|_2}{\|b_{true}\|_2} = 0.1.$$

We evaluate the method using the relative error

$$\text{Rerr} = \|x_{computed} - x_{true}\| / \|x_{true}\|$$

between the computed solution and the exact one.



**Example 1.** “Phillips”. This test problem is obtained by discretizing the first kind Fredholm integral equation  $b(s) = \int_{-6}^6 a(s, t)x(t)dt$ , where

$$\begin{aligned} a(s, t) &= \rho(s - t), \quad x(t) = \rho(t), \\ b(s) &= (6 - |s|)\left(1 + \frac{1}{2} \cos \frac{\pi s}{3}\right) + \frac{9}{2\pi} \sin\left(\frac{\pi|s|}{3}\right), \\ \rho(t) &= \begin{cases} 1 + \cos \frac{\pi t}{3}, & |t| < 3, \\ 0, & |t| \geq 3. \end{cases} \end{aligned}$$

**Example 2.** “Shaw” is a one-dimensional image restoration problem.  $A$  and  $x_{true}$  are obtained by discretizing, on the interval  $-\frac{\pi}{2} \leq s, t \leq \frac{\pi}{2}$ , the functions

$$\begin{aligned} a(s, t) &= (\cos(s) + \cos(t))\left(\frac{\sin u}{u}\right)^2, \quad s, t \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right], \quad u = \pi(\sin(s) + \sin(t)), \\ x(t) &= 2 \exp(-6(t - 0.8)^2) + \exp(-2(t + 0.5)^2). \end{aligned}$$

and  $b_{true} = Ax_{true}$ .

**Example 3.** “Deriv2” constructs  $A$  and  $b_{true}$  by discretizing a first kind Fredholm integral equation  $b(s) = \int_0^1 a(s, t)x(t)dt$ ,  $0 \leq s \leq 1$  where the kernel  $a(s, t)$  is given by the Green’s function for the second derivative:

$$\begin{aligned} a(s, t) &= \begin{cases} s(t - 1), & s < t, \\ t(s - 1), & s \geq t, \end{cases} \\ x(t) &= t, \quad b(s) = (s^3 - s)/6. \end{aligned}$$

**Example 4.** “Baart” constructs  $A$  and  $b_{true}$  by discretizing a first kind Fredholm integral equation  $b(s) = \int_0^\pi a(s, t)x(t)dt$ ,  $0 \leq s \leq \frac{\pi}{2}$ , where

$$\begin{aligned} a(s, t) &= \exp(s \cos t), \quad x(t) = \sin t, \\ b(s) &= \frac{2 \sin hs}{s}. \end{aligned}$$

**Example 5.** “Heat” is an inverse heat equation using the Volterra integral equation of the first kind on  $[0, 1]$  with kernel  $a(s, t) = k(s - t)$  where

$$k(t) = \frac{t^{-\frac{3}{\lambda}}}{2\sqrt{\pi}} \exp\left(-\frac{1}{4t}\right).$$

**Example 6.** “Wing” is the discretization of a first kind Fredholm integral equation with kernel  $K(s, t)$  and right-hand side  $g(s)$  given by

$$\begin{aligned} K(s, t) &= t \exp(-st^2), \quad 0 < s, t < 1, \\ g(s) &= \frac{\exp(-st_1^2) - \exp(-st_2^2)}{2s}, \quad 0 < s < 1. \end{aligned}$$

For the above six examples, we test our method and hybrid method with W-GCV regularization (denoted HyBR) [4]. In the experiments, we set  $x_0$  be zero vector,  $\delta = 0.1$ ,  $M = 5$  and the algorithm is stopped when  $\frac{|M(z_k) - M(z_{k-1})|}{M(z_{k-1})} \leq 10^{-6}$  and  $k > 50$  for our method. The initial values of  $\lambda$  for the six examples are listed in table 6.1.

Table 6.1: Initial value of  $\lambda$  for the six examples.

Problem	Phillips	Shaw	Deriv2	Baart	Heat	Wing
$\lambda_0$	5	800	100000	5000	10000	100000

Table 6.2: Relative error of our method and HyBR for the six examples.

Problem	Phillips	Shaw	Deriv2	Baart	Heat	Wing
Our method	0.0796	0.1749	0.3234	0.2300	0.2538	0.6022
HyBR	0.0759	0.1730	0.3362	0.2762	0.2727	0.6039

HyBR method is stopped when  $\frac{|GCV(k)-GCV(k-1)|}{GCV(1)} \leq 10^{-6}$  and  $k > 50$ . See [4] for details.

The relative errors for both our method and HyBR are listed in table 6.2.

The true data “ $Ax_{true}$ ”, noisy data  $b = Ax_{true} + N$ , true solution  $x_{true}$  and computed solution of our method and HyBR are depicted in figures 6.1 to 6.6. The convergence curves are showed in figure 6.7 and figure 6.8.

According to the figures 6.1 to 6.8, and table 6.2, we see that, our method generally has rapid convergence and accurate results. So we think the proposed method is promising and competitive.

## 7 Conclusions

In this paper, we present a new method for large-scale ill-posed problems based on the Karush-Kuhn-Tucker conditions and the discrepancy principle. We actually provide a framework for the solution of large-scale ill-posed problems. Under this framework, more efficient methods can be developed.

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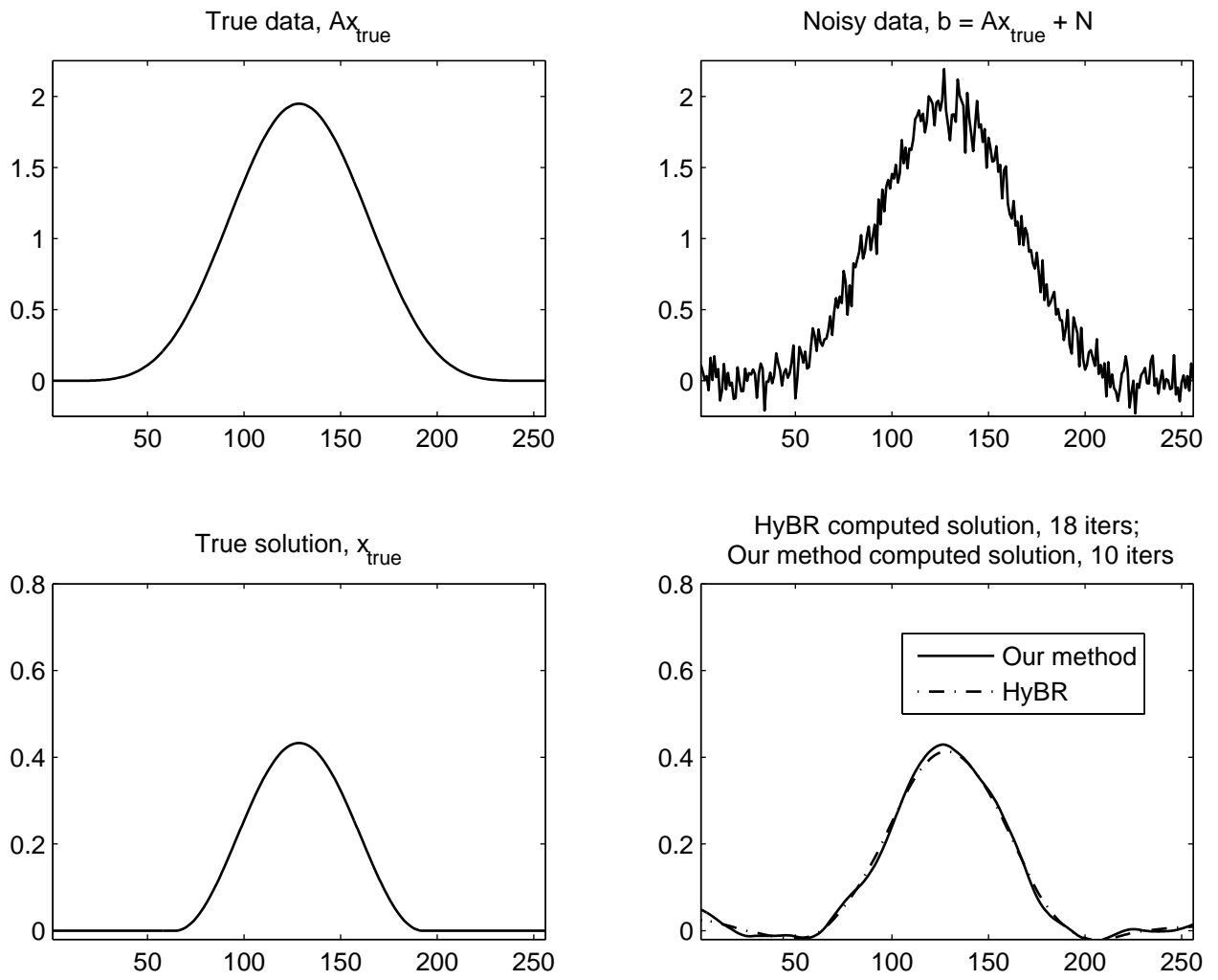


Figure 6.1: "Phillips"

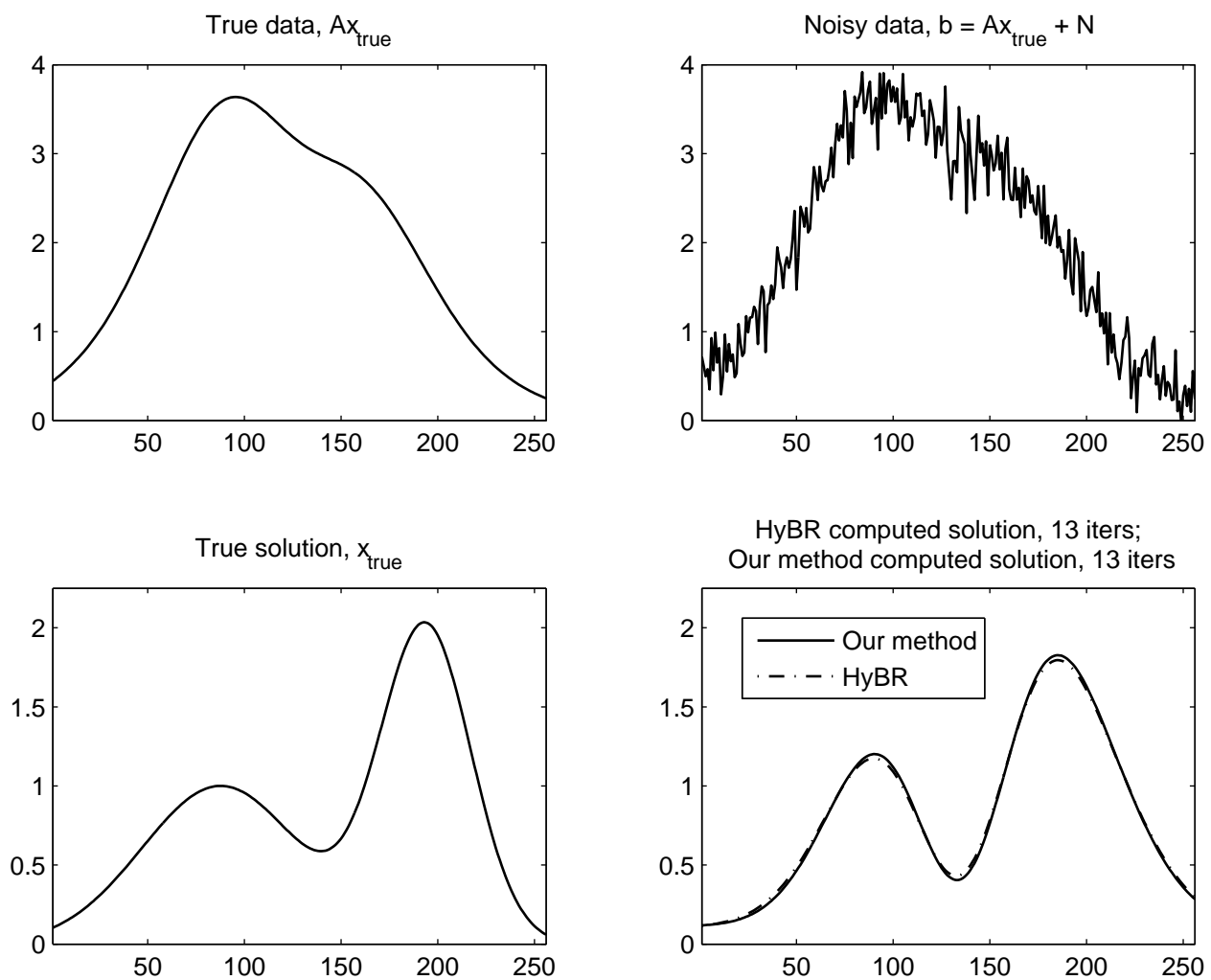


Figure 6.2: "Shaw"

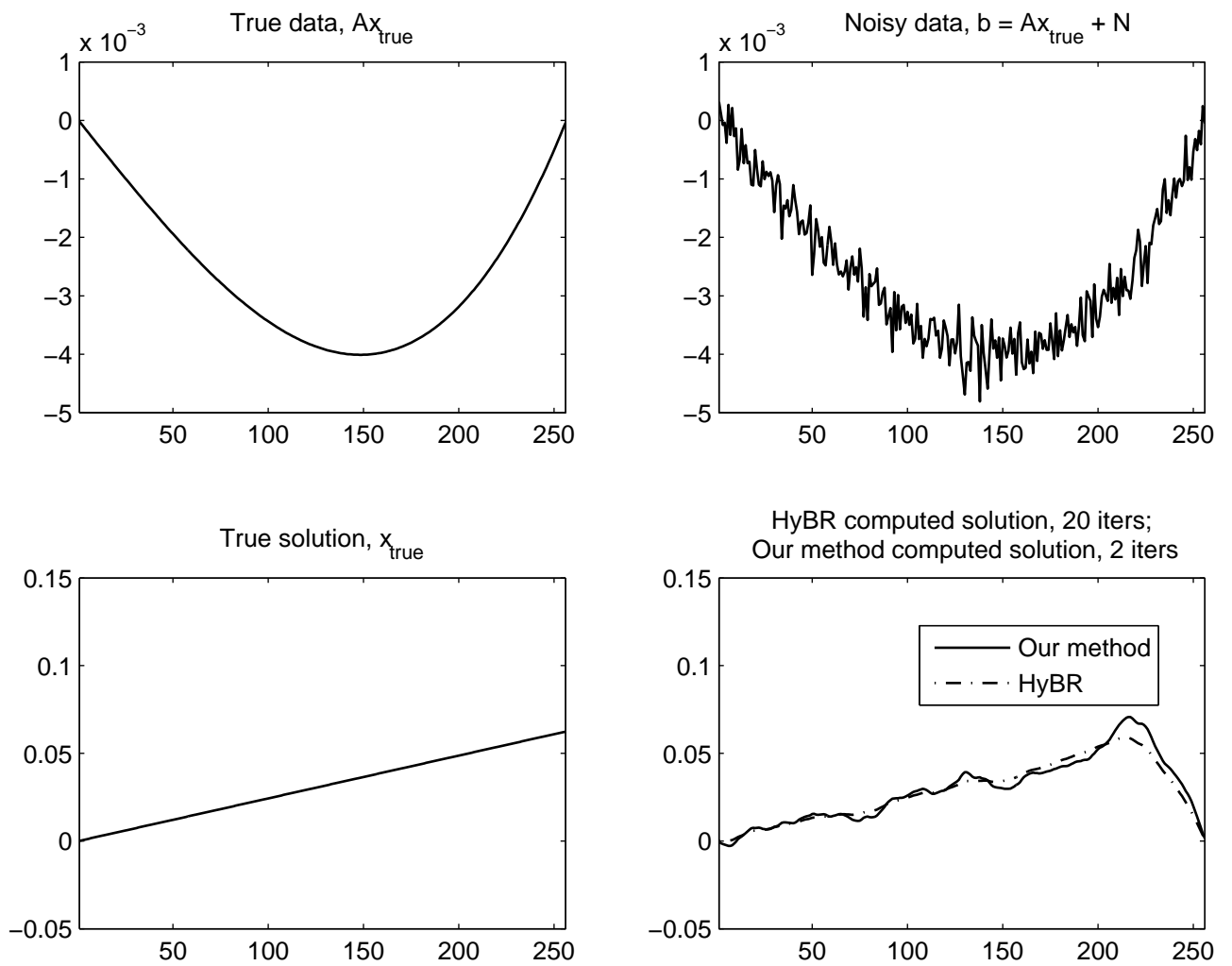


Figure 6.3: "Deriv2"

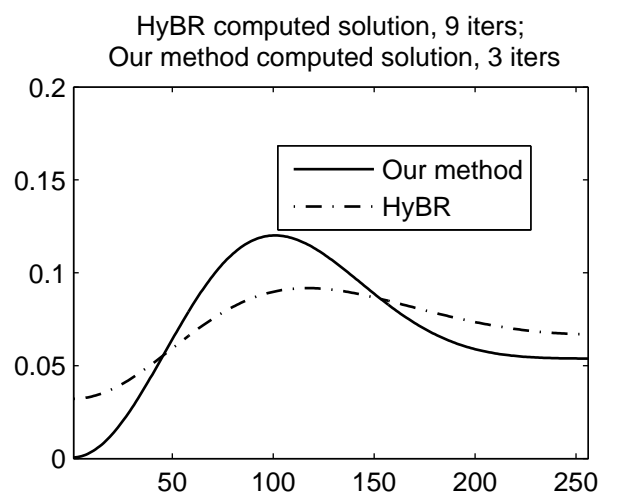
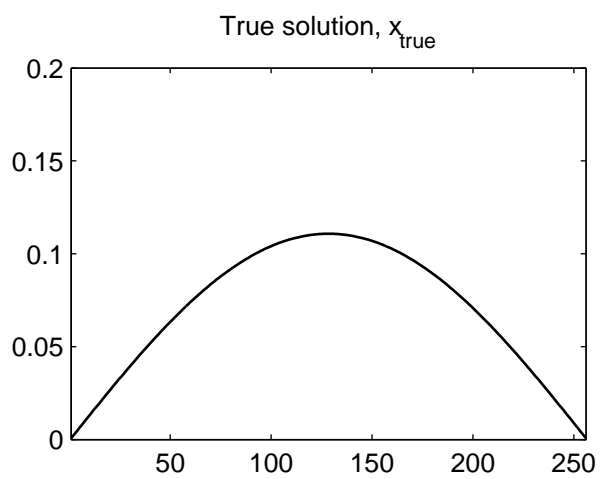
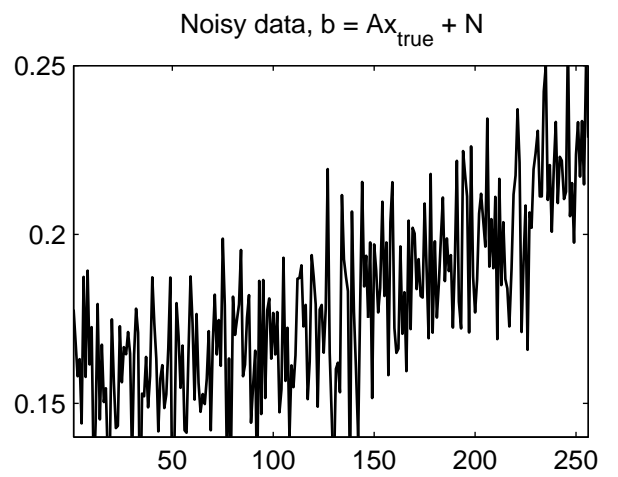
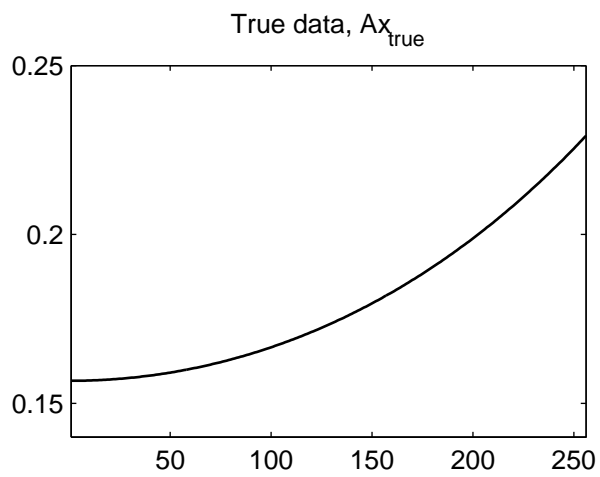


Figure 6.4: "Shaw"

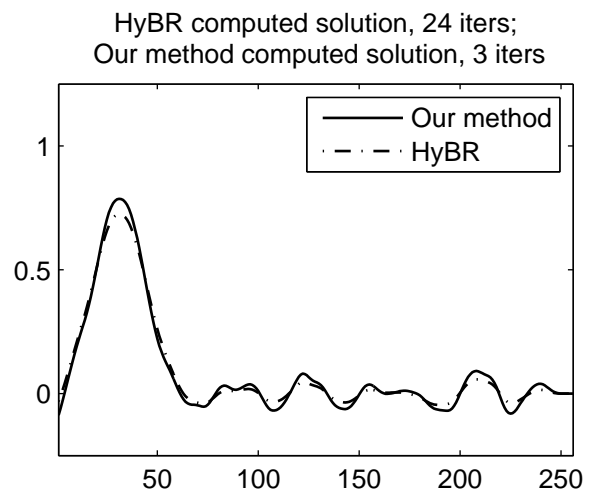
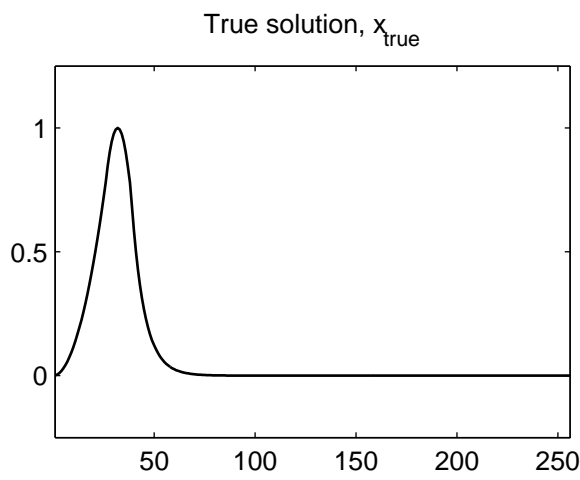
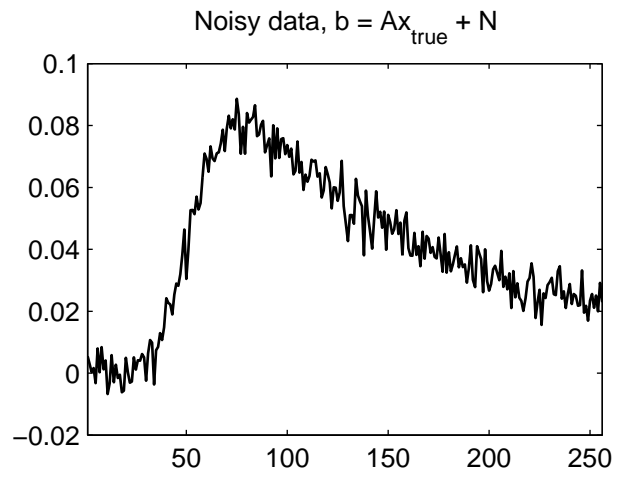
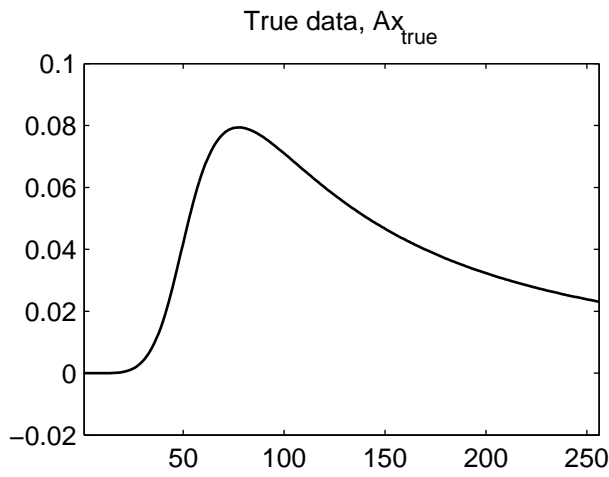


Figure 6.5: "Shaw"

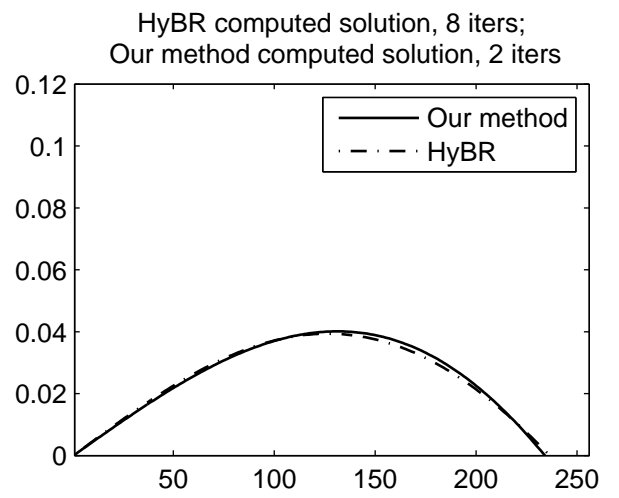
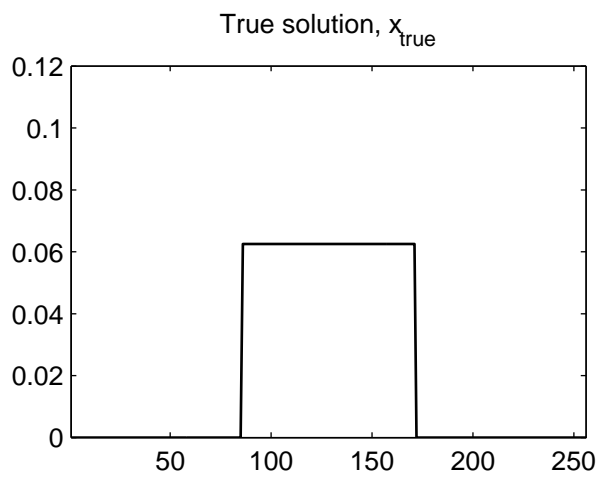
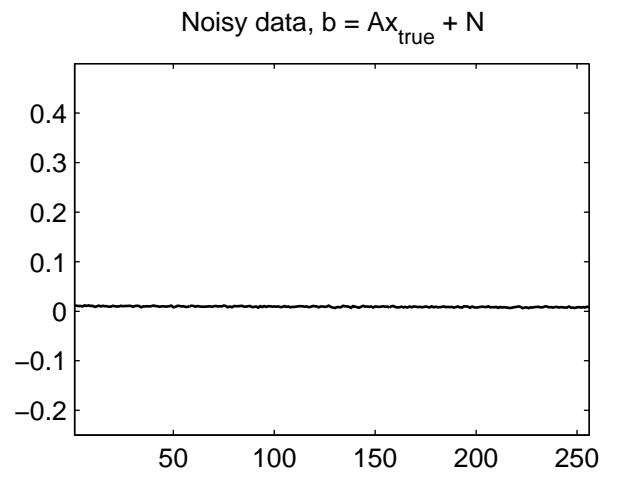
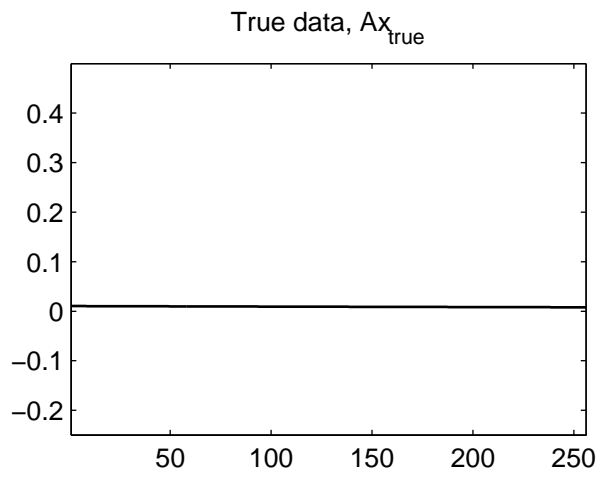
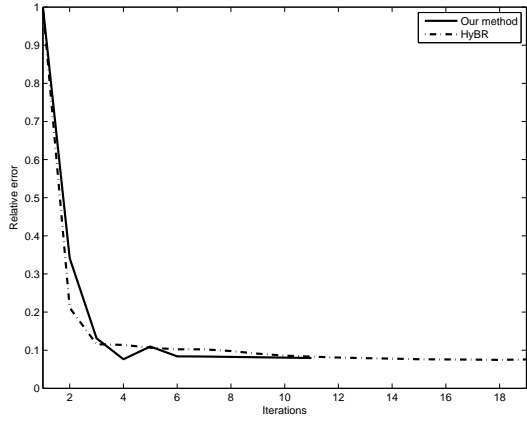
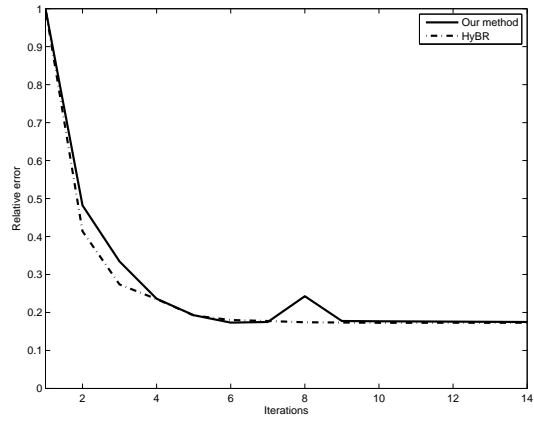


Figure 6.6: "Shaw"

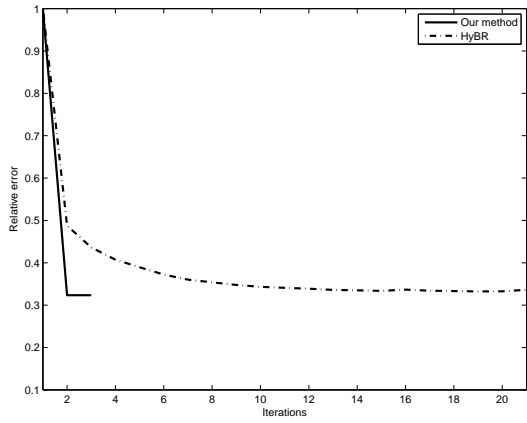




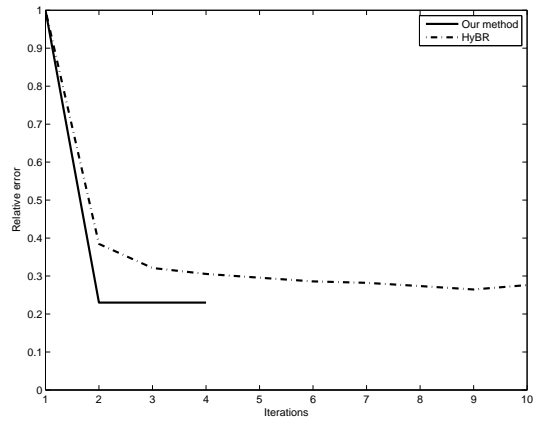
(a)



(b)

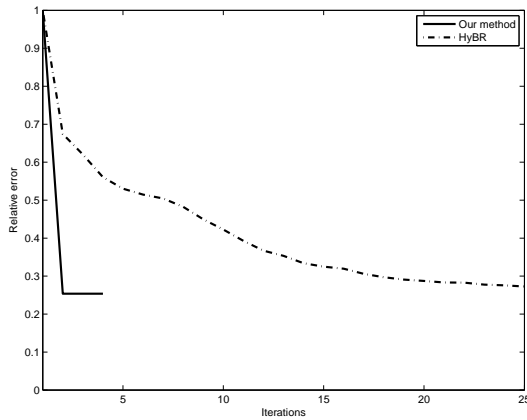


(c)

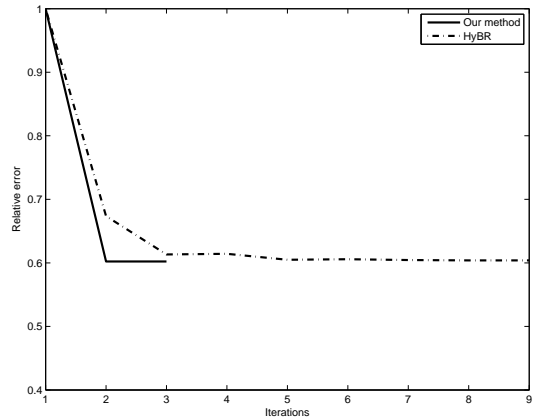


(d)

Figure 6.7: (a) Phillips; (b) Shaw; (c) Deriv2; (d) Baart.



(a)



(b)

Figure 6.8: (a) Heat; (b) Wing.

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