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# Iterative Solution of Weighted Linear Least Squares Problems

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**Abstract**

In this report we show that the iterated regularization scheme due to Riley and Golub, sometimes also called the iterated Tikhonov regularization, can be generalized to damped least squares problems where the weights matrix $D$ is not necessarily the identity but a general symmetric and positive definite matrix. We show that the iterative scheme approaches the same point as the unique solutions of the regularized problem, when the regularization parameter goes to 0. Furthermore this point can be characterized as the solution of a weighted minimum Euclidean norm problem. Finally several numerical experiments were performed in the field of rigid multibody dynamics supporting the theoretical claims.

## 1 Introduction

A timestep problem in rigid multibody dynamics can be formulated with the help of the Jacobian $J : n \times m$, the mass matrix $M : m \times m$ and the impulses $x \in I\!R^n$ as

$$JM^{-1}J^T x - Jc = 0, \tag{1}$$

where the right hand side $c \in I\!R^m$ comes from the rigid body system structural characteristics (see for details [8]). Moreover, as shown in [6], [7], in the case

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of bilateral joints, the problem (1) can be regularized by relaxing the rigidity assumptions as

$$JM^{-1}J^T x - Jc = -sDx, \tag{2}$$

with $s > 0$ and $D : n \times n$ symmetric and positive definite (SPD, for short). Because the mass matrix $M$ is also SPD, we can write (2) as

$$(JM^{-\frac{1}{2}})(JM^{-\frac{1}{2}})^T x - (JM^{-\frac{1}{2}})(M^{\frac{1}{2}} c) = -sDx \quad \Leftrightarrow$$

$$A^T Ax - A^T b = -sDx, \tag{3}$$

with

$$A = (JM^{-\frac{1}{2}})^T : m \times n, \quad b = M^{\frac{1}{2}} c \in I\!R^m. \tag{4}$$

Therefore, we will refer to the problem (3)-(4), and denote by $x^*(s)$ its unique solution (because the matrix $A^T A + sD$ is SPD). The paper is organized as follows. In section 2 we observe that the problem (3) is equivalent with the Tikhonov-type regularization of

$$A^T Ax = A^T b \;\Leftrightarrow\; \parallel Ax - b \parallel^2 = \min! \tag{5}$$

namely

$$\parallel Ax - b \parallel^2 + s \parallel D^{\frac{1}{2}} x \parallel^2 = \min! \tag{6}$$

Moreover, if $x^*_D$ is the (unique) minimal $D$-norm solution of (5), i.e.

$$\parallel x^*_D \parallel_D \quad \leq \quad \parallel x \parallel_D, \;\; \forall x \in LSS(A; b), \tag{7}$$

we show that

$$\lim_{s \to 0} x^*(s) = x^*_D \tag{8}$$

(we denoted by $LSS(A; b)$ the set of least squares solutions of the problem (5)). In section 3 of the paper we propose the (implicit) iterative method

$$x^0 \in I\!R^n, (A^T A + sD)x^{k+1} = sDx^k + A^T b, \quad k \geq 0, \tag{9}$$

show that it generates a sequence of approximations $(x^k)_{k \geq 0}$ which converges linearly to $x^*_D$, and provide a step error reduction factor in terms of a generalized singular value decomposition of the pair $(A, D^{\frac{1}{2}})$. A numerical experiments section together with some conclusions will end the paper.

## 2 Analysis of the Tikhonov-type regularization

We will start this section by first observing that the regularized problem (3) is equivalent with the (global) minimization one

$$H(x^*(s)) = \min_{x \in I\!R^n} H(x), \tag{10}$$

with $H : I\!R^n \longrightarrow I\!R$ be defined by

$$H(x) = \langle A^T Ax, x\rangle - 2\langle A^T b, x\rangle + s\langle Dx, x\rangle. \tag{11}$$

Now, by defining

$$G(x) = H(x) + \| b \|^2, \tag{12}$$

we get that (10) is equivalent with

$$G(x^*(s)) = \min_{x \in I\!R^n} G(x), \tag{13}$$

which can be written as a Tikhonov-type regularization as

$$G(x^*(s)) = \min_{x \in I\!R^n} \| \begin{bmatrix} A \\ \sqrt{s} D^{\frac{1}{2}} \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \|^2 . \tag{14}$$

It is well known that, one of the most useful and famous matrix decompositions is the Singular Value Decomposition (SVD, for short). It says that for any $m \times n$ matrix $A$ of rank $r$, there exists orthogonal matrices $U : m \times m$ and $V : n \times n$ such that

$$A = U\Sigma V^T, \quad \text{with} \quad \Sigma = diag(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0). \tag{15}$$

The positive numbers $\sigma_1, \ldots, \sigma_r$ are uniquelly determined and called the (nonzero) **singular values** of $A$; their squares are the nonzero eigenvalues of the matrix $A^T A$. According to the paper [11]: *Together, E. Beltrami (1873) and C. Jordan (1874) are the progenitors of the singular value decomposition*, but essential developments were obtained also by J.J. Sylvester, E. Schmidt and H. Weyl. Although this powerful decomposition provided many important applications in matrix theory, another crucial step was made by the construction of the Generalized version of SVD (GSVD, for short). The first version of the GSVD was given in [3], in the particular case $m \geq n$, whereas its general version, for any $m$ and $n$ was given in [4]. It refers to a pair of arbitrary matrices $(A, B)$, $A : m \times n$, $B : q \times n$, but we will briefly present in what follows the (particular) case when $B$ is $n \times n$ and invertible (see for details [6]). In this case there exist orthogonal matrices $U_A : m \times m$, $U_B : n \times n$ and an invertible one $X : n \times n$ such that

$$U_A^T AX = D_A = diag(\alpha_1, \ldots, \alpha_r, 0, \ldots, 0),$$

$$U_B^T BX = D_B = diag(\beta_1, \ldots, \beta_n), \tag{16}$$

with $D_A : m \times n$, $D_B : n \times n$,

$$1 > \alpha_1 \geq \cdots \geq \alpha_r > 0, \quad 0 < \beta_1 \leq \cdots \leq \beta_r < \beta_{r+1} = \cdots = \beta_n = 1,$$

$$\alpha_i^2 + \beta_i^2 = 1, i = 1, \ldots, r, \tag{17}$$

and the ratios

$$\frac{\alpha_i}{\beta_i} > 0, \ i = 1, \ldots, r, \tag{18}$$

are the nonzero singular values of the matrix $AB^{-1}$.

We will now use a GSVD of the matrix $\begin{bmatrix} A \\ D^{\frac{1}{2}} \end{bmatrix}$ as in (16)-(17) (for $B = D^{\frac{1}{2}}$)

$$U_A^T AX = diag(\alpha_1, \ldots, \alpha_r, 0, \ldots, 0) = D_A,$$

$$U_B^T D^{\frac{1}{2}} X = diag(\beta_1, \ldots, \beta_n) = D_B. \tag{19}$$

Then, by introducing (19) in (14) and using the orthogonality of $U$ and $V$ and the invertibility of $X$ we successively obtain

$$\min_{x \in I\!\!R^n} \| \begin{bmatrix} A \\ \sqrt{s} D^{\frac{1}{2}} \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \|^2 =$$

$$\min_{x \in I\!\!R^n} \| \begin{bmatrix} U_A^T & 0 \\ 0 & U_B^T \end{bmatrix} \left( \begin{bmatrix} A \\ \sqrt{s} D^{\frac{1}{2}} \end{bmatrix} X(X^{-1}x) - \begin{bmatrix} b \\ 0 \end{bmatrix} \right) \|^2 =$$

$$\min_{z \in I\!\!R^n} \| \begin{bmatrix} D_A \\ \sqrt{s} D_B \end{bmatrix} z - \begin{bmatrix} w \\ 0 \end{bmatrix} \|^2 =$$

$$\sum_{i=1}^{r} (\alpha_i z_i - w_i)^2 + \sum_{i=r+1}^{m} w_i^2 + \sum_{i=1}^{n} s \beta_i^2 z_i^2 = E(z), \tag{20}$$

where $z = (z_1, \ldots, z_n)^T = X^{-1}x$, $w = (w_1, \ldots, w_n)^T = U_A^T b$. The values of $z_i$ which ensure the minimal value of the function $E(z)$ are obtained by solving the system $\frac{\partial E}{\partial z_i}(z) = 0, i = 1, \ldots, n$. These are

$$z_i = \frac{w_i \alpha_i}{\alpha_i^2 + s\beta_i^2}, i = 1, \ldots, r, \quad z_i = 0, i = r+1, \ldots, n. \tag{21}$$

Thus, the unique solution $x^*(s)$ of the problem (13) will be given by

$$x^*(s) = Xz = \sum_{i=1}^{n} z_i X^i = \sum_{i=1}^{r} \frac{w_i \alpha_i}{\alpha_i^2 + s\beta_i^2} X^i. \tag{22}$$

Now let us consider the weighted LSS problem

$$\| D^{\frac{1}{2}} x_D^* \|^2 = \min_{x \in I\!R^n, s.t. \|Ax-b\|=\min!} \| D^{\frac{1}{2}} x \|^2, \tag{23}$$

with the unique solution $x_D^* \in I\!R^n$. That is, we must find $x_D^* \in LSS(A;b)$ for which $\| D^{\frac{1}{2}} x_D^* \|$ is minimal. By using again the GSVD (19) we obtain

$$\| Ax - b \|^2 = \sum_{i=1}^{r} (\alpha_i z_i - w_i)^2 + \sum_{i=r+1}^{n} w_i^2$$

from which we get

$$LSS(A;b) = \{x^* = Xz^*, z_i^* = \frac{w_i}{\alpha_i}, i = 1, \ldots, r; z_i^* \in I\!R, i = r+1, \ldots, n\}. \tag{24}$$

Now, $U_B^T D^{\frac{1}{2}} X = D_B$, i.e. $D^{\frac{1}{2}} = U_B D_B X^{-1}$, thus, for an $x^* \in LSS(A;b)$ we obtain

$$\| D^{\frac{1}{2}} x^* \|^2 = \| D_B z^* \|^2 = \sum_{i=1}^{r} (\frac{\beta_i w_i}{\alpha_i})^2 + \sum_{i=r+1}^{n} (\beta_i z_i^*)^2, \tag{25}$$

which has its minimal value for $z_i^* = 0, i = r+1, \ldots, n$ and gives us

$$x_D^* = Xz^* = \sum_{i=1}^{r} \frac{w_i}{\alpha_i} X^i. \tag{26}$$

Then, from (22) and (26) the desired equality results, i.e.

$$\lim_{s \to 0} x(s) = x_D^*. \tag{27}$$

## 3 The weighted iteration

In this section we will analyse the convergence of the iteration (9) for a general SPD matrix $D$. For $D = I$ this was done in [10] in the case and $A^T A$ invertible, and in [1] for a general $m \times n$ matrix $A$. In our considerations we shall use the proof ideas in [1], but with respect to a GSVD of the pair $(A, D^{\frac{1}{2}})$, where $D^{\frac{1}{2}}$ is the square root of $D$. Firstly we shall observe that, if we write (9) as

$$x^0 \in I\!R^n, \quad x^{k+1} = Gx^k + c \tag{28}$$

where

$$G = s(A^T A + sD)^{-1} D, \quad c = (A^T A + sD)^{-1} A^T b \tag{29}$$

then, for $x^0 = 0$ we obtain

$$x^k = (G^{k-1} + G^{k-2} + \cdots + I)c \tag{30}$$

According to the GSVD decomposition (19) it results

$$G = sX(D_A^T D_A + sD_B^2)^{-1} D_B^2 X^{-1}, c = X(D_A^T D_A + sD_B^2)^{-1} D_A^T w, w = U_A^T b, \tag{31}$$

thus

$$G^j = s^j X(D_A^T D_A + sD_B^2)^{-j} (D_B^2)^j X^{-1}, j = 0, 1, \ldots, k-1 \tag{32}$$

The $n \times n$ matrices $D_A^T D_A$ and $D_B^2$ are diagonal, of the form (see (19))

$$D_A^T D_A = \begin{pmatrix} \alpha_1^2 & & & & \cdots & 0 \\ & \ddots & & & & \vdots \\ & & \alpha_r^2 & & & \\ & & & 0 & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 0 \end{pmatrix}, D_B^2 = \begin{pmatrix} \beta_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \beta_n^2 \end{pmatrix}. \tag{33}$$

From (31)-(33) we then obtain

$$s^j (D_A^T D_A + sD_B^2)^{-j} (D_B^2)^j = \begin{pmatrix} \left(\frac{s\beta_1^2}{\alpha_1^2 + s\beta_1^2}\right)^j & & & & \cdots & 0 \\ & \ddots & & & & \vdots \\ & & \left(\frac{s\beta_r^2}{\alpha_r^2 + s\beta_r^2}\right)^j & & & \\ & & & 1 & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 1 \end{pmatrix} \tag{34}$$

and

$$(D_A^T D_A + sD_B^2)^{-1} D_A^T w = \begin{pmatrix} \frac{w_1 \alpha_1}{\alpha_1^2 + s\beta_1^2} \\ \vdots \\ \frac{w_r \alpha_r}{\alpha_r^2 + s\beta_r^2} \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{35}$$

We observe that

$$0 < \frac{s\beta_i^2}{\alpha_i^2 + s\beta_i^2} < 1 \quad \forall i = 1, \ldots, r. \tag{36}$$

By introducing all these formulas in (30) we get (by also using (36))

$$x^k = X \begin{pmatrix} \sum_{j=0}^{k-1} \left(\frac{s\beta_1^2}{\alpha_1^2+s\beta_1^2}\right)^j \cdot \frac{w_1\alpha_1}{\alpha_1^2+s\beta_1^2} \\ \vdots \\ \sum_{j=0}^{k-1} \left(\frac{s\beta_r^2}{\alpha_r^2+s\beta_r^2}\right)^j \cdot \frac{w_r\alpha_r}{\alpha_r^2+s\beta_r^2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = X \begin{pmatrix} \left(1-\left(\frac{s\beta_1^2}{\alpha_1^2+s\beta_1^2}\right)^k\right)\frac{w_1}{\alpha_1} \\ \vdots \\ \left(1-\left(\frac{s\beta_r^2}{\alpha_r^2+s\beta_r^2}\right)^k\right)\frac{w_r}{\alpha_r} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{37}$$

$$= \sum_{i=1}^{r} \left(1-\left(\frac{s\beta_i^2}{\alpha_i^2+s\beta_i^2}\right)^k\right)\frac{w_i}{\alpha_i} \cdot X^i.$$

Using again (36), (37) and (26) we obtain

$$\lim_{k\to\infty} x^k = x_D^*, \tag{38}$$

i.e. the sequence $\{x^k\}_{k\geq 0}$ generated with the iteration (9) with $x^0 = 0$ and $s > 0$ fixed arbitrary, converges to the unique solution of the weighted least squares problem (23). Moreover, from (26) and (37) it results $x_D^*, x^k \in span\{X^1, \ldots, X^r\}$, thus for the error vector $e^k = x^k - x_D^*$ we have

$$e^k = \sum_{i=1}^{r} e_i^k X^i \in span\{X^1, \ldots, X^r\}, \quad e_i^k \in I\!R. \tag{39}$$

If we define $f^k = X^{-1}e^k$, from (39) it results

$$f^k = \sum_{i=1}^{r} e_i^k X^{-1} X^i = (e_1^k, \ldots, e_r^k, 0, \ldots, 0)^T \in I\!R^n. \tag{40}$$

Now, because $e^k = Ge^{k-1}$ (see (28) and the relation $x_D^* = Gx_D^* + c$), by using (31), (34) (for $j = 1$) and (40) we get

$$f^k = X^{-1}e^k = X^{-1}Ge^{k-1} = sX^{-1}X(D_A^TD_A + sD_B^2)^{-1}D_B^2X^{-1}e^{k-1}$$

$$= \begin{pmatrix} \frac{s\beta_1^2}{\alpha_1^2+s\beta_1^2} & & & & \cdots & 0 \\ & \ddots & & & & \vdots \\ & & \frac{s\beta_r^2}{\alpha_r^2+s\beta_r^2} & & & \\ & & & 1 & & \\ \vdots & & & & \ddots & \\ 0 & \cdots & & & & 1 \end{pmatrix} \begin{pmatrix} e_1^{k-1} \\ \vdots \\ e_r^{k-1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{41}$$

By taking the Euclidean norm of (41) we obtain

$$\begin{aligned} \|f^k\|^2 &= \sum_{i=1}^{r} \left( \frac{s\beta_i^2}{\alpha_i^2 + s\beta_i^2} \right)^2 \left( e_i^{k-1} \right)^2 \leq \max_{1\leq i\leq r} \left( \frac{s\beta_i^2}{\alpha_i^2 + s\beta_i^2} \right)^2 \cdot \|f^{k-1}\|^2 \\ &= \left( \max_{1\leq i\leq r} \frac{s}{s + \left(\frac{\alpha_i}{\beta_i}\right)^2} \right)^2 \|f^{k-1}\|^2 \leq \frac{s^2}{\left( s + \min_{1\leq i\leq r} \left(\frac{\alpha_i}{\beta_i}\right)^2 \right)^2} \|f^{k-1}\|^2, \end{aligned} \tag{42}$$

which gives us information about the step reduction factor (with respect to the Euclidean norm) of the weighted errors $f^k$ from (40). If we consider the relations (17) we obtain that

$$\mu = \min_{1\leq i\leq r} \left( \frac{\alpha_i}{\beta_i} \right)^2 = \frac{\alpha_r^2}{\beta_r^2} = \frac{1-\beta_r^2}{\beta_r^2} = \frac{\alpha_r^2}{1-\alpha_r^2} \tag{43}$$

**Note.** From (42)-(43) we obtain

$$\|f^k\| \leq \frac{s}{s+\mu} \|f^{k-1}\| \tag{44}$$

Thus, if $s \approx \mu$ we obtain a step error reduction factor $\approx \frac{1}{2}$. If $s \gg \mu$, we have $\frac{s}{s+\mu} \approx 1$ which is not a good error reduction factor per iteration. If $s \ll \mu$ it will determine the increase of the condition number of the matrix $A^T A + sD$ in (9), which makes the computation of $x^{k+1}$ difficult.

## 4 Numerical experiments

The numerical experiments of this section are performed with the weighted iteration scheme described (28) - (29). The test problems are time step problems arising in rigid multibody dynamics. The test scenarios are described in detail in [5]. The test cases contain only bilateral constraints so that the resulting systems are least squares problems of the form (5). For each test case the iteration was executed for an unweighted regularization where $D = I$ and for a weighted regularization where $D$ was chosen randomly. The weights were computed by generating a standard normally-distributed random variable, taking the absolute value and adding 1, such that all weights were greater equal and close to 1. The weighted and the unweighted tests were executed with three different values for the parameter $s$. The parameter was chosen such that an error reduction at least of a factor $f \in \{0.1, 0.5, 0.9\}$ was achieved. From (44) we can conclude that $s = \frac{f}{1-f}\mu$, where $\mu$ is the smallest nonzero singular value of $AD^{-1}$ squared.

### 4.1 Test Case: Well

In the well test case $A \in I\!R^{1200\times 6240}$ has full row-rank ($rankA = 1200$) and thus $A^TA \in I\!R^{6240\times 6240}$ is rank deficient ($rankA^TA = rankA = 1200$). A singular value decomposition of $A$ reveals that the smallest nonzero singular value $\sigma_r$ of $A$ is approximately 0.0365. Thus $s$ was $1.4771 \cdot 10^{-4}$ for $f = 0.1$, 0.0013 for $f = 0.5$ and 0.0120 for $f = 0.9$ in the unweighted case where $D = I$. For the weighted case $\sigma_r \approx 0.0222$ and $s$ is thus $5.4840 \cdot 10^{-5}$, $4.9356 \cdot 10^{-4}$ and 0.0044 for $f$ equal to 0.1, 0.5 and 0.9 respectively. The error graphs in Figure 1 plot the Euclidean norm of the difference between the current iterate and the minimum norm solution computed by Matlab. The weighted minimum norm solution can be restated as an unweighted minimum norm solution of a modified system:

$$\begin{aligned} x_D^* &= \text{argmin}\{x^TDx \text{ s.t. } A^TAx = A^Tb\} = \\ &D^{-\frac{1}{2}}\text{argmin}\{y^Ty \text{ s.t. } A^TAD^{-\frac{1}{2}}y = A^Tb\}. \end{aligned} \tag{45}$$

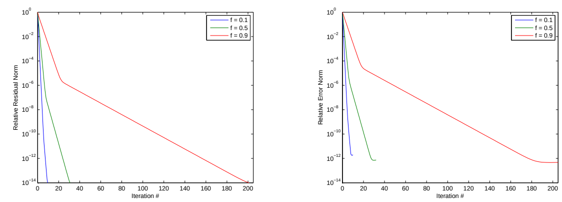
Hence the weighted minimum norm solution $x_D^*$ can be computed by applying the Moore-Penrose pseudo-inverse of $A^TAD^{-\frac{1}{2}}$ to the right-hand side $A^Tb$.

$$x_D^* = (A^TAD^{-\frac{1}{2}})^+A^Tb \tag{46}$$

Thus the reference solution was obtained by using the `pinv` command or in the case where $D = I$ by computing $V\Sigma^+U^Tb$ which is evidently the same. This can be verified by inserting the singular value decomposition of $A$ into (46). The SVD was computed by the standard `svd` command in Matlab. The unweighted minimum norm solution obtained had the norm $\sqrt{x^Tx} = 10.9296$ and the weighted minimum norm solution obtained had the norm $\sqrt{x^TDx} =$ 14.0871. Though the residual does not make any statements on whether the iterate approaches the minimum norm solution (as opposed to an arbitrary solution) it seems to be a good indicator.

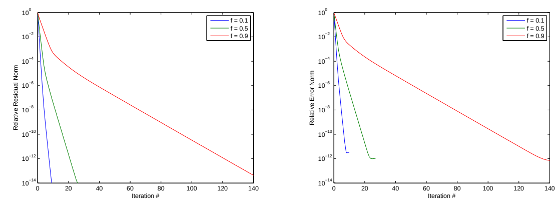
### 4.2 Test Case: Mobile

Here the system matrix $A \in I\!R^{1013\times 570}$ has full column-rank ($rankA = 570$) and thus $A^TA$ has full rank. The smallest singular value $\sigma_r$ of $A$ was determined to be approximately 0.1612. Thus the parameter $s$ was chosen to be 0.0029, 0.0260 and 0.2338 for $f$ equal to 0.1, 0.5 and 0.9 respectively. For the weighted case $\sigma_r \approx 0.1010$ of $AD^{-1}$ and $s$ therefore 0.0011, 0.0102 and 0.0917. The (weighted) norms of the solutions were 0.1549 in the unweighted case and 0.1936 in the weighted case. Figure 2 shows residual and error graphs for the tests.




(a) The residual graphs with unweighted regularization.

(b) The error graphs with unweighted regularization.




(c) The residual graphs with weighted regularization.

(d) The error graphs with weighted regularization.

Figure 1: Residual and error graphs for the well test case with different regularizations.

### 4.3 Test Case: Pyramid

In the last test case $A \in I\!R^{1155\times 1240}$ has full row-rank ($rankA = 1115$) and thus $A^T A$ is again rank deficient. The smallest nonzero singular value $\sigma_r$ of $A$ was determined to be approximately 0.1202. Thus the parameter $s$ was chosen to be 0.0016, 0.0145 and 0.1301 for $f$ equal to 0.1, 0.5 and 0.9 respectively. For the weighted case $\sigma_r \approx 0.0628$ of $AD^{-1}$ and $s$ therefore $4.3839 \cdot 10^{-4}$, 0.0039 and 0.0355. The (weighted) norms of the solutions were 0.6758 in the unweighted case and 0.8973 in the weighted case. Figure 3 shows residual and error graphs for the tests.

**Final comments.** The advantage of the iterative algorithm that we proposed in the paper is that it directly computes a weighted minimal norm solution with an symmetric and positive definite weights matrix, and does not require prior transformation of the weighted least squares problem into an unweighted one.
We will work on a proper computational comparison in future work.

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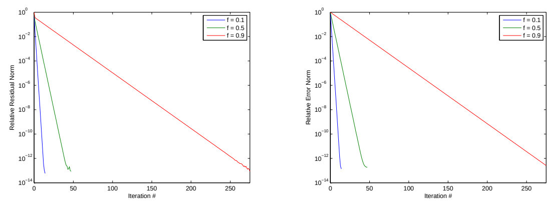
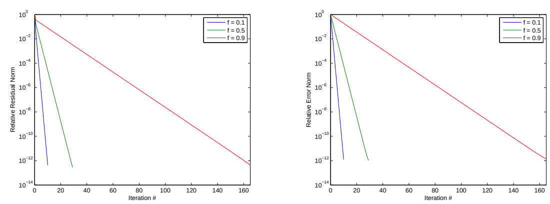
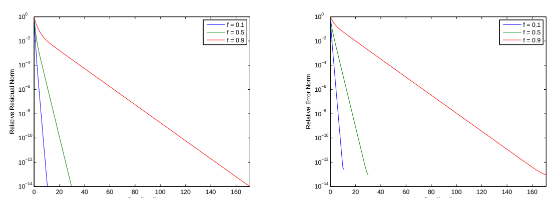



(a) The residual graphs with unweighted regularization.
(b) The error graphs with unweighted regularization.

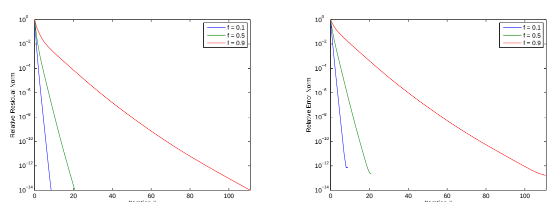



(c) The residual graphs with weighted regularization.
(d) The error graphs with weighted regularization.

Figure 2: Residual and error graphs for the mobile test case with different regularizations.




(a) The residual graphs with unweighted regularization.
(b) The error graphs with unweighted regularization.




(c) The residual graphs with weighted regularization.
(d) The error graphs with weighted regularization.

Figure 3: Residual and error graphs for the pyramid test case with different regularizations.

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