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A WEIGHTED GLOBAL GENERALIZED CROSS VALIDATION FOR GL-CGLS REGULARIZATION

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Abstract. To obtain more accurate approximation of the true images in the deblurring problems, the weighted global generalized cross validation(GCV) function to the inverse problem with multiple right-hand sides is suggested as an efficient way to determine the regularization parameter. We analyze the experimental results for many test problems and was able to obtain the globally useful range of the weight when the preconditioned global conjugate gradient linear least squares(Gl-CGLS) method with the weighted global GCV function is applied.

1. Introduction

The large-scale inverse problems with multiple right-hand sides

$$HX = B$$

arise from the column stacking of each small blocks obtained by partitioning the blurred and noisy image in the image deblurring and reconstruction, where $H \in R^{N\times N}$ is an imaging system and $B \in R^{N\times s}$ $(N \gg s)$ is a collection of noisy images. The multiple right-hand sides B of the system is contaminated by the noise $\mathcal{E}$, $B = B^* + \mathcal{E}$, where the noise-free images of the object B^*. The noise $\mathcal{E}$ accounts for both the error measurements and the process involved in the construction of the discrete model describing the underlying continuous phenomenon. Typically H is a large full rank matrix, having singular values which accumulate at the origin and gradually decay to zero, so that it is difficult to determine its numerical rank. This ill-posed nature of the problem

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may give rise to significant errors in computing approximations of the true image solution.

Regularization methods can be used to deal with a severely ill-conditioning of the matrix H and the presences of noises. Applying the regularization method to deblurring problems, the illustrating general space-invariant imaging systems are often modeled as in the following equivalent minimization problem:

$$\min_{X}(\|HX - B\|_F^2 + \lambda^2 \|X\|_F^2) \tag{1.1}$$

([2, 11, 12]). The positive regularization parameter λ controls the smoothness of the regularized solution and an appropriate value of this parameter λ is not known a priori. The regularization parameter λ plays a crucial role in the quality of the solution and thus a computationally efficient and reliable estimate of the regularization parameter is needed in many regularization methods.

In [11], we applied the preconditioned global conjugate gradient linear least squares (Gl-CGLS) method to image deblurring problems (1.1) and obtained significant improvements in execution times. But for some severe ill-posed problems the iterative method without the appropriate regularization parameters revealed the semiconvergence behaviors in later iterations. In [12], we suggested an efficient way in adapting Gl-CGLS to determine the better regularization parameter λ using the global generalized cross validation(GCV) technique and obtained better reconstruction images by $1.2 \sim 38.7\%$ less relative accuracies than Gl-CGLS method without using the global generalized cross validation(GCV) technique.

To determine the regularization parameter λ for 2-norm based model problems in the case where the number of column stacks $s = 1$ in (1.1), Morozov's discrepancy principle, L-curve criterion, generalized cross validation, and new variants of these methods are suggested in [3, 4, 5, 13]. Especially the GCV method is prominent for the selection of the crucial regularization parameters since GCV has good asymptotic properties for large number of noisy data. For certain classes of problems, however, the method may exhibit the poor performances caused by the suboptimal parameter determining processes.

Chung and et al in [1] used a weighted GCV(W-GCV) function in Lanczos-hybrid methods to regularize large scale ill-posed problems and had more effective results than the standard GCV which has a strong tendency to over-estimate the regularization parameter. They used a different range of weights in the W-GCV method to avoid over and under smoothing difficulties when using GCV in Lanczos-hybrid methods.

Our study adapts the weighted global GCV function in Gl-CGLS methods to determine the Tikhonov parameters λ and proposes a more automated approach of choices of the weight parameter ϖ that is versatile and also can be used on a variety of problems.

An outline of this study is as follows: Section 2 deals with the weighted global GCV function for regularization parameters. Section 3 describes the analysis of preconditioned Gl-CGLS regularization method with weighted global GCV implemented for the image deblurring problems with multiple right hand sides. Numerical experiments and final remarks are described in Section 4 and 5.

2. Weighted global GCV method for regularization parameters

The standard global GCV method in [12] can be a method of choosing an efficient parameter for image deblurring applicatons. For a certain class of problems, the small Tikhonov parameters chosen by GCV causes under-smoothing of the solution, so that Gl-CGLS method with the global GCV method may not perform well. Thus to improve the method to choose regularization parameters, we modify the standard global GCV function by introducing a new parameter ϖ to the trace term as in the following function,

$$\mathcal{T}(\lambda, \varpi) = \text{trace}(I - \varpi H(H^T H + \lambda^2 I)^{-1} H^T). \tag{2.1}$$

Definition 2.1. Let the weighted global GCV function $\mathcal{G}_{\text{global}}(\lambda, \varpi)$ be defined as

$$\mathcal{G}_{\text{global}}(\lambda, \varpi) = \frac{\|HX_\lambda - B\|_F^2}{\mathcal{T}(\lambda, \varpi)^2} \tag{2.2}$$

for an user-defined weight ϖ where $X_\lambda = (H^T H + \lambda^2 I)^{-1} H^T B$.

Notice that choosing $\varpi = 1$ gives the standard global GCV function [Section 3, [12]]. If we choose $\varpi > 1$, we obtain smoother solutions, where $\varpi < 1$ results in less smooth solutions. Our study is to propose a more global and automated approach that can be used on a variety of image deblurring problems rather than using a user-defined parameter choice for ϖ.

To our knowledge, in all work using weighted global GCV, only experimental approaches are used to choose ϖ. For smoothing spline applications, [8] empirically found that standard GCV consistently produced regularization parameters that were too small, while choosing ϖ in the range $1.2 \sim 1.4$ worked well. [1] seek a parameter ϖ in the range $0 < \varpi \leq 1$.

When considering the reflective boundary conditions, the matrix H can be diagonalized by the orthogonal two-dimensional discrete cosine transform matrix $\mathcal{C}$, $H = \mathcal{C}^T \Lambda_H \mathcal{C}$ when $\Lambda_H = diag(\rho_1, \rho_2, \ldots, \rho_N)$. Therefore the next Lemma 2.2 can be obtained.

LEMMA 2.2. *If $\{\rho_i\}_{i=1}^N$ represents the spectrum of H,*

$$\mathcal{G}_{\text{global}}(\lambda, \varpi) = \frac{\sum_{j=1}^{s} \sum_{i=1}^{N} \left(\frac{\lambda^2}{\rho_i^2 + \lambda^2} [\mathcal{C} B_j]_i \right)^2}{\left(N - \varpi \sum_{i=1}^{N} \frac{\rho_i^2}{\rho_i^2 + \lambda^2} \right)^2}, \tag{2.3}$$

where B_j is the j-th column of B.

Proof. Substitute a unitary spectral decomposition of H into $HX_\lambda - B$ and $\mathcal{T}(\lambda, \varpi)$ then we get

$$HX_\lambda - B = \mathcal{C}^T (\Lambda_H (\Lambda_H^2 + \lambda^2 I)^{-1} \Lambda_H - I) \mathcal{C} B, \tag{2.4}$$

and

$$\begin{aligned}
\mathcal{T}(\lambda, \varpi) &= \text{trace}(\mathcal{C}^T (I - \varpi \Lambda_H (\Lambda_H^2 + \lambda^2 I)^{-1} \Lambda_H - I) \mathcal{C}) \\
&= \sum_{i=1}^{N} \left(1 - \varpi \frac{\rho_i^2}{\rho_i^2 + \lambda^2} \right) = N - \varpi \sum_{i=1}^{N} \frac{\rho_i^2}{\rho_i^2 + \lambda^2} \\
&= \sum_{i=1}^{N} \left(1 - \frac{\rho_i^2}{\rho_i^2 + \lambda^2} \right) + (1 - \varpi) \sum_{i=1}^{N} \frac{\rho_i^2}{\rho_i^2 + \lambda^2}.
\end{aligned}$$

From (2.4) we can obtain $\|HX_\lambda - B\|_F^2 = \sum_{j=1}^{s} \sum_{i=1}^{N} \left(\frac{\lambda^2 [\mathcal{C} B_j]_i}{\rho_i^2 + \lambda^2} \right)^2$. Consequently (2.2) can be replaced by (2.3). □

Notice that parameters λ and ϖ are determined by minimizing the weighted global GCV function (2.3). The minimizer usually cannot be determined analytically because $\mathcal{G}_{\text{global}}(\lambda, \varpi)$ is a nonlinear function. Considering the limitation of λ and ϖ, we can determine the value of λ

and ϖ by solving constrained optimization problem

$$\begin{aligned} &\min_{\lambda,\varpi} && \mathcal{G}_{\text{global}}(\lambda,\varpi) \\ &\text{subject to} && \rho_{min} \le \lambda \le \rho_{max} \\ &&& \kappa_1 \le \varpi \le \kappa_2. \end{aligned} \tag{2.5}$$

We used the Matlab toolbox *fmincon* to find λ and ϖ to minimize the constrained function $\mathcal{G}_{\text{global}}(\lambda,\varpi)$ in (2.3).

3. Preconditioned Gl-CGLS regularization method with weighted global GCV

To solve (1.1) numerically with $\lambda = \lambda_{\varpi gGCV}$, we can rewrite it in certain situations as a minimization problem:

$$\min_X \left\| \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} X - \begin{pmatrix} B \\ O \end{pmatrix} \right\|_F \tag{3.1}$$

that is equivalent to the symmetric positive definite Tikhonov system with multiple right-hand sides

$$(H^T H + \lambda^2_{\varpi gGCV} I)X = H^T B. \tag{3.2}$$

Large sparse systems (3.2) can be solved by the global conjugate gradient linear least squares(Gl-CGLS) method as an iterative regularization method.

Algorithm 1. Gl-CGLS

1. X_0 is initial guess and compute $R_0 = \begin{pmatrix} B \\ O \end{pmatrix} - \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} X_0$.
2. $P_0 = S_0 = \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix}^T R_0$, $\gamma_0 = (S_0, S_0)_F$.
3. For k=0, 1, ..., until convergence do
   - i. $Q_k = \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} P_k$, $\alpha_k = \gamma_k/(Q_k, Q_k)_F$,
   - ii. $X_{k+1} = X_k + \alpha_k P_k$, $R_{k+1} = R_k - \alpha_k Q_k$,
   - iii. $S_{k+1} = \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix}^T R_{k+1}$, $\gamma_{k+1} = (S_{k+1}, S_{k+1})_F$,
   - iv. $\beta_k = \gamma_{k+1}/\gamma_k$, $P_{k+1} = S_{k+1} + \beta_k P_k$.

Enddo

The following theorem is about the solution norm where $\|X_k\|_F$ increases monotonically with k if the starting matrix X_0 is zero.

Theorem 3.1. *Let $\psi(X_k)$ denote the error function of Gl-CGLS with the weighted global GCV:*

$$\psi(X_k) = \left(X_{LS} - X_k, (H^T H + \lambda^2_{\varpi gGCV} I)(X_{LS} - X_k)\right)_F, \tag{3.3}$$

where X_{LS} is a solution of (3.1). Then the Gl-CGLS iterate X_k can be written as

$$X_k = X_0 + \sum_{i=0}^{k-1} \frac{\psi(X_i) - \psi(X_k)}{\left(\left(\begin{array}{c} H \\ \lambda_{\varpi gGCV} I \end{array} \right)^T R_i, \left(\begin{array}{c} H \\ \lambda_{\varpi gGCV} I \end{array} \right)^T R_i \right)_F^2} \left(\begin{array}{c} H \\ \lambda_{\varpi gGCV} I \end{array} \right)^T R_i,$$

and if $X_0 = O$ then

$$\|X_k\|_F^2 = \sum_{i=0}^{k-1} \left(\frac{\psi(X_i) - \psi(X_k)}{\left(\left(\begin{array}{c} H \\ \lambda_{\varpi gGCV} I \end{array} \right)^T R_i, \left(\begin{array}{c} H \\ \lambda_{\varpi gGCV} I \end{array} \right)^T R_i \right)_F} \right)^2. \tag{3.4}$$

Proof. See [12]. □

The following suggests an estimate of the magnitude of the error function $\psi(X_k)$ in (3.3).

THEOREM 3.2. *The error matrix $Y = X_{LS} - X_k$, the residual $\mathfrak{R}_k = H^T B - (H^T H + \lambda_{\varpi gGCV}^2 I) X_k$, and the error function $\psi(X_k)$ satisfy*

$$\|\mathfrak{R}_k\|_F^2 / \mu(\mathfrak{R}_k) \le \psi(X_k) \le \|\mathfrak{R}_k\|_F^2 / \mu(Y)$$

where $\mu(Z) = (Z, (H^T H + \lambda_{\varpi gGCV}^2 I) Z)_F / (Z, Z)_F$.

Proof. Using the error function $\psi(X_k) = (Y, (H^T H + \lambda_{\varpi gGCV}^2 I) Y)_F$, the residual $\mathfrak{R}_k = (H^T H + \lambda_{\varpi gGCV}^2 I) Y$, and

$$\begin{aligned} &|(Y, (H^T H + \lambda_{\varpi gGCV}^2 I) Y)_F|^2 \\ &\le (Y, Y)_F ((H^T H + \lambda_{\varpi gGCV}^2 I) Y, (H^T H + \lambda_{\varpi gGCV}^2 I) Y)_F, \end{aligned}$$

the following is obtained:

$$\begin{aligned} \mu(Y) &= (Y, (H^T H + \lambda_{\varpi gGCV}^2 I) Y)_F / (Y, Y)_F \\ &\le \|\mathfrak{R}_k\|_F^2 / \psi(X_k). \end{aligned}$$

Thus $\psi(X_k) \le \|\mathfrak{R}_k\|_F^2 / \mu(Y)$. Similarly, $\|\mathfrak{R}_k\|_F^2 / \mu(\mathfrak{R}_k) \le \psi(X_k)$ can be also obtained. □

If Ω^{-T} is a preconditioning matrix and $Y = \Omega X$, then the preconditioned version of (3.2) is

$$\Omega^{-T} \left((H^T H + \lambda_{\varpi gGCV}^2 I) \Omega^{-1} Y - H^T B \right) = O \tag{3.5}$$

and the matrix $\begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} \Omega^{-1}$ is well conditioned. The overall procedure for preconditioned Gl-CGLS with the weighted global GCV is as follows:

ALGORITHM 2. Preconditioned Gl-CGLS with the weighted global GCV

1. Determine the minimizer $\lambda_{\varpi gGCV}$ for the constrained minimization problem:

$$\begin{array}{ll} \min\limits_{\lambda} & \mathcal{G}_{\text{global}}(\lambda, \varpi) \\ \text{subject to} & \rho_{min} \leq \lambda \leq \rho_{max} \\ & \kappa_1 \leq \varpi \leq \kappa_2. \end{array}$$

2. Solve $\Omega^{-T}(H^T H + \lambda^2_{\varpi gGCV} I)X = \Omega^{-T} H^T B$ using preconditioned Gl-CGLS:

   i. $R_0 = \begin{pmatrix} B \\ O \end{pmatrix} - \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} X_0$.

   ii. $P_0 = S_0 = \Omega^{-T} \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix}^T R_0$, $\gamma_0 = (S_0, S_0)_F$.

   iii. For $k = 0, 1, 2, ...$ until convergence do

   (i) $T_k = \Omega^{-1} P_k$ $Q_k = \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix} T_k$, $\alpha_k = \gamma_k / (Q_k, Q_k)_F$,

   (ii) $X_{k+1} = X_k + \alpha_k T_k$, $R_{k+1} = R_k - \alpha_k Q_k$,

   (iii) $S_{k+1} = \Omega^{-T} \begin{pmatrix} H \\ \lambda_{\varpi gGCV} I \end{pmatrix}^T R_{k+1}$, $\gamma_{k+1} = (S_{k+1}, S_{k+1})_F$,

   (iv) $\beta_k = \gamma_{k+1} / \gamma_k$, $P_{k+1} = S_{k+1} + \beta_k P_k$.

   Enddo

Considering the reflective boundary condition, the preconditioner Ω in (3.5) is set to $\Omega = \mathcal{C}^T(|\Lambda_H|^2 + \lambda^2_{\varpi gGCV} I)^{1/2} \mathcal{C}$ where $\mathcal{C}$ is two dimensional discrete cosine transformation matrix.

4. Numerical experiments

Employing the weighted global GCV in preconditioned Gl-CGLS method for solving image deblurring problems with three test images which are named by *x*, *grain*, and *text* image, we investigated numerical results to illustrate the effectiveness of the regularization parameters chosen from the minimization of the weighted global GCV function. The size of the test image *x* is 32-by-32 and both *grain* and *text* are 256-by-256. Using reflective boundary condition, these images are divided into the collection of small blocks using 32 × 32 sub-blocks. These images are degraded by *Gaussian* blur and Gaussian noise is added. Gaussian blurring parameter is set to 1 for *x* and 3 for *grain* and *text*. Each blocks of test images include 0.5%, 0.9%, and 3% in noise level respectively.

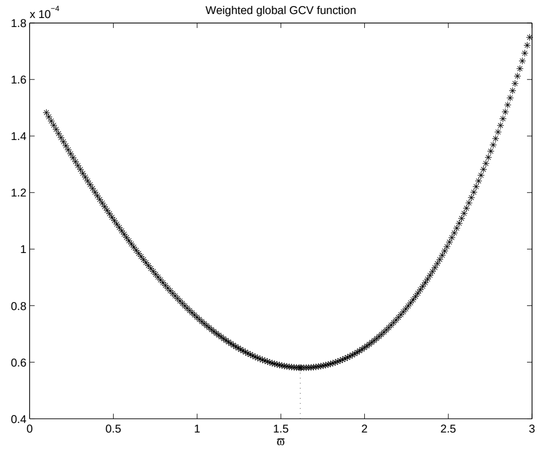

FIGURE 1. Weighted global GCV function $\mathcal{G}_{\text{global}}(\lambda, \varpi)$ for fixed λ in x image with 0.5% noise level has a local minimum at $\varpi \approx 1.616366$.

Noise level(%)		x	*grain*	*text*
0.5	$\varpi = 1$	0.174017	0.228294	1.529964
	$0.1 \leq \varpi \leq 1$	0.174450	0.245501	1.611033
	$1 \leq \varpi \leq 2$	0.165560	0.207119	0.862073
	$2 \leq \varpi \leq 3$	0.166581	0.217749	0.191185
	ϖ, unconstrained	0.166477	0.208517	0.869487
0.9	$\varpi = 1$	0.362061	0.675613	4.711108
	$0.1 \leq \varpi \leq 1$	0.359220	0.654529	3.865294
	$1 \leq \varpi \leq 2$	0.248512	0.305815	2.787565
	$2 \leq \varpi \leq 3$	0.221995	0.221234	0.334344
	ϖ, unconstrained	0.221980	0.386014	2.084861
3	$\varpi = 1$	3.133529	7.160470	40.151111
	$0.1 \leq \varpi \leq 1$	3.202195	8.294281	40.180446
	$1 \leq \varpi \leq 2$	1.925261	3.899219	35.746096
	$2 \leq \varpi \leq 3$	1.580581	0.962814	5.098610
	ϖ, unconstrained	1.580739	5.071711	39.285166

TABLE 1. Relative accuracy

In order to get the local minimizer $\lambda_{\varpi gGCV}$ of $\mathcal{G}_{\text{global}}(\lambda, \varpi)$, (2.3) was solved by using the matlab function *fmincon* to find a constrained minimum of a function of several variables.

Noise level(%)		x	*grain*	*text*
0.5	$\varpi = 1$	1.000000	1.000000	1.000000
	$0.1 \leq \varpi \leq 1$	0.986884	0.989062	0.997578
	$1 \leq \varpi \leq 2$	1.616366	1.089384	1.037937
	$2 \leq \varpi \leq 3$	2.057542	2.028090	2.007250
	ϖ, unconstrained	1.984640	1.063563	1.033435
0.9	$\varpi = 1$	1.000000	1.000000	1.000000
	$0.1 \leq \varpi \leq 1$	0.986883	0.989063	0.997580
	$1 \leq \varpi \leq 2$	1.616343	1.089360	1.037991
	$2 \leq \varpi \leq 3$	2.057542	2.028089	2.007250
	ϖ, unconstrained	1.984623	1.063517	1.033488
3	$\varpi = 1$	1.000000	1.000000	1.000000
	$0.1 \leq \varpi \leq 1$	0.986874	0.989072	0.997603
	$1 \leq \varpi \leq 2$	1.616219	1.089389	1.038674
	$2 \leq \varpi \leq 3$	2.057521	2.028081	2.007244
	ϖ, unconstrained	1.984490	1.063434	1.034158

TABLE 2. Weights corresponding to the results of Table 1

Noise level(%)		x	*grain*	*text*
0.5	$\varpi = 1$	0.448780	0.142343	0.103687
	$0.1 \leq \varpi \leq 1$	0.442439	0.131216	0.098718
	$1 \leq \varpi \leq 2$	0.808796	0.289431	0.192443
	$2 \leq \varpi \leq 3$	0.977290	0.983209	0.994775
	ϖ, unconstrained	0.992795	0.248818	0.181961
0.9	$\varpi = 1$	0.448765	0.142343	0.103729
	$0.1 \leq \varpi \leq 1$	0.442425	0.131217	0.098764
	$1 \leq \varpi \leq 2$	0.808781	0.289391	0.192586
	$2 \leq \varpi \leq 3$	0.977289	0.983209	0.994776
	ϖ, unconstrained	0.992790	0.248728	0.182107
3	$\varpi = 1$	0.448773	0.142483	0.104358
	$0.1 \leq \varpi \leq 1$	0.442427	0.131354	0.099459
	$1 \leq \varpi \leq 2$	0.808756	0.289465	0.194380
	$2 \leq \varpi \leq 3$	0.977294	0.983212	0.994786
	ϖ, unconstrained	0.992781	0.248573	0.183951

TABLE 3. Regularization parameters corresponding to the results of Table 1

In x image with 0.5% noise level, weighted global GCV function has a local minimum at $(\lambda, \varpi) \approx (0.808796, 1.616366)$ when $1 \leq \varpi \leq 2$. Figure 1 is the graph of weighted global GCV function for fixed λ.

The relative accuracy, $\|X^* - X_k\|_F / \|X^*\|_F$, shows how well the true image has been approximated. Table 1 shows the relative accuracy of preconditioned Gl-CGLS method with regularization parameters chosen from both of the weighted global GCV and standard global GCV for three different noise levels. Also, corresponding weights and regularization parameters for each results of Table 1 are given in the Table 2 and 3 respectively.

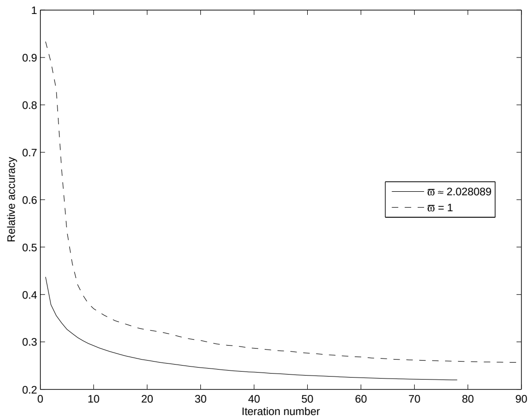

FIGURE 2. Comparison of the relative accuracy for *grain* image when $\varpi = 1$ and $\varpi \approx 2.028089$.

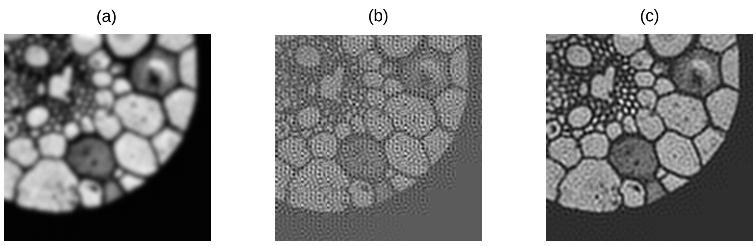

FIGURE 3. (a) is blurred and noisy *grain* image that each block images have 0.9% noisy level. Both (b) and (c) are restored images of (a) when $\varpi = 1$ and $\varpi \approx 2.028089$.

For *grain* image with 0.9% noise level, Figure 2 shows the comparison of the change of relative accuracy along the standard global GCV ($\varpi = 1$) and optimal ϖ from (2.3). Using the weighted global GCV brings appropriate stopping point of the preconditioned Gl-CGLS algorithms. On other side, using the standard global GCV needs more iterations for satisfying stopping condition of the preconditioned Gl-CGLS.

For the optimal $\varpi \approx 2.028089$ using the weighted global GCV, 79 of iterations are required with 60.57 of PSNR, while the standard global GCV needs 418 iterations with 50.87 of PSNR. Degraded and reconstructed images at the stopping point of the preconditioned Gl-CGLS for the given tolerance are shown in Figure 3.

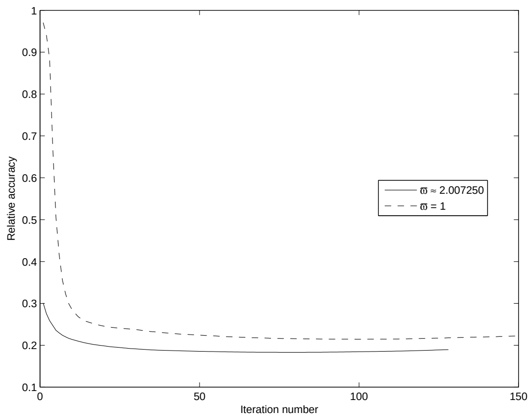

FIGURE 4. Comparison of the relative accuracy for *text* image when $\varpi = 1$ and $\varpi \approx 2.007250$.

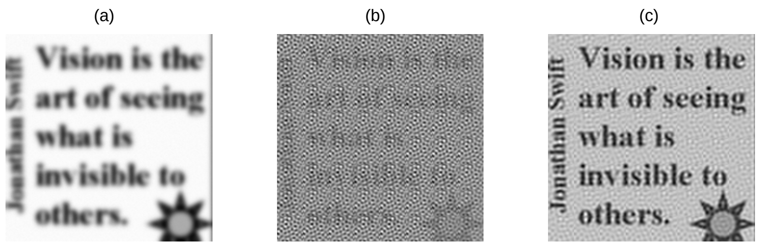

FIGURE 5. (a) is blurred and noisy *text* image that each block images have 0.5% noisy level. Both (b) and (c) are restored images of (a) when $\varpi = 1$ and $\varpi \approx 2.007250$.

The simulation results for *text* image with 0.5% noise level are presented in Figure 4 and 5. For the optimal $\varpi \approx 2.007250$ using the weighted global GCV, 129 of iterations are required with 51.32 of PSNR, while the standard global GCV needs 1403 iterations with 33.26 of PSNR.

5. Conclusions

To obtain more accurate approximation of the true images in deblurring problems, we proposed an efficient way to determine the regularization parameter by applying the weighted global GCV function to the inverse problem with multiple right-hand sides. We analyzed the experimental results for many test problems and was able to obtain the globally useful range of the weight when the Gl-CGLS method with the weighted global GCV function is used.

In the future, our next study is to investigate a variant approach of the global *L*-curve method and also to compare it with the weighted global GCV method in determining the regularization parameter for deblurring problem with multiple right-hand sides.

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