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Convergence analysis of the GKB-GCV algorithm

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Abstract

This paper explores the application of the generic Tikhonov regularization used to stabilize large scale ill-posed problems in deblurring, hyper resolution and other applicable situations. Recently, a new solver for the generic Tikhonov regularization, called the GKB-GCV method was proposed by D. Togashi et al. [GSTF JMSR, Vol. 3, No. 2, pp. 53–58]. This paper, analyzes the convergence properties of the GKB-GCV method.

Key Words. ill-posed problem, Tikhonov regularization, GKB-GCV
AMS(MOS) subject classifications. 65F22

1 Introduction

The stable approximate solution for a large scale ill-posed problem of the form:

$$\boldsymbol{x}_{\mathrm{LS}} = \operatorname*{argmin}_{\boldsymbol{x}\in\mathbb{R}^n} \|\boldsymbol{b} - A\boldsymbol{x}\|_2^2, \tag{1}$$

is computed, where matrix $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is ill-conditioned. The right-hand vector $\boldsymbol{b} \in \mathbb{R}^m$ contains the following error:

$$\boldsymbol{b} = A\boldsymbol{x}_{\mathrm{exact}} + \boldsymbol{\epsilon}, \tag{2}$$

where $\boldsymbol{x}_{\mathrm{exact}} \in \mathbb{R}^n$ is the exact solution, and $\boldsymbol{\epsilon} \in \mathbb{R}^m$ is the unknown noise. A matrix of this form sometimes comes from image resolutions, e.g. image deblurring or hyper resolution. Because matrix A is ill-conditioned, $\boldsymbol{x}_{\mathrm{LS}}$ is dependent on noise. The Tikhonov regularization [7] constructs stable approximations of $\boldsymbol{x}_{\mathrm{exact}}$ by solving the least squares problem of the form:

$$\boldsymbol{x}_\lambda = \operatorname*{argmin}_{\boldsymbol{x}\in\mathbb{R}^n} \{\|\boldsymbol{b} - A\boldsymbol{x}\|_2^2 + \lambda\|L\boldsymbol{x}\|_2^2\}, \tag{3}$$

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where $L \in \mathbb{R}^{p\times n}$ is the regularization matrix, and $\lambda > 0$ is the regularization parameter. The standard form of the Tikhonov regularization is when $L = I_n$, where I_n is the $n \times n$ identity matrix. The general form of the Tikhonov regularization is when $L \neq I_n$. When the common space between the null spaces of A and L is the zero space, the regularization problem (3) has a unique solution. To obtain a good approximate solution for (3), an appropriate regularization parameter is required. There are many methods for determining the regularization parameter without identifying the norm of the noise: $\|\boldsymbol{\epsilon}\|_2$, [1, 5].

For $L = I_n$, there are two hybrid methods, called GKB-FP [2] and W-GCV [4]. These methods do not require identifying the norm $\|\boldsymbol{e}\|_2$, and contain a projection over the Krylov subspace generated by the Golub-Kahan Bidiagonalization (GKB) method. The difference between these two methods is in the approach, i.e. in terms of determining the regularization parameter. The GKB-FP uses the FP scheme, whereas the W-GCV uses the weighed GCV. Bazán et al. [3] proposed an approach without identifying norm $\boldsymbol{\epsilon}$, which is created by the extension of the GKB-FP method. In a recent study, the W-GCV method was extended to a general form of the Tikhonov regularization. This was called the GKB-GCV method [8].

This paper explores the uses of the GKB-GCV method which is a solver for a large scale general form of the Tikhonov regularization. A convergence property of the GKB-GCV was analyzed, and it was proven that when the norm of the noise converged to 0, the GKB-GCV method converged to produce the exact solution at most n iterations.

This paper is organized as follows: After the introduction, Section 2 summarizes the framework of the GKB-GCV method. In Section 3, the convergence analysis of the GKB-GCV is described succinctly. The conclusions are summed-up in Section 4.

2 The GKB-GCV method

The GKB-GCV is one of the algorithms for a general form of the Tikhonov regularization, which is based on the GKB and GCV. When $k < n$ GKB steps are applied to matrix A with the initial vector $\boldsymbol{b}/\|\boldsymbol{b}\|_2$, it results in two matrices $Y_{k+1} = [\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{k+1}] \in \mathbb{R}^{m\times(k+1)}$ and $W_k = [\boldsymbol{w}_1, ..., \boldsymbol{w}_k] \in \mathbb{R}^{n\times k}$ with orthonormal columns, and a lower bidiagonal matrix as follows:

$$B_k = \begin{pmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \beta_3 & \ddots & \\ & & \ddots & \alpha_k \\ & & & \beta_{k+1} \end{pmatrix} \in \mathbb{R}^{(k+1)\times k},$$

such that,

$$\begin{aligned} \beta_1 Y_{k+1}\boldsymbol{e}_1 &= \boldsymbol{b} = \beta_1 \boldsymbol{y}_1, \\ AW_k &= Y_{k+1}B_k, \\ A^T Y_{k+1} &= W_k B_k^T + \alpha_{k+1}\boldsymbol{w}_{k+1}\boldsymbol{e}_{k+1}^T, \end{aligned}$$

where $\boldsymbol{e}_i$ denotes the i-th unit vector in $\mathbb{R}^{k+1}$. Columns of W_k are the orthonormal basis for the generalized Krylov subsupace $\mathcal{K}_k(A^TA,\ A^T\boldsymbol{b})$. The general form of regularization over the generated Krylov subspace is as follows:

$$\boldsymbol{x}_\lambda^{(k)} = \underset{\boldsymbol{x}\in\mathcal{K}_k(A^TA,\ A^T\boldsymbol{b})}{\text{argmin}} \{A\boldsymbol{x}-\boldsymbol{b}\|_2^2 + \lambda\|L\boldsymbol{x}\|_2^2\}. \tag{4}$$

Since the columns of W_k are the orthonormal basis for the generated Krylov subsupace, equation (4) is rewritten as follows:

$$\boldsymbol{x}_\lambda^{(k)} = W_k\boldsymbol{y}_\lambda^{(k)}, \quad \boldsymbol{y}_\lambda^{(k)} = \underset{\boldsymbol{y}\in\mathbb{R}^k}{\text{argmin}}\{\|B_k\boldsymbol{y}-\beta_1\boldsymbol{e}_1\|_2^2 + \lambda\|LW_k\boldsymbol{y}\|_2^2\}. \tag{5}$$

GKB-GCV uses the same reduction to PROJ-L when solving the general form of the Tikhonov regularization of Bazán [3]. By using the reduction QR factorization for matrix products LW_k, equation (5) is rewritten as follows:

$$\boldsymbol{y}_\lambda^{(k)} = \underset{\boldsymbol{y}\in\mathbb{R}^k}{\text{argmin}}\{\|B_k\boldsymbol{y}-\beta_1\boldsymbol{e}_1\|_2^2 + \lambda\|R_k\boldsymbol{y}\|_2^2\}. \tag{6}$$

where $Q_kR_k = LW_k$ and Q_k has orthogonal columns. To increase k, the QR factorization can be updated computing $k+1$ elements by using the summation and a product of the vectors. This reduction technique is a good choice for large scale problems, because this approach reduces the size of the least squares problem: $(m+p)\times n$ to $(2k+1)\times k$.

The GCV determines the regularization parameter for equation (3) by searching for the minimum point of function as follows:

$$G(\lambda) = \frac{\|(I_m - AA_{\lambda,L}^+)b\|_2^2}{(\text{trace}(I_m - AA_{\lambda,L}^+))^2}, \tag{7}$$

where $A_{\lambda,L}^+ = (A^TA+\lambda L^TL)^{-1}A^T$. Using the GSVD for the matrix pair $(A,\ L)$, equation (7) is written as follows:

$$G_(\lambda) = \frac{\sum_{i=1}^n \left(\frac{c_i^2\lambda\boldsymbol{u}_i^T\boldsymbol{b}}{s_i^2+c_i^2\lambda}\right)^2 + \sum_{i=n+1}^m(\boldsymbol{u}_i^T\boldsymbol{b})^2}{\left(m - \sum_{i=1}^n \frac{s_i^2}{s_i^2+c_i^2\lambda}\right)^2}. \tag{8}$$

where $A = USZ^{-1},\ L = VCZ^{-1}$. At the k step, the GKB-GCV uses the same approach as AT-GCV [6] for determining λ. The regularization parameter λ is chosen to minimize the following function:

$$\begin{aligned} G_k(\lambda) &= \frac{\|(I_m - AW_k(B_k)_{\lambda,R_k}^+Y_{k+1}^T)\boldsymbol{b}\|_2^2}{(\text{trace}(I_m - AW_k(B_k)_{\lambda,R_k}^+Y_{k+1}^T))^2}, \\ &= \frac{\beta_1^2\left(\sum_{i=1}^k\left(\frac{\lambda_k\boldsymbol{u}_{i(k)}^T\boldsymbol{e}_1}{\sigma_{i(k)}^2+\lambda_k}\right)^2 + (\boldsymbol{u}_{k+1(k)}^T\boldsymbol{e}_1)^2\right)}{\left(m - \sum_{i=1}^k\frac{\sigma_{i(k)}^2}{\sigma_{i(k)}^2+\lambda_k}\right)^2}. \end{aligned}$$

where $B_k = U_kS_kZ_k^{-1},\ R_k = V_kC_kZ_k^{-1}$ by using the reduction GSVD$(B_k,\ R_k)$.

The GKB-GCV method is compactly summarized in Algorithm 1.

Algorithm 1 GKB-GCV Method

Require: $A, \boldsymbol{b}, L, tol$

Ensure: Regularized solution $\boldsymbol{x}_{\lambda^*}^{(k)}$

1. Apply the GKB step to A with starting vector $\boldsymbol{b}$ at $k = 0$ and set $k = 1$.
2. Perform one more GKB step and update the QR factorization of LW_k.
   $LW_k = Q_k R_k$.
3. Compute GSVD($B_k,\ R_k$). $B_k = U_k S_k Z^{-1},\ R_k = V_k C_k Z^{-1}$.
4. Compute the minimized point λ_k of $G_k(\lambda)$.
5. **If** the stopping criteria is satisfied **do**
   $\lambda^* = \lambda_k$.
   else do
   $k \leftarrow k + 1$
   Go to step 2.
   end if
6. Solve subproblem $\boldsymbol{y}_{\lambda^*}^{(k)}$.
7. Compute the regularized solution $\boldsymbol{x}_{\lambda^*}^{(k)}$.

3 Convergence property

It will be assumed that when $\lambda_k = \text{argmin}\ G_k(\lambda)$, λ_k will not have a monotone convergence. Therefore, the following theorem must be proven to analyze the convergence property of the GKB-GCV method.

Theorem 3.1 *Assume* $\text{rank}(A) = q < m$ *and* $A\boldsymbol{x}_{\text{exact}} \neq \mathbf{0}$. *Whenever the noise's norm converges to* 0, *the regularization parameter determined by GKB-GCV method converges to* 0 *at the* q *step:*

$$(\|\boldsymbol{\epsilon}\|_2 \to 0) \Rightarrow (\lambda_q \to 0).$$

Proof: 1 *At the* q *step, the GKB method generates these matrices:*

$$B_q = \begin{bmatrix} \alpha_1 & & & & \\ \beta_2 & \alpha_2 & & & \\ & \beta_3 & \ddots & & \\ & & \ddots & \alpha_{q-1} & \\ & & & \beta_q & \alpha_q \\ & & & & 0 \end{bmatrix} = \begin{bmatrix} \hat{B}_q \\ 0 \end{bmatrix} \quad \textit{with} \quad \alpha_q \neq 0,$$

$$\boldsymbol{b} = \beta_1 Y_{q+1} \boldsymbol{e}_1 = A\boldsymbol{x}_{\text{exa}} + \boldsymbol{\epsilon},$$

$$A = Y_{q+1} B_q W_q^T = Y_q \hat{B}_q W_q^T,$$

The reduction GSVD for matrix pair $(\hat{B}_q,\ R_q)$ *is considered, and then the diagonal matrix* D_q *is defined as follows:*

$$[D_q]_{i,i} = [\tilde{C}_q]_{i,i}^2 / ([\tilde{S}_q]_{i,i}^2 + \lambda[\tilde{C}_q]_{i,i}^2) \quad \textit{with} \quad \hat{B}_q = \tilde{U}_q \tilde{S}_q \tilde{X}_q, R_q = \tilde{V}_q \tilde{C}_q \tilde{X}_q.$$

From the triangle inequality, it follows that:

$$\begin{aligned}\|\boldsymbol{r}_{q,\lambda}\|_2 &= \|(I_m - Y_q\hat{B}_q(\hat{B}_q^T\hat{B}_q + \lambda R_q^T R_q)^{-1}\hat{B}_q^T Y_q^T)\boldsymbol{b}\|_2,\\ &= \|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T)\boldsymbol{b}\|_2,\\ &\le \|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^T)^{-1}\tilde{U}_q^T Y_q^T)A\boldsymbol{x}_{\text{exa}}\|_2,\\ &+ \|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T)\boldsymbol{\epsilon}\|_2.\end{aligned}$$

Since $Y_q\tilde{U}_q\tilde{U}_q^T Y_q^T$ is an orthogonal projection from $Y_q^T Y_q = \tilde{U}_q^T\tilde{U}_q = I_q$, the following inequalty is approved:

$$\begin{aligned}&\|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T)\boldsymbol{\epsilon}\|_2\\ &\le \|(I_q - \tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1})\tilde{U}_q^T Y_q^T\boldsymbol{\epsilon}\|_2 + \|\boldsymbol{\epsilon}\|_2,\\ &= \|\lambda\tilde{C}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T\boldsymbol{\epsilon}\|_2 + \|\boldsymbol{\epsilon}\|_2,\\ &= \|\lambda D_q\tilde{U}_q^T Y_q^T\boldsymbol{\epsilon}\|_2 + \|\boldsymbol{\epsilon}\|_2,\\ &\le 2\|\boldsymbol{\epsilon}\|_2.\end{aligned}$$

The last inequality comes from $\|\lambda D_q\boldsymbol{f}\|_2 \le \|\boldsymbol{f}\|_2$. This follows for all λ and $\boldsymbol{f}$ from the definition of the D_q.

From $A = Y_q\hat{B}_q W_q^T$, and $Y_q^T Y_q = \tilde{U}_q^T\tilde{U}_q = I_q$,

$$\begin{aligned}&\|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T)A\boldsymbol{x}_{\text{exa}}\|_2,\\ &= \|(I_m - Y_q\tilde{U}_q\tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{U}_q^T Y_q^T)Y_q\tilde{U}_q\tilde{S}_q\tilde{X}_q W_q^T\boldsymbol{x}_{\text{exa}}\|_2,\\ &= \|Y_q\tilde{U}_q(I_q - \tilde{S}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1})\tilde{S}_q\tilde{X}_q W_q^T\boldsymbol{x}_{\text{exa}}\|_2,\\ &= \|\lambda\tilde{C}_q^2(\tilde{S}_q^2 + \lambda\tilde{C}_q^2)^{-1}\tilde{S}_q\tilde{X}_q W_q^T\boldsymbol{x}_{\text{exa}}\|_2,\\ &= \|\lambda D_q\tilde{U}_q^T Y_q^T Y_q\tilde{U}_q\tilde{S}_q\tilde{X}_q W_q^T\boldsymbol{x}_{\text{exa}}\|_2,\\ &= \lambda\|D_q\tilde{U}_q^T Y_q^T A\boldsymbol{x}_{\text{exa}}\|_2.\end{aligned}$$

Note that since $\|D_q\tilde{U}_q^T Y_q^T A\boldsymbol{x}_{\text{exa}}\|_2 > 0$ from the assumption and the definition of the matrices, it has a minimum value 0 at $\lambda = 0$. Therefore, from $G_k(\lambda) \ge 0$ for all k and $\text{trace}(A(A^TA)^+A^T) = m - q > 0$,

$$(\|\boldsymbol{\epsilon}\|_2 \to 0) \Rightarrow (\|\boldsymbol{r}_{q,0}\|_2 \le 2\|\boldsymbol{\epsilon}\|_2 \to 0) \Rightarrow (\lambda_q \to 0).$$

Theorem 3.2 *Assume that $\text{rank}(A) = q < m$, $\boldsymbol{x}_{\text{exact}} \in (\text{Ker}(A))^\perp$. Then, if the $\|\boldsymbol{\epsilon}\| \to 0$, GKB-GCV method converges to a true solution at most q iterations. That is:*

$$(\|\boldsymbol{\epsilon}\|_2 \to 0) \Rightarrow (\boldsymbol{x}_{q,\lambda_q} \to \boldsymbol{x}_{\text{exa}}).$$

Proof: 2 *At the q step, from the triangle inequality:*

$$\begin{aligned}\|\boldsymbol{x}_{q,\lambda_q} - \boldsymbol{x}_{\text{exa}}\|_2 &\le \|(W_q(\hat{B}_q^T\hat{B}_q + \lambda_q R_q^T R_q)^{-1}\hat{B}_q^T Y_q^T A - I_n)\boldsymbol{x}_{\text{exa}}\|_2,\\ &+ \|W_q(\hat{B}_q^T\hat{B}_q + \lambda_q R_q^T R_q)^{-1}\hat{B}_q^T Y_q^T\boldsymbol{\epsilon}\|_2.\end{aligned}$$

From $A = Y_q \hat{B}_q W_q^T$, *and* $W_q W_q^T \boldsymbol{x}_{\text{exa}} = \boldsymbol{x}_{\text{exa}}$, *the first term in the inequality rewrites:*

$$
\begin{aligned}
&\|(W_q(\hat{B}_q^T \hat{B}_q + \lambda_q R_q^T R_q)^{-1} \hat{B}_q^T Y_q^T A - I_n)\boldsymbol{x}_{\text{exa}}\|_2, \\
&= \|(W_q(\hat{B}_q^T \hat{B}_q + \lambda_q R_q^T R_q)^{-1} \hat{B}_q^T \hat{B}_q W_q^T - I_n)\boldsymbol{x}_{\text{exa}}\|_2, \\
&= \|(W_q \tilde{X}_q^{-1}(\tilde{S}_q^2 + \lambda_q \tilde{C}_q^2)^{-1} \tilde{S}_q^2 \tilde{X}_q W_q^T - I_n)\boldsymbol{x}_{\text{exa}}\|_2, \\
&= \|\tilde{X}_q^{-1}((\tilde{S}_q^2 + \lambda_q \tilde{C}_q^2)^{-1} \tilde{S}_q^2 - I_q)\tilde{X}_q W_q^T \boldsymbol{x}_{\text{exa}}\|_2, \\
&= \| - \lambda_q \tilde{X}_q^{-1} D_q \tilde{X}_q W_q^T \boldsymbol{x}_{\text{exa}}\|_2, \\
&= \lambda_q \|\tilde{X}_q^{-1} D_q \tilde{X}_q W_q^T \boldsymbol{x}_{\text{exa}}\|_2.
\end{aligned}
$$

From Theorem 3.1: $(\|\boldsymbol{\epsilon}\|_2 \to 0) \Rightarrow (\lambda_q \to 0)$. *So,*

$$\lambda_q \|\tilde{X}_q^{-1} D_q \tilde{X}_q W_q^T \boldsymbol{x}_{\text{exa}}\|_2 \to 0 \quad (\|\boldsymbol{\epsilon}\|_2 \to 0)$$

From the property of the norm, it follows that:

$$
\begin{aligned}
&\|W_q(\hat{B}_q^T \hat{B}_q + \lambda_q R_q^T R_q)^{-1} \hat{B}_q^T Y_q^T \boldsymbol{\epsilon}\|_2, \\
&= \|W_q \tilde{X}_q^{-1}(\tilde{S}_q^2 + \lambda_q \tilde{C}_q^2)^{-1} \tilde{S}_q \tilde{U}_q^T Y_q^T \boldsymbol{\epsilon}\|_2, \\
&= \|\hat{B}_q^{-1} \tilde{U}_q (\tilde{S}_q^2 + \lambda_q \tilde{C}_q^2)^{-1} \tilde{S}_q^2 \tilde{U}_q^T Y_q^T \boldsymbol{\epsilon}\|_2, \\
&\leq \|\hat{B}_q^{-1}\|_2 \cdot \|(\tilde{S}_q^2 + \lambda_q \tilde{C}_q^2)^{-1} \tilde{S}_q^2\|_2 \cdot \|\boldsymbol{\epsilon}\|_2 \to 0.
\end{aligned}
$$

In the last limits, this is used since $\hat{B}_q$ *is a full rank and in Theorem 3.1:* $\|(\tilde{S}_q^2 + \lambda \tilde{C}_q^2)^{-1} \tilde{S}_q^2\|_2 \to 1$. *From the above,*

$$
\begin{aligned}
\|\boldsymbol{x}_{q,\lambda} - \boldsymbol{x}_{\text{exa}}\|_2 &\leq \lambda_q \|\tilde{X}_q^{-1} D_q \tilde{X}_q W_q^T \boldsymbol{x}_{\text{exa}}\|_2 + \|B_q^{-1}\|_2 \cdot \|\boldsymbol{\epsilon}\|_2, \\
&\to 0 \quad (\|\boldsymbol{\epsilon}\|_2 \to 0).
\end{aligned}
$$

4 Conclusion

The GKB-GCV algorithm was explored and the convergence property of the GKB-GCV algorithm was analyzed. As a result, it was proven that when rank(A) is less than m, the norm of the noise converged to 0 and the true solution is orthogonal to the kernel of A, then the GKB-GCV algorithm converges to produce the true solution at most matrix size iterations. The results show that if the GKB-GCV is applied to well-posed problems, the computed solution converges to a true solution.

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