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Residual smoothing for complex symmetric systems

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Abstract

We present a residual smoothing algorithm for the complex symmetric conjugate gradients method. As in the real case, the residual smoothing method reproduces the (quasi-minimising) QMR method, and is considerably simpler to compute.

1 Introduction

The proper inner product for complex vectors is $(x, y)_* = y^* x$. In the case of complex symmetric systems, i.e., $A = A^t$ but not necessarily $A = A^*$, there is also value in considering the real inner product[1] $(x, y)_t = x^t y$. Applying the conjugate gradient method to a complex symmetric system, and letting all inner products be the t-inner product leads to a three-term recurrence.

By contrast, while the conjugate gradient method using the $*$-inner product applied to a Hermitian system satisfies a three-term recurrence, on a complex symmetric system it would give longer recurrences, much like the GMRES method when applied to real nonsymmetric systems.

In [2], Freund derived a variant of his QMR method [3] for complex symmetric methods. As in the real case, it is based on minimising the coefficient vector on the Krylov basis, rather than minimising the residuals themselves. Correspondingly, this version of QMR effects a quasi-minimisation of the residuals.

Zhou and Walker showed in [6] that the QMR method in the real case can be derived by so-called 'residual smoothing'. In this paper we apply the same

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[1] Which is not an inner product, strictly speaking.

Let A be complex symmetric and let b be given,
let x_1 by arbitrary, and $r_1 = Ax_1 - b$.
Iterate for $i = 1, \ldots$:
  let $\omega_i = r_i^t r_i$
  if $i = 1$, $p_i = r_i$,
  otherwise $\beta = \omega_i / \omega_{i-1}$
    and $p_i = r_i + \beta p_{i-1}$;
  with $\alpha = \omega_i / p_i^t A p_i$
    update $x_{i+1} = x_i - \alpha p_i$ and $r_{i+1} = r_i - \alpha A p_i$

Figure 1: The conjugate gradient algorithm for complex symmetric systems.

residual smoothing strategy to the complex symmetric CG method, thereby deriving a different way of computing the vectors of Freund's complex symmetric QMR method. The advantage of the residual smoothing algorithm for the QMR vectors is a greatly simplified algorithm.

2 Derivation of the method

Let R be the sequence of residuals of the (three-term) conjugate gradient method for complex symmetric systems (figure 1), and define $\Theta = diag(R^* R)$, and the normalisation $R = N\Theta^{1/2}$. Since $R^* R$ is not a diagonal matrix, neither is $N^* N$, but we have

$$\|N_n\|_2 \leq \sqrt{n} \tag{1}$$

(where the n subscript denotes that we take the block consisting of the first n columns).

In [1] we showed that any convex combination vector g_n of the residuals $r_1, \ldots, r_n$ satisfies the following formula:

$$g_{n+1} - g_1 = -AR_n v_n = -R_{n+1} H_n u_n$$

where H_n is the $(n+1) \times n$ Hessenberg matrix describing the iterative method, and $R_n = (r_1, \ldots, r_n)$. Since $g_1 = r_1 = R_n e_1$ (for any n), this leads to the minimisation problem

$$\min \|g_{n+1}\| = \min \|R_{n+1}(e_1 - H_n u_n)\|.$$

In the real case, this is used to generate minimising or quasi-minimising residuals in methods such as MinRes [4] and GMRES [5], or QMR [3] respectively.

Since H_n can be factored as $H_n = (J - I)U$ with

$$J - I = \begin{pmatrix} -1 & & & \\ 1 & -1 & & \emptyset \\ \emptyset & \ddots & \ddots & \end{pmatrix}, \qquad U \text{ upper triangular,}$$

there is likewise a vector z_n such that

$$g_{n+1} = R_{n+1}(e_1 - (J - I)z_n). \tag{2}$$

The minimisation problem to be solved is then

$$\min_{z_n} \|g_{n+1}\|. \tag{3}$$

For future reference we define $v_n = e_1 - (J - I)z_n$.

We consider the minimisation problem (3), and note that from (1):

$$\begin{aligned} \|g_{n+1}\|_2 &= \|R_{n+1}v_n\|_2 = \|N_{n+1}\Theta^{1/2}v_n\|_2 \\ &\leq \|N_{n+1}\|_2\,\|\Theta^{1/2}v_n\|_2 = \sqrt{n+1}\|\Theta^{1/2}v_n\|_2. \end{aligned} \tag{4}$$

Hence, solving the minimisation problem

$$\min_{z_n} \|\Theta^{1/2}v_n\|_2 \tag{5}$$

gives the optimal solution in the Krylov basis up to a factor of $\sqrt{n}$. The minimisation problem (5) is also essentially the one considered in [2], though this theoretical justification was not given there.

In the traditional derivation of the QMR method, the minimisation problem (5) was solved by QR factorisations, as in [2]. We will here derive the residual smoothing method of solving the same minimisation problem, hence deriving the same iterates. We follow the discussion in [6].

The minimisation problem

$$\tau_k^2 = \min_{z_n \in C^n} \|\Theta^{1/2}(e_1 - (J - I)z_n)\|_2$$

is of the form $\min_x \|Ax - b\|$ with A and b real, so the solution, given by $x = (A^*A)^{-1}A^*b$ is real too.

An explicit form for the minimum, and the value of v for which it is taken, can be given.

With $z_n = (\zeta_1, \ldots, \zeta_n)^t$,

$$\tau_k^2 = \min_z \theta_1(1 - \zeta_1)^2 + \theta_2(\zeta_1 - \zeta_2)^2 + \cdots + \theta_n(\zeta_{n-1} - \zeta_n)^2 + \theta_{n+1}\zeta_n^2.$$

Changing variables $\xi_1 = 1 - \zeta_1$, $\xi_k = \zeta_{k+1} - \zeta_k$ for $k = 2, .., n$, $\xi_{n+1} = \zeta_n$, the minimisation problem becomes

$$\tau_n^2 = \min_{\sum \xi_i = 1} \sum \theta_i \xi_i^2$$

Let A be complex symmetric and let b be given,
let x_1 by arbitrary, and $g_1 = r_1 = Ax_1 - b$.
Iterate for $i = 1, \ldots$:
    let $\omega_i = r_i^t r_i$ and $\theta_1 = r_i^* r_i$
    if $i = 1$, $p_i = r_i$, $\tau_1 = \theta_1$
    otherwise, $\beta = \omega_i / \omega_{i-1}$
        and $p_i = r_i + \beta p_{i-1}$;
    with $\alpha = \omega_i / p_i^t A p_i$
        update $x_{i+1} = x_i - \alpha p_i$ and $r_{i+1} = r_i - \alpha A p_i$
    and with $\tau_{i+1} = (\tau_i^{-1} + \theta_i^{-1})^{-1}$
        update $g_{i+1} = \tau_{i+1}(\tau_i^{-1} g_i + \theta_i^{-1} r_{i+1})$

Figure 2: The conjugate gradient algorithm for complex symmetric systems.

for which the unique minimiser gives

$$\tau_n = \sqrt{\frac{1}{\sum_i^n 1/\theta_i}}.$$

We thus find that L_2 quasi-minimisation of the norm of the coefficient vector z_k gives coefficients τ_k satisfying

$$\frac{1}{\tau_k^2} = \frac{1}{\tau_{k-1}^2} + \frac{1}{\theta_k}, \quad \tau_1^2 = \theta_1, \qquad \text{where } \theta_k = \|r_k\|_2. \tag{6}$$

From the discussion in [6] we know that these τ_k coefficients generate the (quasi) minimising residuals:

$$\tau_{k+1}^{-2} g_{k+1} = \tau_k^{-2} g_k + \theta_k^{-1} r_{k+1}.$$

Note that this method needs the $(r_k, r_k)_*$ inner products, which do not arise naturally from the complex symmetric conjugate gradients method. Thus, some extra amount of computation is required.

We summarise the resulting algorithm in figure 2.

3 Conclusion

We have applied the residual-smoothing technique of [6] to the complex symmetric conjugate gradients method. The resulting method gives the same iterates as the QMR method of [2], but computed in a far simpler fashion. These QMR iterates constitute a quasi-minimisation, giving the optimal approximations based on the given Krylov space up to a small factor.

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