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Paper 23

Modified Versions of QMR-Type Methods

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Abstract

The quasi-minimal residual methods, these are QMR (Freund and Nachtigal [4]), TFQMR (Freund [5]) and QMRCGSTAB (Chan et al [1]), are biorthogonalization methods for solving nonsymmetric linear systems of equations which improve the irregular behaviour of BiCG, CGS and BiCGSTAB algorithms [8], respectively. They are based on the quasi-minimization of the residual using the standard Givens rotations that lead to methods with short term recurrences.

In this paper, the quasi-minimization problem is solved using a similar procedure to that developed in [6] for the minimization problem arising in GMRES method. It consists of a direct solver which provides new versions of QMR-type methods, the so called modified QMR methods (MQMR). MQMR algorithms have different convergence behaviour in finite arithmetic although are equivalent to the standard ones in exact arithmetic. The new implementations not only reduce the number of iterations but also reach convergence in some cases where the standard algorithms do not work well.

On the other hand, we study the effect of preconditioning, for example with Jacobi, ILU, SSOR or sparse approximate inverse [9], and reordering [2] on the performance of these algorithms is studied.

Finally, some numerical experiments are solved in order to compare the results obtained by standard and modified algorithms.

Keywords: nonsymmetric linear systems, sparse matrices, Krylov subspace methods, quasi-minimal residual methods, preconditioning, reordering.

1 Introduction

The approximate solution using QMR method for the Krylov subspace of order k is,

$$x_k = x_0 + V_k\,u \tag{1}$$

where u minimizes the norm,

$$\left\|\gamma e_1 - \overline{T}_k\,u\right\|_2 \tag{2}$$

which is a simplification of the residual norm,

$$\|\,r\|_2 = \left\|V_{k+1}\left(\gamma e_1 - \overline{T}_k\,u\right)\right\|_2 \tag{3}$$

where V_k is the matrix which columns are the vectors v_i, $i = 1, ..., k$, obtained by Lanczos biorthogonalization procedure, $\gamma = \|r_0\|_2$, and matrix $\overline{T}_k$ is,

$$\overline{T}_k = \begin{pmatrix} T_k \\ \delta_{k+1}e_k^t \end{pmatrix} \tag{4}$$

with,

$$T_k = \begin{pmatrix} \alpha_1 & \beta_2 & & . & & & \\ \delta_2 & \alpha_2 & \beta_3 & . & & & \\ & \delta_3 & \alpha_3 & . & & & \\ . & . & . & . & . & . & . \\ & & & . & \alpha_{k-2} & \beta_{k-1} & \\ & & & . & \delta_{k-1} & \alpha_{k-1} & \beta_k \\ & & & . & & \delta_k & \alpha_k \end{pmatrix} \tag{5}$$

α_i, $i = 1, ..., k$; β_j, $j = 2, ..., k$; δ_l, $l = 2, ..., k+1$, are the parameters obtained during Lanczos process (see 2.2.1).

In this paper we will directly solve the minimum square problem arising from the minimization of the quadratic functional (2), instead of using the QR factorization of matrix $\overline{T}_k$; see e.g. [7].

2 Modified QMR method

Consider the orthogonal projection on the subspace of solutions of the quasi-minimization problem (2) multiplying by $\overline{T}_k^T$ we obtain,

$$\overline{T}_k^T\,\overline{T}_k\,u = \overline{T}_k^T\gamma e_1 \tag{6}$$

where the structure of the $(k+1)\times k$ matrix $\overline{T}_k$ is,

$$\overline{T}_k = \begin{pmatrix} \boxed{\quad d_k^T \quad} \\ \boxed{\begin{matrix} & U_k \\ \mathbf{0} & \end{matrix}} \end{pmatrix}$$

the first row of $\overline{T}_k$ is a k dimension vector d_k^t, and the rest is an upper triangular matrix U_k,

$$d_k = \begin{pmatrix} \alpha_1 & \beta_2 & 0 & . & . & . & 0 \end{pmatrix}$$

$$U_k = \begin{pmatrix} \delta_2 & \alpha_2 & \beta_3 & . & & & \\ & \delta_3 & \alpha_3 & \beta_4 & & & \\ & & & . & & & \\ . & . & . & . & . & . & . \\ & & & . & \delta_{k-1} & \alpha_{k-1} & \beta_k \\ & (0) & & . & & \delta_k & \alpha_k \\ & & & . & & & \delta_{k+1} \end{pmatrix}$$

where,

$$\{d_k\}_i = d_i = \{\overline{T}\}_{1i} \qquad i = 1, ..., k \tag{7}$$

$$\{U_k\}_{ij} = u_{ij} = \begin{cases} \{\overline{T}\}_{i+1,\,j} & 1 \le i \le j \le k \\ 0 & \text{in the rest} \end{cases} \tag{8}$$

then, the decomposition of the product $\overline{T}_k^T \overline{T}_k$ in (6) becomes in a sum,

$$\left\{\overline{T}_k^T \overline{T}_k\right\}_{ij} = d_i d_j + \sum_{m=1}^{k} u_{mi} u_{mj} \tag{9}$$

Taking into account the descomposition of $\overline{T}_k^T \overline{T}_k$, the equation (6), can be written as,

$$\left(d_k d_k^T + U_k^T U_k\right) u = \overline{T}_k^T \gamma e_1 \tag{10}$$

and, from $\overline{T}_k^T e_1 = d_k$, we obtain,

$$\left(d_k d_k^T + U_k^T U_k\right) u = \gamma d_k \tag{11}$$

Using the associative and distributive properties of matrix product, the equation above can be written as,

$$U_k^T U_k u = d_k \left(\gamma - \langle d_k, u\rangle\right) \tag{12}$$

from,

$$\lambda_i = \gamma - \langle d_k, u\rangle \tag{13}$$

$$u = \lambda_i p_k \tag{14}$$

we obtain,

$$U_k^T U_k p_k = d_k \tag{15}$$

Which is a double triangular system, where U_k^T y U_k are triangular matrices and only two substitution process are required for the solution.

Once we solve (15), we compute λ_i to obtain u from equation (14),

$$\lambda_i = \gamma - \langle d_k, u\rangle = \gamma - \lambda_i \langle d_k, p_k\rangle \tag{16}$$

thus,

$$\lambda_i = \frac{\gamma}{1 + \langle d_k,\, p_k\rangle} \tag{17}$$

Note that $1 + \langle d_k, p_k\rangle \neq 0$, because,

$$\langle d_k, p_k\rangle = \left\langle U_k^T U_k p_k, p_k\right\rangle = \|U_k p_k\|_2^2 \geq 0 \tag{18}$$

therefore λ_i never degenerates.

The proposed method requires:

1. Given d_k and U_k defined in (7) and (8), solve in a double triangular system given in (15) ,

$$U_k^T \bar{p}_k = d_k \tag{19}$$
$$U_k p_k = \bar{p}_k \tag{20}$$

2. Compute λ_i in equation (17).

3. Obtain u solving equation (14)

The residual vector whose norm is given in (3) can be obtained from,

$$r_i = V_{k+1}\widehat{r_i} \tag{21}$$

where $\widehat{r_i}$ is the $(k+1)$-vector,

$$\widehat{r_i} = \gamma e_1 - \overline{T}_k\, u \tag{22}$$

and its entries can be computed as follow,

$$\{\widehat{r_i}\}_j = \begin{cases} \lambda_i & \text{if} \quad j = 1 \\ -\lambda_i \bar{p}_k & \text{if} \quad j = 2, ..., k+1 \end{cases} \tag{23}$$

Since, from partition of $\overline{T}_k$, the first entrie from $(k+1)$-vector $(\overline{T}_k\, u)$ is $\langle d_k, u\rangle$, and the rest of the entries are given by k-vector $(U_k u)$. Then the first entry of $\hat{r}_i$ is λ_i, and the rest are,

$$-U_k u = -\lambda_i U_k p_k = -\lambda_i \bar{p}_k \tag{24}$$

where $\bar{p}_k$ can be kept in the resolution of the first triangular system given in (19).

Note that the residuals are not equivalent (as in GMRES), because vectors v_i are not orthonormal, $\|r_i\|_2 \neq \|\widehat{r_i}\|_2$

The MQMR algorithm obtained with direct solving of the quasi-minimization problem results as follows, *MQMR algorithm*

Initial guess x_0. $r_0 = b - Ax_0$

$\beta_1 = \delta_1 = 0$

$v_0 = w_0 = 0$

$\gamma = \|r_0\|$

$v_1 = w_1 = \frac{1}{\gamma} r_0$

Do while $\sqrt{k+1} \parallel \widehat{r}_{k-1} \parallel / \parallel r_0 \parallel \geq \varepsilon \quad (k = 1, 2, 3, ...)$,

$\alpha_k = \langle Av_k, w_k \rangle$

$\widehat{v}_{k+1} = Av_k - \alpha_k v_k - \beta_k v_{k-1}$

$\widehat{w}_{k+1} = A^T w_k - \alpha_k w_k - \delta_k w_{k-1}$

$\delta_{k+1} = |\langle \widehat{v}_{k+1}, \widehat{w}_{k+1} \rangle|^{1/2}$

$\beta_{k+1} = \langle \widehat{v}_{k+1}, \widehat{w}_{k+1} \rangle / \delta_{k+1}$

$v_{k+1} = \widehat{v}_{k+1} / \delta_{k+1}$

$w_{k+1} = \widehat{w}_{k+1} / \beta_{k+1}$

Solve $U_k^T \bar{p} = d_k$ and $U_k p = \bar{p}$

$$\text{where} \left\{ \begin{array}{l} \{d_k\}_m = \{\overline{T}\}_{1m} \\ \{U_k\}_{lm} = \{\overline{T}\}_{l+1m} \end{array} \right. \qquad l, m = 1, ..., k$$

$$\lambda_k = \frac{\gamma}{1 + \langle d_k,\, p \rangle}$$

$u_k = \lambda_k \, p$

$x_k = x_0 + V_k u_k$; being $V_k = [v_1, v_2, ..., v_k]$

$r_k = V_{k+1} \widehat{r}_k$; being $V_{k+1} = [v_1, v_2, ..., v_{k+1}]$

$$\text{where} \left\{ \begin{array}{l} \{\widehat{r}_k\}_1 = \lambda_k \\ \{\widehat{r}_k\}_{l+1} = -\lambda_k \, \{\bar{p}\}_l \end{array} \right. \qquad l = 1, ..., k$$

End

We must take into account that the convergence criterion depends on $\widehat{r}_k$, which is the residual computed from Modified QMR.

3 Modified TFQMR Method

The approximation obtained using TFQMR method in a Krylov subespace of dimension k, is,

$$x_0 + Y_k u_k \tag{25}$$

where $Y_k = [y_1, y_2, ..., y_k]$, $y_k = t_{i-1}$ si $k = 2i-1$ is odd, and $y_k = q_i$ if $k = 2i$ is even, and u_k minimizes the norm $\left\| \left(\delta_1 e_1 - \bar{T}_k \, u \right) \right\|_2$, which represents a quasi-minimum of the residual la norm (see Saad [10]),

$$\| \, r_k \|_2 = \left\| W_{k+1} \Delta_{k+1}^{-1} \left(\delta_1 e_1 - \Delta_{k+1} \overline{B}_k u_k \right) \right\|_2 \tag{26}$$

being,

$$\overline{\overline{T}}_k = \mathbf{\Delta}_{k+1}\overline{B}_k \tag{27}$$

Where W_{k+1} is the matrix whose columns are the vectors,

$$W_{k+1} = [w_1, w_2, ..., w_{k+1}] \tag{28}$$

and $\mathbf{\Delta}_{k+1}$ is a diagonal matrix, such that W_{k+1} is scaled up ($\delta_k = \| r_i\|$, if $k = 2i+1$ is odd, or $\delta_k = \sqrt{\| r_{i-1}\| \ \ \| r_i\|}$, if $k = 2i$ is even),

$$\mathbf{\Delta}_{k+1} = \begin{pmatrix} \delta_1 & & . & & \\ & \delta_2 & . & & \\ . & . & . & . & . \\ & & . & \delta_k & \\ & & . & & \delta_{k+1} \end{pmatrix} \tag{29}$$

and $\overline{B}_k$ is the $(k+1) \times k$ matrix,

$$\overline{B}_k = \begin{pmatrix} \alpha_0^{-1} & & & . & & \\ -\alpha_0^{-1} & \alpha_0^{-1} & & . & & \\ & -\alpha_0^{-1} & \alpha_1^{-1} & . & & \\ . & . & . & . & . & . \\ & & & . & \alpha_{(k-1)/2}^{-1} & \\ & & & . & -\alpha_{(k-1)/2}^{-1} & \alpha_{(k-1)/2}^{-1} \\ & & & . & & -\alpha_{(k-1)/2}^{-1} \end{pmatrix} \tag{30}$$

The MTFQMR algorithm obtained with direct solving of the quasi-minimization problem is as follows.

MTFQMR algorithm

Initial guess x_0. $r_0 = b - Ax_0$

r_0^* is arbitrary, such that $\langle r_0, r_0^* \rangle \neq 0$

$s_0 = t_0 = r_0$

$v_0 = As_0$

$\rho_0 = \langle r_0, r_0^* \rangle$

$\delta_1 = \| r_0\|$

Do while $\sqrt{i+1} \ \| \widehat{r}_{i-1} \| \ / \ \| r_0 \| \geq \varepsilon \quad (i = 1, 2, 3, ...)$

  $\sigma_{i-1} = \langle v_{i-1}, r_0^* \rangle$

  $\alpha_{i-1} = \rho_{i-1}/\sigma_{i-1}$

  $q_i = t_{i-1} - \alpha_{i-1}v_{i-1}$

  $r_i = r_{i-1} - \alpha_{i-1}A\,(t_{i-1} + q_i)$

  From $k = 2i-1, 2i$ do

    If k is odd do

$\delta_{k+1} = \sqrt{\| r_{i-1}\| \ \| r_i\|}; y_k = t_{i-1}$

Else

$\delta_{k+1} = \| r_i\|; y_k = q_i$

End

End

Solve $U_k^T \bar{p} = d_k$ and $U_k p = \bar{p}$

$$\text{where} \begin{cases} \{d_k\}_m = \left\{\overline{\overline{T}}\right\}_{1m} \\ \{U_k\}_{lm} = \left\{\overline{\overline{T}}\right\}_{l+1m} \end{cases} \qquad l, m = 1, ..., k$$

$$\lambda_k = \frac{\delta_1}{1 + \langle d_k, \, p \rangle}$$

$u_k = \lambda_k \, p$

$x_k = x_0 + Y_k u_k$; with $Y_k = [y_1, y_2, ..., y_k]$

$$\begin{cases} \{\widehat{r}_i\}_1 = \lambda_{2i} \\ \{\widehat{r}_i\}_{l+1} = -\lambda_{2i} \, \{\bar{p}\}_l \end{cases} \qquad l = 1, ..., 2i$$

$\rho_i = \langle r_i, r_0^* \rangle$

$\beta_i = \rho_i / \rho_{i-1}$

$t_i = r_i + \beta_i q_i$

$s_i = t_i + \beta_i (q_i + \beta_i s_{i-1})$

$v_i = \ A s_i$

End

Now the convergence criterion depends on $\widehat{r}_k$, which represents the residual, computed from Modified TFQMR.

4 Modified QMRCGSTAB Method

The QMRCGSTAB algorithm proposed by Chan et al [1], makes two quasi-minimizations per iterations. If we define $Y_k = [y_1, y_2, ..., y_k]$, being $y_{2l-1} = g_l$ for $l = 1, ..., [(k+1)/2]$ ($[(k+1)/2]$ the integer part of $(k+1)/2$) and $y_{2l} = s_l$ for $l = 1, ..., [k/2]$($[k/2]$ the integer part of $k/2$). The approximate solution of the system $Ax = b$, starting from the k-th Krylov subspace, is built as $x_0 + Y_k u_k$, where u_k minimizes the norm $\left\| \left(\delta_1 e_1 - \bar{T}_k \, u \right) \right\|_2$, which is again a quasi-minimum of the residual norm,

$$\| r_k\|_2 = \left\| W_{k+1} \Delta_{k+1}^{-1} \left(\delta_1 e_1 - \Delta_{k+1} \overline{B}_k \, u_k \right) \right\|_2 \tag{31}$$

being,

$$\overline{\overline{T}}_k = \mathbf{\Delta}_{k+1} \overline{B}_k \tag{32}$$

W_{k+1} is the matrix whose columns are the residual vectors,

$$W_{k+1} = [w_1, w_2, ..., w_{k+1}] \tag{33}$$

with $w_{2l-1} = s_l$ for $l = 1, ..., [(k+1)/2]$ and $w_{2l} = r_l$ for $l = 1, ..., [k/2]$; and $\mathbf{\Delta}_{k+1}$ is a diagonal matrix, such that W_{k+1} is scaled up ($\delta_i = \| w_i \|$),

$$\mathbf{\Delta}_{k+1} = \begin{pmatrix} \delta_1 & & . & & \\ & \delta_2 & . & & \\ . & . & . & . & . \\ & & . & \delta_k & \\ & & . & & \delta_{k+1} \end{pmatrix} \tag{34}$$

$\overline{B}_k$ is the $(k+1) \times k$ matrix,

$$\overline{B}_k = \begin{pmatrix} \sigma_1^{-1} & & & . & & \\ -\sigma_1^{-1} & \sigma_2^{-1} & & . & & \\ & -\sigma_2^{-1} & \sigma_3^{-1} & . & & \\ . & . & . & . & . & . \\ & & & . & \sigma_{k-1}^{-1} & \\ & & & . & -\sigma_{k-1}^{-1} & \sigma_k^{-1} \\ & & & . & & -\sigma_k^{-1} \end{pmatrix} \tag{35}$$

with $\sigma_{2l} = \omega_l$ for $l = 1, ..., [(k+1)/2]$, and $\sigma_{2l-1} = \alpha_l$ for $l = 1, ..., [(k+1)/2]$.

The MQMRCGSTAB algorithm obtained with direct solving of the quasi-minimization problem is written below.

MQMRCGSTAB algorithm

Initial guess x_0, $r_0 = b - Ax_0$

r_0^* is arbitrary, such that $\langle r_0, r_0^* \rangle \neq 0$

$\rho_0 = \alpha_0 = \omega_0 = 1$

$g_0 = v_0 = 0$

Do while $\sqrt{2i+1} \parallel \widehat{r}_{i-1} \parallel / \parallel r_0 \parallel \geq \varepsilon \quad (i = 1, 2, 3, ...)$

$\rho_i = \langle r_0^*, r_{i-1} \rangle$

$\beta_i = (\rho_i / \rho_{i-1})(\alpha_{i-1} / \omega_{i-1})$

$g_i = r_{i-1} + \beta_i (g_{i-1} - \omega_{i-1} v_{i-1})$

$v_i = A g_i$

$\alpha_i = \dfrac{\rho_i}{\langle v_i, r_0^* \rangle}$

$s_i = r_{i-1} - \alpha_i v_i$

$\delta_{2i-1} = \|s_i\|$, $y_{2i-1} = g_i$

$t_i = A s_i$

$\omega_i = \dfrac{\langle t_i, s_i \rangle}{\langle t_i, t_i \rangle}$

$r_i = s_i - \omega_i t_i$

$\delta_{2i} = \|r_i\|$, $y_{2i} = s_i$

Solve $U_{2i}^t \bar{p} = d_{2i}$ and $U_{2i} p = \bar{p}$

$$\text{where}\begin{cases} \{d_{2i}\}_m = \{\overline{T}\}_{1m} \\ \{U_{2i}\}_{lm} = \{\overline{T}\}_{l+1m} \end{cases} \quad l,m = 1,...,2i$$

$$\lambda_{2i} = \frac{\delta_1}{1 + \langle d_{2i},\, p\rangle}$$

$$u_{2i} = \lambda_{2i}\, p$$

$$x_i = x_0 + Y_{2i}u_{2i} \text{ with } Y_{2i} = [y_1, y_2, ..., y_{2i}]$$

$$\begin{cases} \{\widehat{r}_i\}_1 = \lambda_{2i} \\ \{\widehat{r}_i\}_{l+1} = -\lambda_{2i}\,\{\bar{p}\}_l \end{cases} \quad l = 1,...,2i$$

End

Here, the convergence criterion is depends on $\widehat{r}_k$, which represents the residual computed from Modified QMRCGSTAB.

5 Numerical experiments

The first nonsymmetric linear system that has been selected is *orsreg1* matrix corresponding to an oil reservoir problem from the *Harwell-Boeing Sparse Matrix Collection*, which yields a system of 2205 equations with 14133 non zero entries.

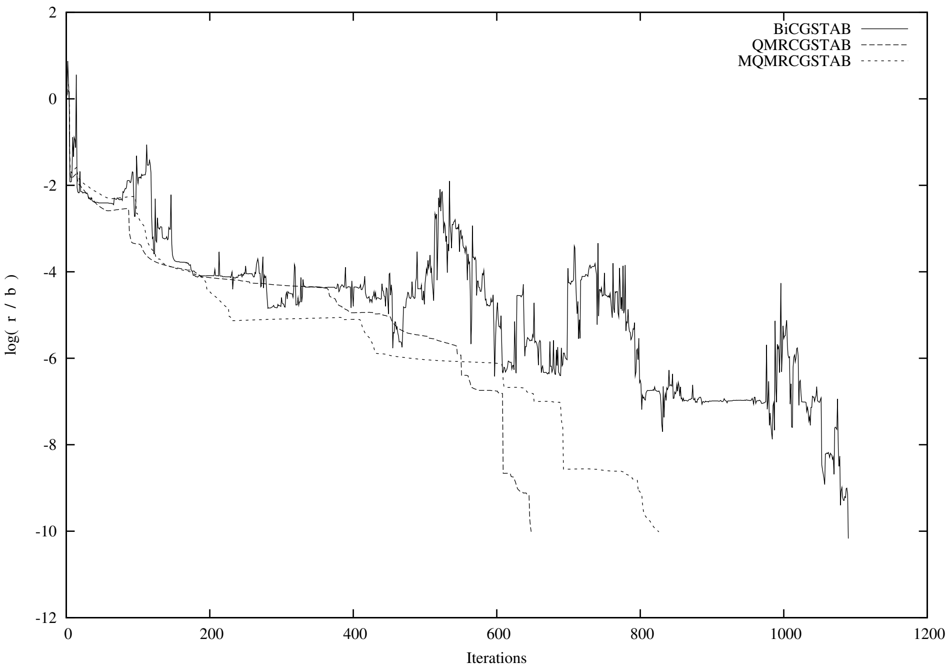

Figure 1: Convergence of stabilized biortogonalization methods for *orsreg1*

The convergence behaviour of non preconditioned BiCGSTAB, QMRCGSTAB and MQMRCGSTAB algorithms is represented in figure 1. We can see the smoother convergence of QMR type methods compared to that of BiCGSTAB. In addition, the modified version of QMRCGSTAB reduces the number of iterations required by the standard algorithm for reaching convergence.

The second example has been selected from the *Harwell-Boeing Sparse Matrix Collection* too. In this case, *watt1* matrix arises from an oil reservoir engineering problem and has 1856 equations with 11360 non zero entries.

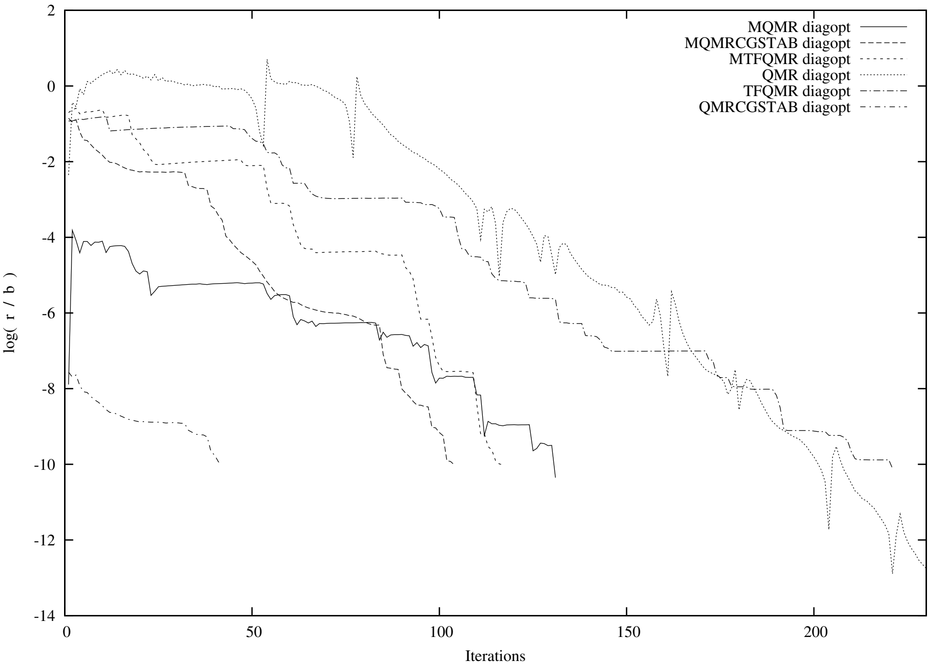

Figure 2: Convergence of modified and standard QMR algorithms with diagonal approximate inverse preconditioning for *watt1*

Figure 2 shows the performance of modified and standard QMR type methods using an approximate inverse preconditioner with diagonal pattern. In this case, although the modified versions of QMR and TFQMR reach convergence before the standard ones, however the QMRCGSTAB is faster than MQMRCGSTAB.

The third numerical experiment (*cuaref*) is related to the convection-diffusion equation in a square $\Omega = (0,1) \times (0,1)$

$$v_1 \frac{\partial u}{\partial x} + v_2 \frac{\partial u}{\partial y} - K \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0$$

with velocity field,

$$v_1 = C\,(y - 1/2)\left(x - x^2\right), \quad v_2 = C\,(1/2 - x)\left(y - y^2\right)$$

An adaptive finite element discretization leads to a nonsymmetric linear system of 7520 equations.

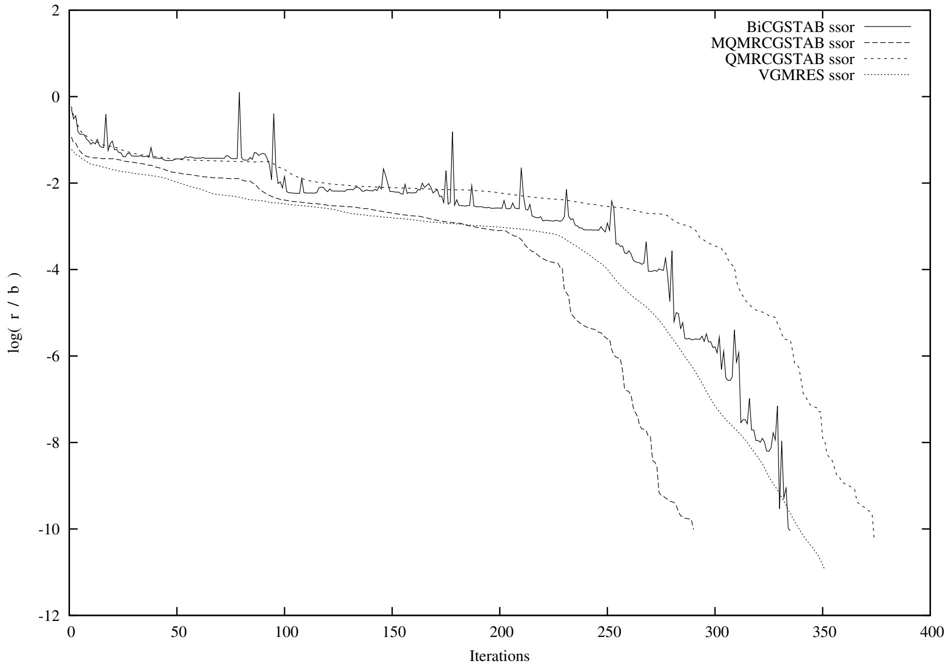

Figure 3: Performance of several Krylov subspace methods with SSOR preconditioning for *cuaref* (7520 equations)

In figure 3 we represent the convergence of some Krylov subspace methods with SSOR preconditioning. Note that MQMRCGSTAB reaches convergence at a lower number of iterations than BiCGSTAB, QMRCGSTAB and VGMRES. At first, MQMRCGSTAB curve is close to VGMRES one, while at the end it has the same behaviour than QMRCGSTAB. This phenomenon has been repeated in many others experiments not included here.

The last linear system arise from a two-dimensional convection-diffusion problem (*convdifhor*) defined in a square Ω,

$$v_1 \frac{\partial u}{\partial x} - K \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = F$$

with a velocity field given by,

$$v_1 = 10^4 \left(y - 1/2\right) \left(x - x^2\right) \left(1/2 - x\right)$$

Again, an adaptive finite element discretization yields a nonsymmetric system of 3423 equations. Figure 4 illustrates the effect of ordering on the convergence of Preconditioned MTFQMR when we use ILU(0). In this example Minimun Degree, Minimun Neighbouring and Reverse Cuthill-McKee reordering algorithms have been applied (see e.g. [3]). The results show that some reordering techniques may reduce about 50% the number of iterations.

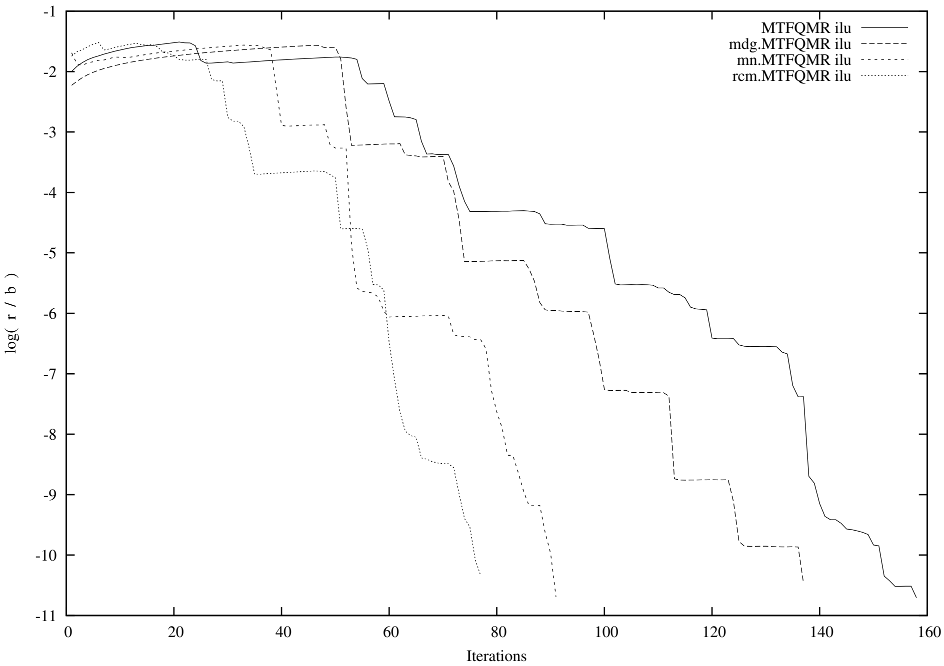

Figure 4: Effect of ordering on the convergence of MTFQMR with ILU(0) preconditioning *convdifhor* (3423 equations)

6 Conclusion

The modified versions of QMR methods generally lead to smoother convergence curves than the standard ones. The studied numerical experiments shows that the modified algorithms are closer to GMRES at the beginning of the convergence process but at lower computational cost, and work like the standard QMR methods at the last iterations. This robust behaviour of the modified versions has allowed to reach convergence even when the standard QMR methods could not.

We have verified that ordering techniques improve the rate of convergence and the computational cost of the modified algorithms, specially with ILU and SSOR preconditioning.

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