Estimates of the norm of the error in FOM and GMRES

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Introduction

We solve

$$Ax = b$$

with non symmetric Krylov solvers : FOM or GMRES

We would like to compute estimates of the error norm $\|\epsilon^k\| = \|x - x^k\|$ during the iterations

This goal has already been achieved for CG (Conjugate Gradient) for symmetric positive definite matrices

The CG case

Let A be SPD of order n. For CG we have the nice formula

$$\|\epsilon^k\|_A^2 = (A\epsilon^k, \epsilon^k) = \|r^0\|^2[(T_n^{-1}e^1, e^1) - (T_k^{-1}e^1, e^1)]$$

where T_k is the (tridiagonal) Jacobi matrix obtained from the CG (or Lanczos) coefficients

The formula for $\|\epsilon^k\|_A^2$ is equivalent to a formula proved in Hestenes and Stiefel (1952)

$$\|\epsilon^k\|_A^2 = \sum_{j=k}^{n-1} \gamma_j \|r^k\|^2$$

$\|\epsilon^k\|_A^2$ is the remainder of a Gauss quadrature formula for $(A\epsilon^0, \epsilon^0) = (A^{-1}r^0, r^0)$

Gauss quadrature gives a lower bound. If we have a lower bound of the smallest eigenvalue of A Gauss-Radau gives an upper bound

For the l_2 norm we have

$$\|\epsilon^k\|^2 = \|r^0\|^2[(e^1, T_n^{-2}e^1) - (e^1, T_k^{-2}e^1)] - 2\frac{(e^k, T_k^{-2}e^1)}{(e^k, T_k^{-1}e^1)}\|\epsilon^k\|_A^2$$

Observe that all these formulas involve unknown quantities (T_n or coefficients which have not yet been computed at iteration k)

To deal with this we introduce a delay d and compute an estimate (or a bound) of $\|\epsilon^{k-d}\|$ at CG iteration k

The goal of this work is to achieve the same program for FOM and GMRES :

1) Derive exact formulas for the l_2 norm of the error

2) Use these formulas to obtain estimates of the norm of the error by looking "backwards"

Notations for FOM and GMRES

Let A be real and non singular

Let V_k be the matrix whose columns are orthogonal basis vectors v^j, $j = 1, \dots, k$ of the Krylov subspace $\mathcal{K}_k(r^0, A)$ generated by the Arnoldi process (using MGS)

$$x^k = x^0 + V_k z^k$$

$$AV_k = V_k H_k + h_{k+1,k} v^{k+1} (e^k)^T$$

where H_k is an upper Hessenberg matrix of order k with elements $h_{i,j}$

We also have $H_k = V_k^T A V_k$ and $AV_n = V_n H_n$ if we suppose that the Arnoldi process does not terminate early

In FOM we ask the residual to be orthogonal to the Krylov subspace

$$H_k z^k = V_k^T r^0 = \|r^0\| e^1$$

Let

$$H_k^{(e)} = \begin{pmatrix} H_k \\ h_{k+1,k}(e^k)^T \end{pmatrix}$$

In GMRES we minimize the norm of the residual

$$\min_z \| \, \|r^0\| e^1 - H_k^{(e)} z \|$$

Formulas for the error norm in FOM

Theorem

In the FOM method the square of the l_2 norm of the error is given by

$$\begin{aligned} \|\epsilon^k\|^2 &= \|r^0\|^2 \, [(H_n^{-1}e^1, H_n^{-1}e^1) - (H_k^{-1}e^1, H_k^{-1}e^{)}) \\ &+ 2h_{k+1,k}(H_k^{-1}e^1, e^k)((H_n^{-1}e^{k+1})^k, H_k^{-1}e^1)] \end{aligned}$$

where $(H_n^{-1}e^{k+1})^k$ denotes the k first components of the $k+1$ st column of the inverse of H_n

Sketch of the proof

$$\|\epsilon^k\|^2 = (A^{-1}r^0, A^{-1}r^0) - 2(A^{-1}r^0, V_k z^k) + (V_k z^k, V_k z^k)$$

and we have

$$(A^{-1}r^0, A^{-1}r^0) = \|r^0\|^2 (H_n^{-1}e^1, H_n^{-1}e^1)$$
$$(V_k z^k, V_k z^k) = \|r^0\|^2 (H_k^{-1}e^1, H_k^{-1}e^1)$$
$$(A^{-1}r^0, V_k z^k) = \|r^0\| (e^1, V_k^T A^{-T} V_k z^k)$$

and we remark that

$$V_k^T A^{-T} V_k = H_k^{-T} - h_{k+1,k} H_k^{-T} e^k (v^{k+1})^T A^{-T} V_k$$

Finally we obtain

$$\begin{aligned}(A^{-1}r^0, V_k z^k) &= \|r^0\|^2 [(H_k^{-1}e^1, H_k^{-1}e^1) \\ &- h_{k+1,k} (H_k^{-1}e^1, e^k)((H_n^{-1}e^{k+1})^k, H_k^{-1}e^1)]\end{aligned}$$

and some terms cancel

This formula is interesting but not very well suited to computation

1) There can be some dangerous cancellations in
$(H_n^{-1}e^1, H_n^{-1}e^1) - (H_k^{-1}e^1, H_k^{-1}e^{)})$

2) We do not know the sign of the others terms

Hence, it is useful to look for alternate formulas

The idea is to express H_n^{-1} in terms of H_k^{-1}

"Simplifications" of the formula for the error norms in FOM

Let

$$H_n = \begin{pmatrix} H_k & W_k \\ Y_k^T & \tilde{H}_k \end{pmatrix}$$

Note that $Y_k^T = h_{k+1,k} e^1 (e^k)^T$

Let $S_k = H_k - W_k \tilde{H}_k^{-1} Y_k^T$ be the Schur complement

$$H_n^{-1} = \begin{pmatrix} S_k^{-1} & -S_k^{-1} W_k \tilde{H}_k^{-1} \\ -\tilde{H}_k^{-1} Y_k^T S_k^{-1} & \tilde{H}_k^{-1} + \tilde{H}_k^{-1} Y_k^T S_k^{-1} W_k \tilde{H}_k^{-1} \end{pmatrix}$$

Because of the special structure of Y_k^T we have

$$S_k = H_k - h_{k+1,k} (W_k \tilde{H}_k^{-1} e_1)(e^k)^T$$

so, S_k is a rank-one modification of H_k

By using the Sherman-Morrison formula we obtain

$$S_k^{-1} = H_k^{-1} + \frac{h_{k+1,k}}{1 - h_{k+1,k}(e^k, H_k^{-1} W_k \tilde{H}_k^{-1} e^1)} H_k^{-1} W_k \tilde{H}_k^{-1} e^1 (e^k)^T H_k^{-1}$$

Lemma

Let $w^k = W_k \tilde{H}_k^{-1} e^1$ *and*

$$\gamma_k = \frac{h_{k+1,k}(e^k, H_k^{-1} e^1)}{1 - h_{k+1,k}(e^k, H_k^{-1} w^k)}$$

Then,

$$\begin{aligned}
(H_n^{-1} e^1, H_n^{-1} e^1) &- (H_k^{-1} e^1, H_k^{-1} e^1) \\
&= (h_{k+1,k}(e^k, S_k^{-1} e^1))^2 (\tilde{H}_k^{-1} e^1, \tilde{H}_k^{-1} e^1) \\
&+ 2\gamma_k (H_k^{-1} e^1, H_k^{-1} w^k) + \gamma_k^2 (H_k^{-1} w^k, H_k^{-1} w^k)
\end{aligned}$$

Lemma

Using the notations of the previous lemma, we have

$$(H_n^{-1} e^{k+1})^k = -\frac{\gamma_k}{h_{k+1,k}(e^k, H_k^{-1} e^1)} H_k^{-1} w^k$$

Theorem

Assume the block partitioning of H_n *and denote* $w^k = W_k \tilde{H}_k^{-1} e^1$
Then $\|\epsilon^k\|^2 / \|r^0\|^2$ *is given by*

$$\{h_{k+1,k}\,(\,(e^k, H_k^{-1} e^1) + \gamma_k (e^k, H_k^{-1} w^k))\,\}^2 \|\tilde{H}_k^{-1} e^1\|^2 + \gamma_k^2 \|H_k^{-1} w^k\|^2$$

Note that in this formula we have the sum of 2 positive terms
This is the main interest of this formula

Relations with the residual norm

Theorem

Assuming that H_k *is nonsingular,*

$$\|r^k\|^2 = \|r^0\|^2 h_{k+1,k}^2 (H_k^{-1} e^1, e^k)^2$$

Theorem

Assume the block partitioning of H_n *and denote* $w^k = W_k \tilde{H}_k^{-1} e^1$

$$\|\epsilon^k\|^2 = \|r^k\|^2 \frac{\|\tilde{H}_k^{-1} e^1\|^2 + \|H_k^{-1} w^k\|^2}{[1 - h_{k+1,k}(e^k, H_k^{-1} w^k)]^2}$$

Estimates of the norm of the error in FOM

$$H_k = \begin{pmatrix} H_{k-d} & W_{k-d} \\ Y_{k-d}^T & \tilde{H}_{k-d} \end{pmatrix}$$

(Note that the notations are different from the previous ones since H_k is of order k)

At iteration k we approximate the norm of the error $\|\epsilon^{k-d}\|^2$ at iteration $k-d$ ($d \geq 1$) by

$$\begin{aligned} & \|r^0\|^2 \left[\left\{ h_{k-d+1,k-d} \left((e^{k-d}, H_{k-d}^{-1} e^1) \right. \right. \right. \\ + \quad & \left. \left. \left. \gamma_{k-d} (e^{k-d}, H_{k-d}^{-1} w^{k-d}) \right) \right\}^2 \|\tilde{H}_{k-d}^{-1} e^1\|^2 + \gamma_{k-d}^2 \|H_{k-d}^{-1} w^{k-d}\|^2 \right] \end{aligned}$$

with $w^{k-d} = W_{k-d} \tilde{H}_{k-d}^{-1} e^1$ and

$$\gamma_{k-d} = \frac{h_{k-d+1,k-d}(e^{k-d}, H_{k-d}^{-1} e^1)}{1 - h_{k-d+1,k-d}(e^{k-d}, H_{k-d}^{-1} w^{k-d})}$$

Numerical experiments

Examples from the Matrix Market and a PDE :

E05r0500 : driven cavity fluid dynamics problem with a Reynolds number $Re = 500$, $n = 236, \kappa = 1.16\ 10^6$, complex eigenvalues with a negative real part

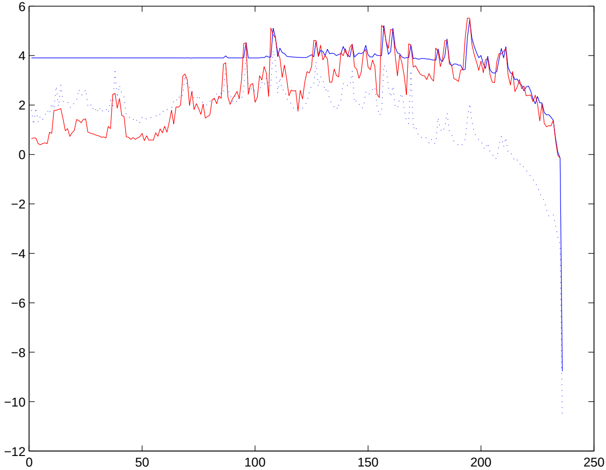
Steam1 : 3D steam model of oil reservoir, $n = 240, \kappa = 2.82\ 10^7$, the eigenvalues of the matrix are real and negative

Steam2 : 3D steam model of oil reservoir, $n = 600, \kappa = 3.78\ 10^6$, the eigenvalues of the matrix are real and negative

Convection-diffusion :

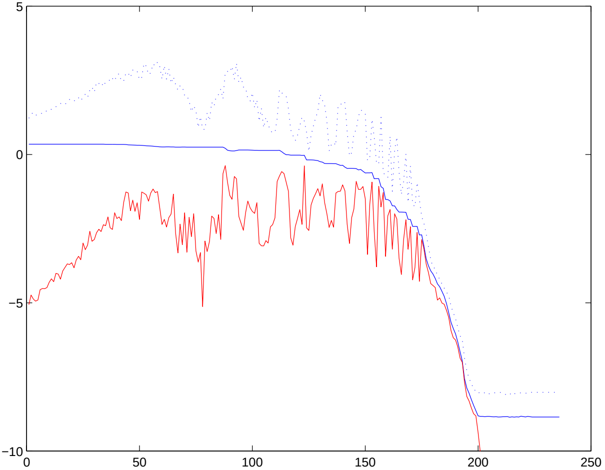
$$-\Delta u + 2e^{2(x^2+y^2)}\frac{\partial u}{\partial x} = f$$

in the unit square, upwind differencing, $n = 2500, \kappa = 1360$

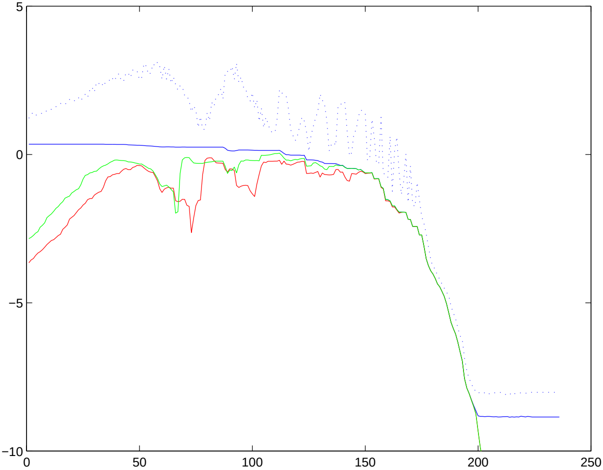


E05r0500 : $n = 236, \kappa = 1.16\ 10^6$, FOM, d=1

Error (solid), residual (dotted), estimate (red)

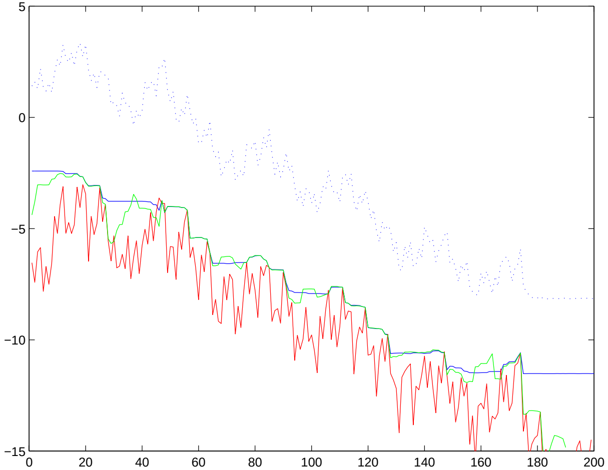


Steam1 : $n = 240, \kappa = 2.82\ 10^7$, FOM, d=1
Error (solid), residual (dotted), estimate (red)



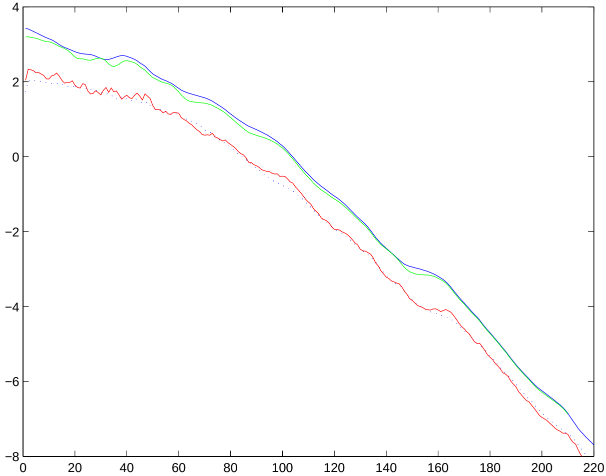
Steam1 : $n = 240, \kappa = 2.82\ 10^7$, FOM

Error (solid), residual (dotted), estimate d=10 (red), d=20 (green)



Steam2 : $n = 600, \kappa = 3.78\ 10^6$, FOM

Error (solid), residual (dotted), estimate d=1 (red), d=10 (green)



Convection-diffusion : $n = 2500, \kappa = 1360$, FOM
Error (solid), residual (dotted), estimate d=1 (red), d=10 (green)

Relations between FOM and GMRES

We use the relations between FOM (F) and GMRES (G) to obtain the GMRES norm of the error

Theorem

Let t^k be the last column of $(H_k^T H_k)^{-1}$ and

$$\delta_{k+1} = \frac{h_{k+1,k}^2}{1 + h_{k+1,k}^2 t_k^k}$$

and $u^k = \delta_{k+1} t^k$. Then

$$x_G^k = x_F^k - (z_F^k)_k V_k u^k$$

$$\epsilon_G^k = \epsilon_F^k + (z_F^k)_k V_k u^k$$

where z_F^k is the coordinate vector of the FOM method given by $z_F^k = \|r^0\| H_k^{-1} e^1$

It is well known that there are relations between the residual norms They can be written in the following way :

Theorem

Let $t_k^k = (e^k, (H_k^T H_k)^{-1} e^k) = \|H_k^{-T} e^k\|^2$. *Then*

$$\|r_G^k\|^2 = \frac{\|r_F^k\|^2}{1 + h_{k+1,k}^2 t_k^k}$$

Formulas for the error norm in GMRES

Theorem

Assume the block partitioning of H_n *and denote* $w^k = W_k \tilde{H}_k^{-1} e^1$

$$\gamma_k = \frac{h_{k+1,k}(e^k, H_k^{-1} e^1)}{1 - h_{k+1,k}(e^k, H_k^{-1} w^k)}$$

Let t^k *be the last column of* $(H_k^T H_k)^{-1}$ *and*

$$\delta_{k+1} = \frac{h_{k+1,k}^2}{1 + h_{k+1,k}^2 t_k^k}$$

and $u^k = \delta_{k+1} t^k$. *Then,*

$$\|\epsilon_G^k\|^2 = \|\epsilon_F^k\|^2 + \|r^0\|^2 [2\gamma_k (H_k^{-1} e^1, e^k)(H_k^{-1} w^k, u^k) + (H_k^{-1} e^1, e^k)^2 \|u^k\|^2]$$

Sketch of the proof

Let $\omega_k = (z_F^k)_k$, we have

$$\epsilon_G^k = \epsilon_F^k + \omega_k V_k u^k$$

and

$$\|\epsilon_G^k\|^2 = \|\epsilon_F^k\|^2 + 2\omega_k(\epsilon_F^k, V_k u^k) + \omega_k^2(V_k u^k, V_k u^k)$$

The problem is to compute $(\epsilon_F^k, V_k u^k)$

$$\epsilon_F^k = \|r^0\| V_n H_n^{-1} e^1 - V_k z_F^k \Rightarrow V_k^T \epsilon_F^k = \|r^0\|(H_n^{-1}e^1)^k - z_F^k$$

$$\begin{aligned}(\epsilon_F^k, V_k u^k) &= \|r^0\|((H_n^{-1}e^1)^k, u^k) - (z_F^k, u^k) \\ &= \|r^0\|[((H_n^{-1}e^1)^k, u^k) - (H_k^{-1}e^1, u^k)]\end{aligned}$$

But $(H_n^{-1}e^1)^k = H_k^{-1}e^1 + \gamma_k H_k^{-1} w^k \Rightarrow$

$$(\epsilon_F^k, V_k u^k) = \|r^0\|\gamma_k(H_k^{-1}w^k, u^k)$$

Estimates of the error norm in GMRES

We use the formula for $\|\epsilon_F^{k-d}\|^2$

The additional term is estimated as

$$\|r^0\|^2[2\gamma_{k-d}(H_{k-d}^{-1}e^1, e^{k-d})(H_{k-d}^{-1}w^{k-d}, u^{k-d})$$

$$+(H_{k-d}^{-1}e^1, e^{k-d})^2\|u^{k-d}\|^2]$$

Numerical experiments

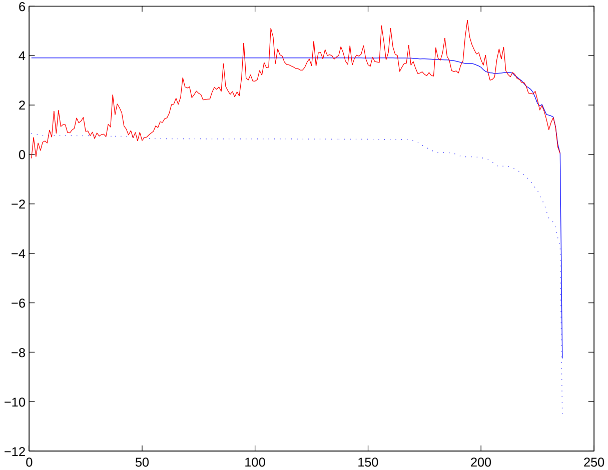
We use the same examples as for FOM

Remarks :

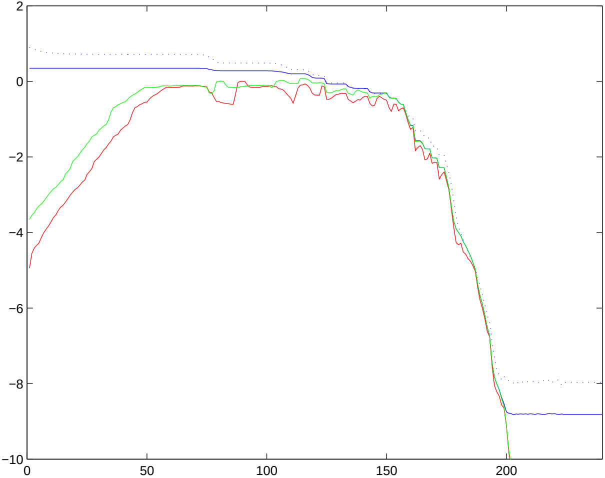
1) The results are a little better

2) The curves of the estimate are less oscillating

3) Increasing the delay d improves the results

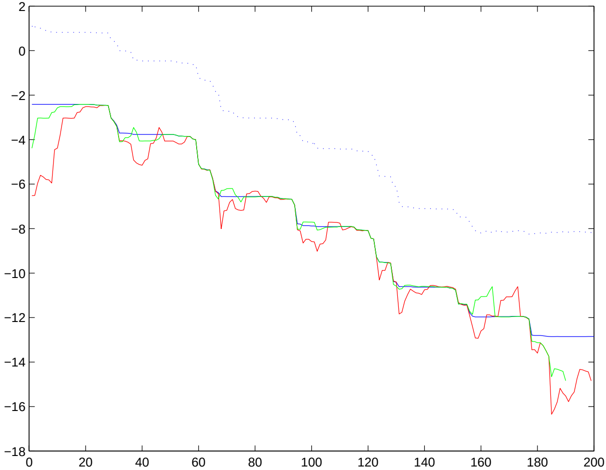


E05r0500 : $n = 236, \kappa = 1.16\ 10^6$, GMRES, d=1
Error (solid), residual (dotted), estimate (red)

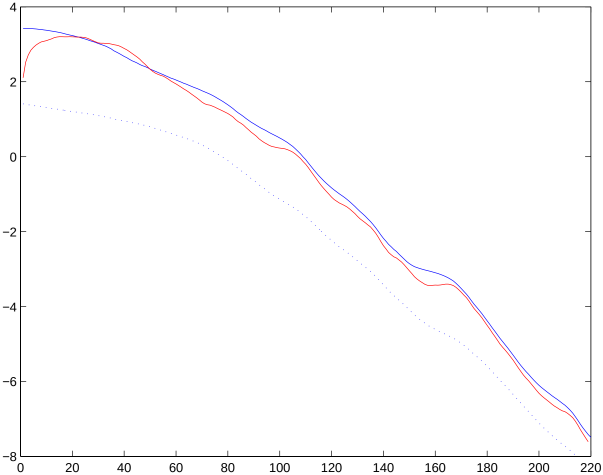


Steam1 : $n = 240, \kappa = 2.82\ 10^7$, GMRES

Error (solid), residual (dotted), estimate d=1 (red), d=10 (green)



Steam2 : $n = 600, \kappa = 3.78\ 10^6$, GMRES
Error (solid), residual (dotted), estimate d=1 (red), d=10 (green)



Convection-diffusion : $n = 2500, \kappa = 1360$, GMRES, d=1

Error (solid), residual (dotted), estimate (red)

Conclusions

We have obtained expressions for the error norms in terms of submatrices of the Arnoldi Hessenberg matrix

We used this to compute estimates of the norms of the error with a (small) delay

The estimates are good except at the beginning of long stagnation phases

It remains to be seen if these expressions of the norms of the error could help to understand GMRES convergence ?