On the convergence of Q-OR and Q-MR Krylov methods for solving linear systems

Gérard MEURANT

Joint work with J. DUINTJER TEBBENS

HH XIX, June 2014

Many Krylov methods have been proposed over the years for solving linear systems

Most of them can be classified as quasi-orthogonal (Q-OR) or quasi-minimum residual (Q-MR)

Q-OR: FOM, BiCG, Hessenberg, ...

Q-MR: GMRES, QMR, CMRH, ...

Whatever their definition, these methods share many fundamental properties

See the nice paper by M. Eiermann and O.G. Ernst, *Geometric aspects in the theory of Krylov subspace methods*, Acta Numerica, v 10 n 10 (2001), pp. 251–312

The methods differ by the basis of the Krylov space that is constructed:

- orthogonal for FOM/GMRES (true OR/MR methods)
- bi-orthogonal for BiCG/QMR
- based on an LU factorization for Hessenberg/CMRH

Our aim is to show that some results about GMRES convergence can be extended to other Q-OR/Q-MR methods

GMRES

GMRES uses the Arnoldi process to construct an orthonormal basis of the Krylov susbpsace

$$\mathcal{K}_n(A, b) = \{b \quad Ab \quad \cdots \quad A^{n-1}b\}$$

Assume the basis vectors are linearly independent. Then,

$$AV = VH, \quad V^*V = I,$$

and H is (unreduced) upper Hessenberg

With $x_0 = 0$, the GMRES iterates $x_k = V_k y_k$ are computed by solving

$$\min_{x_k \in \mathcal{K}_k(A,b)} \|b - Ax_k\|$$

with V_k $n \times k$, k first columns of V

What do we know about GMRES?

Let

$$K = \begin{pmatrix} b & Ab & A^2b & \cdots & A^{n-1}b \end{pmatrix}$$

be the Krylov matrix that we assume of full rank. Then

$$K = VU$$

with V orthogonal (or unitary) and U upper triangular with positive real diagonal entries

As we know, the matrix $H = V^*AV$ is upper Hessenberg

We have

$$H = UCU^{-1}$$

where C is the companion matrix for the eigenvalues of A

[This is a consequence of $AK = KC$]

Let x_k^G (resp. x_k^F) be the iterates for GMRES (resp. FOM) and the residual vectors $r_k^G = b - Ax_k^G$ (resp. $r_k^F = b - Ax_k^F$)

We assume $x_0 = 0$ and $\|b\| = 1$

We know that

- every non-increasing residual norm convergence curve is possible for GMRES

- one can construct matrices A with a prescribed spectrum and right-hand sides b such that GMRES yields a prescribed decreasing residual norm convergence curve. In addition one can prescribe the Ritz values for all iterations

- a first parametrization of this class of matrices and right-hand sides was introduced by Arioli, Pták and Strakoš

For these properties see

A. Greenbaum and Z. Strakoš, *Matrices that generate the same Krylov residual spaces*, in Recent advances in iterative methods, G.H. Golub, A. Greenbaum and M. Luskin, eds., Springer, (1994), pp. 95–118

A. Greenbaum, V. Pták and Z. Strakoš, *Any nonincreasing convergence curve is possible for GMRES*, SIAM J. Matrix Anal. Appl., v 17 (1996), pp. 465–469

M. Arioli, V. Pták and Z. Strakoš, *Krylov sequences of maximal length and convergence of GMRES*, BIT Numerical Mathematics, v 38 n 4 (1998), pp. 636–643

J. Duintjer Tebbens and G. Meurant, *Any Ritz value behavior is possible for Arnoldi and for GMRES*, SIAM J. Matrix Anal. Appl., v 33 n 3 (2012), pp. 958–978

Another parametrization, JDT-GM

Assume we are given n positive numbers

$$1 = f_0 \geq f_1 \geq \cdots \geq f_{n-1} > 0$$

and n complex numbers $\lambda_1, \ldots, \lambda_n$ all different from 0. Let A be a matrix of order n and b an n-dimensional vector of unit norm. The following assertions are equivalent:

1- The spectrum of A is $\{\lambda_1, \ldots, \lambda_n\}$ and GMRES applied to A and b yields residuals $r_j^G,\ j = 0, \ldots, n-1$ such that

$$\|r_j^G\| = f_j, \quad j = 0, \ldots, n-1$$

2- The matrix A is of the form $A = VUCU^{-1}V^*$ and $b = Ve_1$, where V is any unitary matrix, U is nonsingular upper triangular such that

$$U^{-1}_{1,1} = 1, \quad U^{-1}_{1,j} = \left(\frac{1}{f^2_{j-1}} - \frac{1}{f^2_{j-2}} \right)^{\frac{1}{2}}, \; j = 2, \ldots, n$$

and C is the companion matrix corresponding to the prescribed eigenvalues

This type of parametrization can also be used to prescribe all the Ritz values at every iteration

From the relation between FOM and GMRES residual norms we have

- $|(U^{-1})_{1,k}| = 1/\|r^F_{k-1}\|$

Moreover
- $\|r^G_k\|^2 = 1/(M^{-1}_{k+1})_{1,1}$ with $M_{k+1} = U^*_{k+1} U_{k+1}$

This last result has been proved by several people: Stewart, Zitko, Ipsen, Liesen, Rozložník and Strakoš, and Sadok

To compute $(M^{-1}_{k+1})_{1,1}$, following ideas from H. Sadok, we use two simple tools:

- Cramer's rule (1750 but known before that)
- The Cauchy-Binet formula (1812) for $\det(AB)$ with A and B rectangular

Diagonalizable matrices

Let $A = X\Lambda X^{-1}$ and $c = X^{-1}b$. Then

$$K = X \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix}$$

Therefore

$$M = K^*K = \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix}^* X^*X \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix}$$

and

$$M_{k+1} = \mathcal{V}_{k+1}^* D_{\bar{c}} X^* X D_c \mathcal{V}_{k+1}$$

with D_c diagonal with c_i as diagonal entries and ...

$$\mathcal{V}_{k+1} = \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^k \\ 1 & \lambda_2 & \cdots & \lambda_2^k \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_n & \cdots & \lambda_n^k \end{pmatrix}$$

an $n \times (k+1)$ Vandermonde matrix

Then using Cramer's rule for the first column of the inverse and twice the Cauchy-Binet formula we obtain the following (complicated but exact) result for the GMRES residual norms

The residual norms

Let A be a diagonalizable matrix with $A = X\Lambda X^{-1}$, $c = X^{-1}b$. Then

$$\|r_k^G\|^2 = \sigma_{k+1}^N / \sigma_k^D$$

with

$$\sigma_{k+1}^N = \sum_{I_{k+1}} \left| \sum_{J_{k+1}} \det(X_{I_{k+1},J_{k+1}}) c_{j_1} \cdots c_{j_{k+1}} \prod_{j_1 \le j_l < j_p \le j_{k+1}} (\lambda_{j_p} - \lambda_{j_l}) \right|^2$$

$$\sigma_1^D = \sum_{i=1}^{n} \left| \sum_{j=1}^{n} X_{i,j} c_j \lambda_j \right|^2$$

and

$$\sigma_k^D = \sum_{I_k} \left| \sum_{J_k} \det(X_{I_k,J_k}) c_{j_1} \cdots c_{j_k} \lambda_{j_1} \cdots \lambda_{j_k} \prod_{j_1 \le j_l < j_p \le j_k} (\lambda_{j_p} - \lambda_{j_l}) \right|^2, \quad k > 1$$

where the summations are over all sets of indices $I_{k+1}, J_{k+1}, I_k, J_k$ defined as I_ℓ to be a set of ℓ indices $(i_1, i_2, \ldots, i_\ell)$ such that $1 \le i_1 < \cdots < i_\ell \le n$, X_{I_ℓ, J_ℓ} is the submatrix of X whose row and column indices are defined by I_ℓ and J_ℓ

If the matrix A is normal, we have $X^*X = I$ and simpler formulas

$$\sigma_{k+1}^N = \sum_{I_{k+1}} |c_{j_1}|^2 \cdots |c_{j_{k+1}}|^2 \prod_{j_1 \le j_l < j_p \le j_{k+1}} \left|(\lambda_{j_p} - \lambda_{j_l})\right|^2$$

$$\sigma_1^D = \sum_{i=1}^{n} |c_j|^2 \, |\lambda_j|^2$$

and

$$\sigma_k^D = \sum_{I_k} |c_{j_1}|^2 \cdots |c_{j_k}|^2 \, |\lambda_{j_1}|^2 \cdots |\lambda_{j_k}|^2 \prod_{j_1 \le j_l < j_p \le j_k} \left|(\lambda_{j_p} - \lambda_{j_l})\right|^2, \; k > 1$$

See the paper by J. Duintjer Tebbens, GM, H. Sadok and Z. Strakoš, LAA v 450 (2014)

The results for diagonalizable matrices can somehow be extended to the case of non-diagonalizable matrices using the Jordan canonical form

In particular we can obtain nice expressions of the residual norms for one Jordan block

Q-OR and Q-MR methods

Can we extend some of these results to Q-OR and Q-MR methods?

We assume that we have an ascending basis V of the Krylov space (with columns of unit norm) such that $K = VU$ with V nonsingular and U upper triangular

We define $H = UCU^{-1}$. As a consequence $AV = VH$. The iterates are

$$x_k = V_k y_k$$

where V_k is the matrix of the k first columns of V. The residual r_k is

$$V_k e_1 - AV_k y_k = V_k(e_1 - H_k y_k) - h_{k+1,k}(y_k)_k v_{k+1} = V_{k+1}(e_1 - \underline{H}_k y_k)$$

The Q-OR method is defined (provided that H_k is nonsingular) by

$$H_k y_k^O = e_1$$

where H_k is the principal submatrix of order k. This annihilates the first term in the residual

In the Q-MR method y_k^M is computed as the solution of the least squares problem

$$\min_y \|e_1 - \underline{H}_k y\|$$

where $\underline{H}_k$ is $(k+1) \times k$

The vector $z_k^M = e_1 - \underline{H}_k y_k^M$ is referred as the quasi-residual

The residual vector is $r_k^M = V_{k+1} z_k^M$

Generally, the two problems are solved using Givens rotations with sines s_j and cosines c_j. It is known that

$$\|z_k^M\| = |s_1 s_2 \cdots s_k|$$

Moreover we have a relation between the Q-OR residual norms and the Q-MR quasi-residual norms

$$\frac{1}{\|r_k^O\|^2} = \frac{1}{\|z_k^M\|^2} - \frac{1}{\|z_{k-1}^M\|^2}$$

See Eiermann and Ernst (2001), Freund and Nachtigal (1991)

Properties of Q-OR and Q-MR methods

From these results we can show that

$$|(U^{-1})_{1,k}| = \frac{1}{\|r_{k-1}^O\|}$$

This is proved by using the rotation matrices G_j such that

$$G_{n-1} \cdots G_1 H = \mathcal{R}$$

From $H = UCU^{-1}$ we have

$$U^{-1} G_1^{-1} \cdots G_{n-1}^{-1} = CU^{-1} \mathcal{R}^{-1}$$

The first row of the matrix on the right-hand side is zero except from the last entry

Looking at the product of the inverses of the rotation matrices, we can show by induction that

$$U^{-1}_{1,j+1} = \frac{c_j}{s_1 \cdots s_j} = \pm \left(\frac{1}{(s_1 \cdots s_j)^2} - \frac{1}{(s_1 \cdots s_{j-1})^2} \right)^{1/2}, \ j = 1, \ldots, n-1$$

Let $M_{k+1} = U_{k+1}^* U_{k+1}$. Since $M_{k+1}^{-1} = U_{k+1}^{-1} U_{k+1}^{-*}$ and from the first row of U^{-1}, a consequence of the previous result is the following

$$\|z_k^M\|^2 = \frac{1}{(M_{k+1}^{-1})_{1,1}}$$

The difference with GMRES is that we only have the norm of the quasi-residual

Then, we obtain expressions of the quasi-residual norms

The quasi-residual norms

Let A be a diagonalizable matrix with $A = X \Lambda X^{-1}$, $Z = V^{-1}X$ and $c = X^{-1}b$. Then

$$\|z_k^M\|^2 = \sigma_{k+1}^N / \sigma_k^D$$

with

$$\sigma_{k+1}^N = \sum_{I_{k+1}} \left| \sum_{J_{k+1}} \det(Z_{I_{k+1},J_{k+1}}) c_{j_1} \cdots c_{j_{k+1}} \prod_{j_1 \le j_l < j_p \le j_{k+1}} (\lambda_{j_p} - \lambda_{j_l}) \right|^2$$

$$\sigma_1^D = \sum_{i=1}^{n} \left| \sum_{j=1}^{n} Z_{i,j} c_j \lambda_j \right|^2$$

and

$$\sigma_k^D = \sum_{I_k} \left| \sum_{J_k} \det(Z_{I_k,J_k}) c_{j_1} \cdots c_{j_k} \lambda_{j_1} \cdots \lambda_{j_k} \prod_{j_1 \le j_l < j_p \le j_k} (\lambda_{j_p} - \lambda_{j_l}) \right|^2, \quad k > 1$$

where the summations are over all sets of indices $I_{k+1}, J_{k+1}, I_k, J_k$ where I_ℓ is a set of ℓ indices $(i_1, i_2, \ldots, i_\ell)$ such that $1 \le i_1 < \cdots < i_\ell \le n$, Z_{I_ℓ,J_ℓ} is the submatrix of Z whose row and column indices are defined by I_ℓ and J_ℓ

This result arises from $\|z_k^M\|^2 = 1/(M_{k+1}^{-1})_{1,1}$ and

$$\begin{aligned} M &= U^*U = K^*V^{-*}V^{-1}K \\ &= \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix}^* Z^*Z \begin{pmatrix} c & \Lambda c & \cdots & \Lambda^{n-1}c \end{pmatrix} \end{aligned}$$

It yields

$$M_{k+1} = \mathcal{V}_{k+1}^* D_{\bar{c}} Z^* Z D_c \mathcal{V}_{k+1}$$

where D_c is diagonal and $\mathcal{V}_{k+1}$ is an $n \times (k+1)$ Vandermonde matrix

As for GMRES, we compute the $(1,1)$ entry of the inverse using Cramer's rule and the Cauchy-Binet determinant formula

Note that there is no simplification when A is normal

Construction of linear systems with a prescribed convergence curve

Can we construct linear systems with a prescribed convergence curve and a prescribed spectrum for Q-OR and Q-MR methods?

For FOM/GMRES this is easy since we just have to construct an upper triangular matrix U^{-1} with the inverses of the FOM residual norms (obtained from the GMRES norms) on the first row. Then we take

$$A = VUCU^{-1}V^*, \qquad b = Ve_1$$

where C is the companion matrix of the given eigenvalues and V is any unitary matrix

Things are more difficult for some Q-OR/Q-MR methods because we may ask for some non-zero structure in H

BiCG

We would like to find matrices H (with a given spectrum) and U such that

$$H = \begin{pmatrix} \gamma_1 & \beta_2 & 0 & 0 & 0 \\ \rho_2 & \gamma_2 & \beta_3 & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \rho_{n-1} & \gamma_{n-1} & \beta_n \\ 0 & 0 & 0 & \rho_n & \gamma_n \end{pmatrix} = UCU^{-1}$$

and the first row of U^{-1} is prescribed as $\begin{pmatrix} 1 & g_1 & \cdots & g_{n-1} \end{pmatrix}$ with $g_j \neq 0$

Let $\omega_2, \ldots, \omega_n$ be arbitrary chosen entries of the last column of U^{-1} with $\omega_n \neq 0$, $\omega_1 = g_{n-1}$ and $-\alpha_0, \ldots, -\alpha_{n-1}$ be the entries of the last column of C that we know from the prescribed spectrum

We compute U^{-1} and H recursively column-wise
The last column of $U^{-1}H = CU^{-1}$ yields

$$\begin{pmatrix} g_{n-2}\beta_n + g_{n-1}\gamma_n \\ \vdots \\ \omega_n\gamma_n \end{pmatrix} = \begin{pmatrix} -\alpha_0\omega_n \\ \vdots \\ \omega_{n-1} - \alpha_{n-1}\omega_n \end{pmatrix}$$

We use the first and last equations

$$\begin{pmatrix} g_{n-2} & g_{n-1} \\ 0 & \omega_n \end{pmatrix} \begin{pmatrix} \beta_n \\ \gamma_n \end{pmatrix} = \begin{pmatrix} -\alpha_0\omega_n \\ \omega_{n-1} - \alpha_{n-1}\omega_n \end{pmatrix}$$

The solution of this 2×2 non singular linear system yields γ_n, β_n

From the other equations that we discarded we can compute the unknown entries $\nu_{j,n-1}$ of column $n-1$ of U^{-1}

Then we go on backwards with column $n-1$

We have three unknowns $\beta_{n-1}, \gamma_{n-1}$ and ρ_n
We first take the first and the last two equations
This gives us a linear system with an upper triangular matrix

$$\begin{pmatrix} g_{n-3} & g_{n-2} & g_{n-1} \\ 0 & \nu_{n-1,n-1} & \omega_{n-1} \\ 0 & 0 & \omega_n \end{pmatrix} \begin{pmatrix} \beta_{n-1} \\ \gamma_{n-1} \\ \rho_n \end{pmatrix} = \begin{pmatrix} 0 \\ \nu_{n-2,n-1} \\ \nu_{n-1,n-1} \end{pmatrix}$$

And so on... Then $A = VHV^{-1}$ and $b = Ve_1$ for an appropriately chosen matrix V

So far we don't know how to completely handle the case with zero entries on the first row of U^{-1}

This algorithm can be extended to a larger upper bandwidth but what about stability?

This allows to prescribe BiCG residual norm convergence (or QMR quasi-residual norms)

Summary

Many known properties of FOM/GMRES are also valid for general Q-OR/Q-MR methods

We express the Q-MR quasi-residual norms as functions of the eigenvalues, the eigenvectors, the right-hand side and the basis of the Krylov space

We (almost) have a parametrization of the class of matrices with a prescribed spectrum and a prescribed Q-OR/Q-MR convergence curve

In particular we can construct examples with a BiCG (finite) convergence curve