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

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

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, truncated 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

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

where n is the order of A. Assume the basis vectors are linearly independent. Then, V gives a basis of $\mathcal{K}_n(A, b)$ and

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

the matrix 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

With $x_0 = 0$ we have

$$\|r_k\| = \|b - Ax_k\| = \min_{p \in \Pi_k} \|p(A)b\|$$

where Π_k is the set of polynomials of degree k with a value 1 at the origin

This leads to bounds for the residual norms. If A is diagonalizable, $A = X\Lambda X^{-1}$, it yields

$$\|r_k\| \leq \kappa(X) \min_{p \in \Pi_k} \|p(\Lambda)\| \, \|b\|$$

The main question is: What quantities does GMRES convergence depend on?

What do we know about GMRES?

In exact arithmetic GMRES is a *direct* method

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. $r_k^F = b - Ax_k^F$)

Without loss of generality 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

- we have two parametrizations of this class of matrices and right-hand sides

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

The APS parametrization

Greenbaum and Strakoš (1994) proved that any convergence curve for the residual norm that can be generated with GMRES can be obtained with a matrix having prescribed eigenvalues

Greenbaum, Pták and Strakoš (1996) showed that any nonincreasing sequence of residual norms can be given by GMRES

Arioli, Pták and Strakoš (1998) gave a complete parametrization of all pairs $\{A, b\}$ generating a prescribed residual norm convergence curve

Theorem (APS)

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. 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 $A = WYCY^{-1}W^*$ and $b = Wh$, where W is any unitary matrix, Y is given by

$$Y = \begin{pmatrix} h & \begin{matrix} R \\ 0 \end{matrix} \end{pmatrix}$$

R being any nonsingular upper triangular matrix of order $n-1$, h a vector such that

$$h = (\eta_1, \dots, \eta_n)^T, \quad \eta_j = (f_{j-1}^2 - f_j^2)^{1/2}$$

and C is the companion matrix corresponding to the polynomial q,

$$q(z) = (z - \lambda_1) \cdots (z - \lambda_n) = z^n + \sum_{j=0}^{n-1} \alpha_j z^j$$

$$C = \begin{pmatrix} 0 & \dots & & 0 & -\alpha_0 \\ 1 & 0 & \dots & 0 & -\alpha_1 \\ 0 & 1 & 0 & \dots & -\alpha_2 \\ & & \ddots & \ddots & \vdots \\ & & & 1 & -\alpha_{n-1} \end{pmatrix}$$

These results have led some people to write that "GMRES convergence for non-normal matrices does not depend on the eigenvalues"

We are going to see in a moment that this statement is not correct

It must be: "GMRES convergence for non-normal matrices does not depend only on the eigenvalues"

Another parametrization, GM-JDT

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. 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

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

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

Moreover

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

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

Following ideas from H. Sadok, to compute $(M^{-1}_{k+1})_{1,1}$ 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

G. Cramer

1704-1752

A.L. Cauchy

(1789-1857)

J. Binet

(1786-1856)

The residual norms for diagonalizable matrices

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

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

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

Using Cramer's rule, we have

$$\begin{aligned} (M_{k+1}^{-1})_{1,1} &= \frac{1}{\det(M_{k+1})} \det \begin{pmatrix} 1 & m_{1,2} & \cdots & m_{1,k} \\ 0 & & & \\ \vdots & & M_{2:k+1,2:k+1} & \\ 0 & & & \end{pmatrix} \\ &= \frac{\det(M_{2:k+1,2:k+1})}{\det(M_{k+1})} \end{aligned}$$

Let $F = XD_c\mathcal{V}_{k+1}$, an $n \times (k+1)$ matrix. Then $M_{k+1} = F^*F$ and by the Cauchy-Binet formula

$$\det(M_{k+1}) = \sum_{I_{k+1}} |\det(F_{I_{k+1},:})|^2$$

the sum is over all sets I_{k+1} of $k+1$ row indices $(i_1, i_2, \ldots, i_{k+1})$ such that $1 \leq i_1 < \cdots < i_{k+1} \leq n$ and $F_{I_{k+1},:}$ is the submatrix of F whose row indices belong to I_{k+1}

$$F_{I_{k+1},:} = (XD_c)_{I_{k+1},:}\mathcal{V}_{k+1}, \quad [(k+1) \times n] * [n \times (k+1)]$$

Hence we can again apply the Cauchy-Binet formula

$$\det(F_{I_{k+1},:}) = \sum_{J_{k+1}} \det(X_{I_{k+1},J_{k+1}}) c_{j_1} \cdots c_{j_{k+1}} \det(\mathcal{V}(\lambda_{j_1}, \ldots, \lambda_{j_{k+1}}))$$

with the Vandermonde matrix

$$\mathcal{V}(\lambda_{j_1}, \ldots, \lambda_{j_{k+1}}) = \begin{pmatrix} 1 & \lambda_{j_1} & \cdots & \lambda_{j_1}^k \\ 1 & \lambda_{j_2} & \cdots & \lambda_{j_2}^k \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_{j_{k+1}} & \cdots & \lambda_{j_{k+1}}^k \end{pmatrix}$$

But $\det(\mathcal{V}(\lambda_{j_1}, \ldots, \lambda_{j_{k+1}}))$ is known

We apply the same technique for computing $\det(M_{2:k+1,2:k+1})$

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, $X^*X = I$ and we have 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

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

$c = X^* b$

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

Bounds for the residual norms (diagonalizable matrices)

Using a result by Bellalij, Jbilou and Sadok we can prove that

$$\|r_k\|^2 \leq \frac{\|X\|^2}{e_1^T(\mathcal{V}_{k+1}^* D_{\bar{c}} D_c \mathcal{V}_{k+1}^*)^{-1} e_1}$$

It yields

$$\|r_k\|^2 \leq \|X\|^2 \frac{\sum_{1\leq i_1<\cdots<i_{k+1}\leq n} \prod_{j=1}^{k+1} \omega_{i_j} \prod_{i_1\leq i_\ell<i_p\leq i_{k+1}} |\lambda_{i_p}-\lambda_{i_\ell}|^2}{\sum_{1\leq i_1<\cdots<i_k\leq n} \prod_{j=1}^{k} \omega_{i_j}|\lambda_{i_j}| \prod_{i_1\leq i_\ell<i_p\leq i_k} |\lambda_{i_p}-\lambda_{i_\ell}|^2}$$

where $\omega_j = |c_j|^2$ with $c = X^{-1}b$

We can also obtain a similar lower bound where the multiplying factor is $\sigma_{\min}(X)^2$ (min of the singular values)

Hence, the residual norms depend on the (differences of the) eigenvalues, the eigenvectors and the right-hand side (through $X^{-1}b$)

If $\sigma_{\min}(X) \approx \|X\|$, the convergence depends essentially on the eigenvalues (and the right-hand side)

- 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. 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

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

Properties of Q-OR and Q-MR methods

From these results we can show by induction that

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

A consequence of this result is the following

Let $M_{k+1} = U_{k+1}^* U_{k+1}$. Then

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

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

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

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

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

and

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

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 $1 \leq i_1 < \cdots < i_\ell \leq n$, 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 $(Z^*Z \neq I)$

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 tridiagonal (with a given spectrum) and U upper triangular 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 easily extended to a larger upper bandwidth but what about stability?

This allows to prescribe BiCG (finite) 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