An optimal Q-OR Krylov method for solving linear systems

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Joint work with J. Duintjer Tebbens

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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, truncated GMRES, QMR, CMRH, ...

Whatever their definition, these methods share many fundamental properties

See 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

They differ by the basis of the Krylov space that is constructed:

- orthogonal for FOM/GMRES,
- bi-orthogonal for BiCG/QMR,
- based on an LU factorization for Hessenberg/CMRH

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

The matrix $H = V^*AV$ is upper Hessenberg

We have

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

where C is the companion matrix for the eigenvalues of A

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

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

We know that

- every residual norm convergence curve is possible for GMRES (and FOM)

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

- $\|r_k^G\|^2 = 1/(M_{k+1}^{-1})_{1,1}$ with $M_{k+1} = U_{k+1}^* U_{k+1} = K_{k+1}^* K_{k+1}$

- 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

- we have two parametrizations of this class of matrices

Moreover we can express the GMRES residual norms as functions of the eigenvalues and eigenvectors of A

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

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

with

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

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

and

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

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 and $c = X^{-1}b$

If the matrix A is normal 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

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

with $c = X^* b$

For all 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

G. Meurant and J. Duintjer Tebbens, *The role eigenvalues play in forming GMRES residual norms with non-normal matrices*, Numerical Algorithms, v 68, n 1 (2015), pp. 143–165

Q-OR and Q-MR methods

Our aim is to see if some of these properties can be extended to Q-OR and Q-MR methods

We assume that we have a 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

$$H_k y^{(k)} = e_1$$

This annihilates the first term in the residual

In the Q-MR method $y^{(k)}$ 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 $z_k^M = e_1 - \underline{H}_k y^{(k)}$ 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

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

The inverses of the Q-OR residual norms can be read from the first row of the inverse of U

A consequence of this result is the following

Let $M_{k+1} = U_{k+1}^* U_{k+1} \neq K_{k+1}^* K_{k+1}$. 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

Let A be a diagonalizable matrix with $A = X\Lambda X^{-1}$ and $Z = V^{-1}X$. 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 $I_{k+1}, J_{k+1}, I_k, J_k$ defined as I_ℓ to be 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 and $c = X^{-1}b$

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

We compute the $(1,1)$ entry of the inverse using Cramer's rule and the Cauchy-Binet determinant formula as suggested by H. Sadok

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 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

BiCG

We would like to find a matrix

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

such that 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 $\omega_n \neq 0$ and $\omega_1 = g_{n-1}$

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 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 system

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

And so on...

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

Construction of "good" bases

We would like to find bases which lead to a "good" convergence of the Q-OR method

The matrix V of the basis is related to the Krylov matrix K by $K = VU$ with U upper triangular

The entries of the first row of U^{-1} are the inverses of the Q-OR residual norms

Constructing a "good" basis may seem easy since one can think that we can just construct any upper triangular matrix U^{-1} with entries of large modulus on the first row

But, it is not so since the columns of V have to be of unit norm

The inverse of U_k is given recursively as

$$U_k^{-1} = \begin{pmatrix} U_{k-1}^{-1} & -\frac{1}{u_{k,k}} U_{k-1}^{-1} U_{1:k-1,k} \\ 0 & \frac{1}{u_{k,k}} \end{pmatrix}$$

Let $\nu_{i,j}$ be the entries of U^{-1}
At step k we already know the entries of U_{k-1}^{-1}. We would like to choose the entries $u_{j,k}$ of column k of U to maximize the quantity

$$\frac{1}{u_{k,k}} \left| \sum_{j=1}^{k-1} \nu_{1,j} u_{j,k} \right|$$

However, the columns of V have to be of unit norm and we must have

$$u_{k,k} = \left\| \sum_{j=1}^{k-1} u_{j,k-1} A v_j - \sum_{j=1}^{k-1} u_{j,k} v_j \right\|$$

At step k the first sum is known

Something simpler

A first step and a way to approximately obtain large entries on the first row of of U^{-1} is to have small diagonal entries $u_{k,k}$

We choose $u_{2,2} = \|Av_1 - u_{1,2}v_1\|$ and we would like to pick $u_{1,2}$ to minimize $u_{2,2}$
This is a least squares problem whose solution is given by

$$u_{1,2} = \frac{v_1^T A v_1}{v_1^T v_1} = v_1^T A v_1$$

It yields $v_2 = \frac{1}{u_{2,2}}[Av_1 - (v_1^T A v_1)v_1]$
It follows that

$$v_1^T v_2 = \frac{1}{u_{2,2}} v_1^T [Av_1 - (v_1^T A v_1)v_1] = 0$$

Therefore we have v_2 orthogonal to v_1

At the next step we choose $u_{1,3}$ and $u_{2,3}$ to minimize
$\|u_{2,2}Av_2 + u_{1,2}Av_1 - u_{2,3}v_2 - u_{1,3}v_1\|$
This is a least squares problem $\min \|b - By\|$ with

$$b = u_{2,2}Av_2 + u_{1,2}Av_1, \quad B = \begin{pmatrix} v_1 & v_2 \end{pmatrix}, \quad y = \begin{pmatrix} u_{1,3} \\ u_{2,3} \end{pmatrix}$$

The normal equations are

$$B^T By = \begin{pmatrix} 1 & v_1^T v_2 \\ v_2^T v_1 & 1 \end{pmatrix} y = B^T b = \begin{pmatrix} v_1^T [u_{2,2}Av_2 + u_{1,2}Av_1] \\ v_2^T [u_{2,2}Av_2 + u_{1,2}Av_1] \end{pmatrix}$$

But $B^T B = I$ since $v_2 \perp v_1$ and we obtain $y = B^T b$

$$v_3 = \frac{1}{u_{3,3}}[b - By] = \frac{1}{u_{3,3}}[b - BB^T b]$$

Let us consider $v_1^T v_3$. We have $v_1^T B = [1\ 0]$, therefore

$$v_1^T BB^T b = v_1^T [u_{2,2} A v_2 + u_{1,2} A v_1] = v_1^T b$$

Hence, $v_1^T v_3 = 0$. Similarly $v_2^T v_3 = 0$

And we can go on...

At every step (in exact arithmetic) the matrices $B^T B$ in the least squares problems are identity matrices

Minimizing the diagonal entries of U yields an orthonormal basis

Then Q-OR $\rightarrow$ FOM, Q-MR $\rightarrow$ GMRES

This is optimal for Q-MR

What about Q-OR?

We can try directly computing U^{-1} from $V = KU^{-1}$

In this way we obtain the vectors v_j straightforwardly, but the columns of V have to be of unit norm

Let $\nu_{i,j}$ be the entries of U^{-1} and

$$v_k = \nu_{1,k} v + \nu_{2,k} A^2 v + \cdots + \nu_{k,k} A^{k-1} v$$

We would like to have $\|v_k\| = 1$ and $|\nu_{1,k}|$ as large as possible

Can we solve this problem?

Let ν be the vector of the components $\nu_{i,k}, i = 1, \ldots, k$

We want $\|K_k \nu\| = 1$. This corresponds to

$$\nu^T K_k^T K_k \nu = \nu^T \mathcal{M}_k \nu = 1$$

This is the equation of an (hyper) ellipsoid in $\mathbb{R}^k$ centered at the origin

We have to find a point on the surface of this ellipsoid with a maximum of the absolute value of the first coordinate

Let us consider $k = 2$. The matrix is

$$\mathcal{M}_2 = \begin{pmatrix} 1 & v^T A v \\ v^T A^T v & v^T A^T A v \end{pmatrix}$$

and the quadratic form is
$x^2 + (v^T A v + v^T A^T v)xy + (v^T A^T A v)y^2 - 1 = 0$ with $x = \nu_{1,2}$
and $y = \nu_{2,2}$
We need to maximize $|x|$ on the ellipse

Let us write the equation as $x^2 + 2\alpha xy + \beta y^2 - 1 = 0$
We find that the solution is

$$x = \pm \left(\frac{\beta}{\beta - \alpha^2} \right)^{\frac{1}{2}}$$

The value of y is

$$y = \pm \frac{\alpha}{\sqrt{\beta(\beta - \alpha^2)}}$$

We remark that $x = \pm\sqrt{(\mathcal{M}_2)_{1,1}}$

More generally the solution is obtained by writing the equation of a tangent hyperplane and asking that it is orthogonal to the x-axis

One can show that a solution is $x = \sqrt{(\mathcal{M}_k^{-1})_{1,1}}$ and the other components are obtained by solving a linear system of order $k-1$ whose matrix and right-hand side are $\mathcal{M}_{2:k,2:k}$ and $-x\mathcal{M}_{2:k,1}$

This yields U^{-1}. If we apply Q-OR with the basis $V = KU^{-1}$ we obtain residual vectors whose norms are

$$\|r_k^O\|^2 = \frac{1}{(\mathcal{M}_{k+1}^{-1})_{1,1}}$$

These values are those that are obtained from GMRES
Therefore, they are the best ones that we can get with the given Krylov subspace. In a sense it defines an optimal Q-OR method

Avoiding the use of U

The previous construction is not practical because
1) we do not want to compute $\mathcal{M}_k^{-1}$
2) in many cases the matrix U is almost singular and must be (numerically) avoided

Instead we would like to construct H column by column. We have

$$H_j = U_j E_j U_j^{-1} + \begin{pmatrix} 0 & \cdots & 0 & \frac{1}{u_{j,j}} U_{1:j,j+1} \end{pmatrix}$$

It yields

$$\sum_{j=1}^{k+1} \nu_{1,j} h_{j,k} = 0 \;\Rightarrow\; \nu_{1,k+1} = -\frac{1}{h_{k+1,k}} \sum_{j=1}^{k} \nu_{1,j} h_{j,k}$$

At the first step, we have

$$\nu_{1,2} = -\frac{1}{h_{2,1}} \nu_{1,1} h_{1,1}$$

But, $\nu_{1,1} = 1$ and $\nu_{1,2} = -h_{1,1}/h_{2,1}$ with $h_{2,1} = \|Av_1 - h_{1,1}v_1\|$

We want to find the minimum of the inverse

$$\frac{\|Av_1 - y\, v_1\|}{|\nu_{1,1} y|}$$

with $\nu_{1,1} = 1$. We consider the square of this ratio and we look for a lower bound γ

$$\frac{v_1^T A^T A v_1 - 2y\, v_1^T A v_1 + y^2}{y^2} \geq \gamma$$

We would like to find the largest possible value of γ such that

$$v_1^T A^T A v_1 - 2y\, v_1^T A v_1 + y^2(1-\gamma) \geq 0$$

In matrix form this can be written as

$$\begin{pmatrix} y & 1 \end{pmatrix} \begin{pmatrix} 1-\gamma & -v_1^T A v_1 \\ -v_1^T A v_1 & v_1^T A^T A v_1 \end{pmatrix} \begin{pmatrix} y \\ 1 \end{pmatrix} \geq 0$$

The value

$$\gamma_{opt} = 1 - \frac{(v_1^T A v_1)^2}{v_1^T A^T A v_1}$$

yields

$$\begin{pmatrix} 1-\gamma & -v_1^T A v_1 \\ -v_1^T A v_1 & v_1^T A^T A v_1 \end{pmatrix} \begin{pmatrix} y \\ 1 \end{pmatrix} = 0$$

The solution is

$$h_{1,1} = y = \frac{v_1^T A^T A v_1}{v_1^T A v_1}$$

and $h_{2,1} = \|Av_1 - h_{1,1} v_1\|$

More generally, at step k we wish to find the largest γ satisfying

$$\frac{1}{|\nu_{1,k+1}|^2} = \frac{\|b - By\|^2}{(\nu^T y)^2} \geq \gamma$$

with

$$b = Av_k, \quad B = \begin{pmatrix} v_1 & \cdots & v_k \end{pmatrix} = V_k, \quad y = \begin{pmatrix} h_{1,k} & \cdots & h_{k,k} \end{pmatrix}^T,$$

$$\nu = \begin{pmatrix} \nu_{1,1} & \cdots & \nu_{1,k} \end{pmatrix}$$

Since $(\nu^T y)^2 = y^T \nu \nu^T y$, in matrix form we have

$$\begin{pmatrix} y^T & 1 \end{pmatrix} \begin{pmatrix} B^T B - \gamma \nu \nu^T & -B^T b \\ -b^T B & b^T b \end{pmatrix} \begin{pmatrix} y \\ 1 \end{pmatrix} \geq 0$$

The value

$$\gamma_{opt} = \frac{\alpha}{\alpha\nu^T(B^TB)^{-1}\nu + \omega^2} = \frac{1}{\nu^T(B^TB)^{-1}\nu + \frac{\omega^2}{\alpha}}.$$

with $\alpha = b^Tb - b^TB(B^TB)^{-1}B^Tb \geq 0$ and $\omega = b^TB(B^TB)^{-1}\nu$ yields the solution

$$(B^TB - \gamma_{opt}\nu\nu^T)y = B^Tb$$

for which we have

$$\begin{pmatrix} B^TB - \gamma_{opt}\nu\nu^T & -B^Tb \\ -b^TB & b^Tb \end{pmatrix} \begin{pmatrix} y \\ 1 \end{pmatrix} = 0$$

Using the Sherman-Morrison formula, we can write

$$y = (B^TB)^{-1}B^Tb + \frac{\gamma}{1-\gamma\nu^T(B^TB)^{-1}\nu}[\nu^T(B^TB)^{-1}B^Tb](B^TB)^{-1}\nu$$

Hence, to compute y we have to solve two $k \times k$ linear systems for $(B^TB)^{-1}B^Tb$ and $(B^TB)^{-1}\nu$

Finally $h_{k+1,k} = \|b - By\|$, $\nu_{1,k+1} = -\nu^Ty/h_{k+1,k}$ and $v_{k+1} = (b - By)/h_{k+1,k}$

We can do this by computing incrementally the Cholesky factorization of $B^TB = V_k^TV_k$

The Q-OR optimal algorithm

Let A be real and $v_k^A = Av_k$

1- $L_{k-1}\ell_k = V_{k-1}^T v_k$ and $\ell_{k,k} = \sqrt{1 - \ell_k^T \ell_k}$

2 -

$$q_k = \frac{1}{\ell_{k,k}} \left[\nu_{1,k} - \ell_k^T \begin{pmatrix} q_1 \\ \vdots \\ q_{k-1} \end{pmatrix} \right]$$

$$p_k = \frac{1}{\ell_{k,k}^2} \left[\nu_{1,k} - \ell_k^T \begin{pmatrix} q_1 \\ \vdots \\ q_{k-1} \end{pmatrix} \right]$$

$$L_{k-1}^T \begin{pmatrix} p_1 \\ \vdots \\ p_{k-1} \end{pmatrix} = \begin{pmatrix} q_1 \\ \vdots \\ q_{k-1} \end{pmatrix} - p_k \ell_k$$

3 - solve of $L_k L_k^T s = w = V_k^T v_k^A$
4 - $\omega = w^T p$, $\alpha = (v_k^A)^T v_k^A - w^T s$ and $\gamma = \alpha / (\alpha \nu^T p + \omega^2)$
5 -

$$H_{1:k,k} = \begin{pmatrix} h_{1,k} \\ \vdots \\ h_{k,k} \end{pmatrix} = s + \frac{\gamma \nu^T s}{1 - \gamma \nu^T p} p$$

6 -

$$h_{k+1,k} = \left\| v_k^A - V_k \, H_{1:k,k} \right\|, \; \nu_{1,k+1} = -\frac{1}{h_{k+1,k}} \nu^T H_{1:k,k}$$

7 - $v_{k+1} = \frac{1}{h_{k+1,k}} [v_k^A - V_k \, H_{1:k,k}]$ and $v_{k+1}^A = A v_{k+1}$

Using Q-OR with this basis must yield the same residual norms as GMRES

However, computing this basis is more costly than Arnoldi

The basis being non-orthogonal we have more inner products to compute, but they are all independent

A numerical experiment

From Liesen and Strakoš, SIAM J. Sci. Comput., v 26 n 6 (2005)

$$-\nu\Delta u + w \cdot \nabla u = 0,$$

with $w = [0,1]^T$ in $\Omega = (0,1)^2$ with Dirichlet boundary conditions

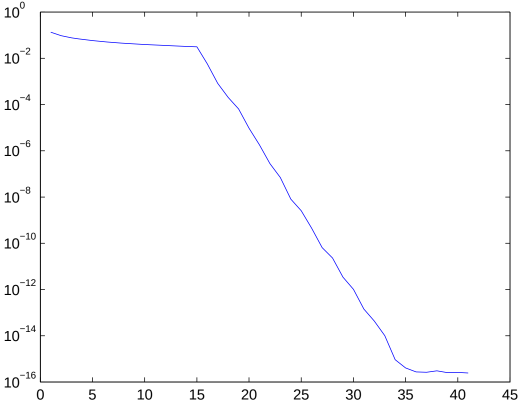
Stabilized Petrov–Galerkin SUPG method with bilinear finite elements on a regular Cartesian mesh

$$A = \nu K \otimes M + M \otimes ((\nu + \delta h)K + C)$$

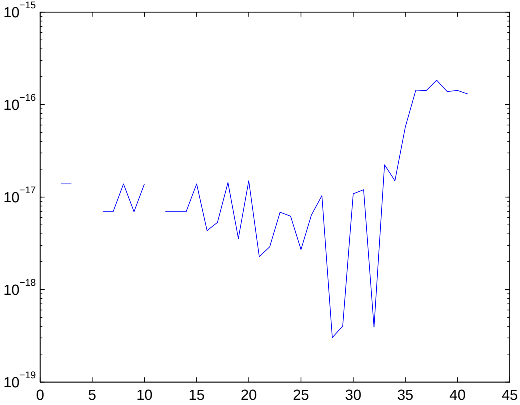
where δ is the stabilization parameter and

$$M = \frac{h}{6}\mathrm{tridiag}(1,4,1), \quad K = \frac{1}{h}\mathrm{tridiag}(-1,2,-1)$$

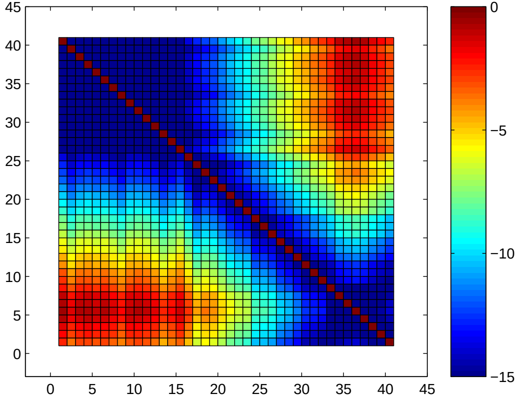
$$C = \frac{1}{2}\mathrm{tridiag}(-1,0,-1)$$



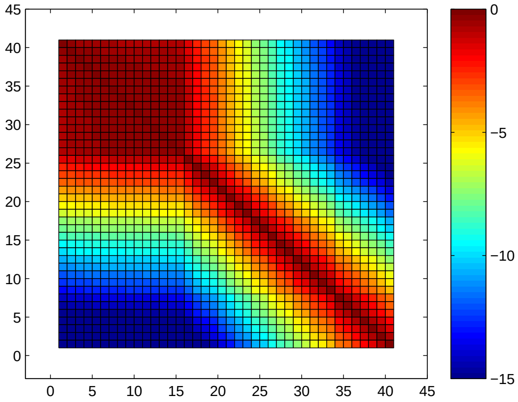
Residual norms for GMRES



Difference of the residual norms of GMRES and Q-OR optimal



$\log_{10}$ of $|V^T V|$, GMRES (Arnoldi) without reorthogonalization



$\log_{10}$ of $|V^T V|$, Q-OR optimal

Conclusion

We studied the properties of the Q-OR methods

We were able to construct a non-orthogonal basis for which Q-OR gives the same residual norms as GMRES

However, the algorithm is more expensive than GMRES

Can we find a better (cheaper) way to compute this basis? (or a basis which gives almost the same residual norms?)