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Worst-case and Ideal GMRES for a Jordan Block

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Introduction. The GMRES method of Saad and Schultz is a very popular iterative method for solving systems of linear algebraic equations $Ax = b$. Starting from an initial guess x_0, this method computes the initial residual $r_0 = b - Ax_0$ and a sequence of iterates $x_1, x_2, \ldots$, so that the kth residual $r_k \equiv b - Ax_k$ satisfies

$$\|r_k\| \;=\; \min_{p\in\pi_k} \|p(A)\, r_0\|\,, \tag{1}$$

where π_k denotes the set of polynomials of degree at most k and with value one at the origin and $\|\cdot\|$ denotes the Euclidean norm. For simplicity we consider that $x_0 = 0$ and $\|b\| = 1$.

The GMRES convergence behavior has been investigated for many years, but a complete understanding still remains elusive. A general approach is to replace the complicated minimization problem (1) by another one that is easier to analyze and that, in some sense, approximates the original problem (1). Natural bounds on the GMRES residual norm arise by excluding the influence of initial residual r_0 (in our case equal to b),

$$\begin{aligned} \|r_k\| &= \min_{p\in\pi_k} \|p(A)b\| && \text{(GMRES)} \\ &\le \max_{\|b\|=1} \min_{p\in\pi_k} \|p(A)b\| && \text{(worst-case GMRES)} \quad (2) \\ &\le \min_{p\in\pi_k} \|p(A)\| && \text{(ideal GMRES).} \quad (3) \end{aligned}$$

The bound (2) corresponds to the *worst-case* GMRES behavior and represents a sharp upper bound, i.e. a bound that is attainable by the GMRES residual norm. In this sense, (2) is the best bound on $\|r_k\|$ that is independent of b. Despite the independence of b, it is not clear in general, which properties of A influence the bound (2). Finally, (2) can be bounded by the *ideal* GMRES approximation (3), that represents a matrix approximation problem.

To justify the relevance of the bound (3), several researchers tried to identify cases in which (2) is equal to (3). The best known result of this type is that (2) is equal to (3) whenever A is normal [4, 5]. Despite the existence of some counterexamples [2, 8], it is still an open question whether (2) is equal or close to (3) for larger classes of nonnormal matrices. To understand the more complicated cases of nonnormal matrices that stem from practical problems, one needs first to understand the relevant "simple" cases. In this talk we concentrate on the case of a

Jordan block, a prototype of a nonnormal matrix. Understanding of this case appears to be a prerequisite for the analysis of other classes of nonnormal matrices, particularly the general triangular Toeplitz matrices, for which some results were obtained by Faber et al. [2].

Results (see [7]). Consider the n by n Jordan block,

$$J_\lambda = \begin{bmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda \end{bmatrix}, \qquad \lambda \in \mathbf{R}, \quad \lambda > 0\,. \tag{4}$$

In our analysis we concentrate on ideal GMRES steps k such that k divides n. In these steps, we discover a special structure behind the convergence of ideal GMRES that allows to prove interesting results. For such k we show that (2) is equal to (3) if $A = J_\lambda$. Our main tool is the equivalence between the kth step of ideal GMRES for $J_\lambda \in \mathbf{R}^{n\times n}$ and the first step of ideal GMRES for $J_{\lambda^k} \in \mathbf{R}^{n/k\times n/k}$, which allows us to characterize the ideal GMRES related quantities in these steps k. In particular, the exact form of the kth ideal GMRES polynomial φ_k that solves

$$\|\varphi_k(J_\lambda)\| = \min_{p\in\pi_k} \|p(J_\lambda)\|$$

is given by

$$\varphi_k(z) = \alpha + \beta\,(\lambda - z)^k,$$

where α and β are some particular real numbers that depend on λ, k and n. The ideal GMRES approximation $\|\varphi_k(J_\lambda)\|$ is bounded by

$$\lambda^{-k}\cos\left(\tfrac{\pi}{n/k+1}\right) \;\le\; \|\varphi_k(J_\lambda)\| \;\le\; \lambda^{-k},$$

whenever $\lambda^k > \cos(\frac{\pi}{n/k+1})$, and

$$\|\varphi_k(J_\lambda)\| \;= 1$$

for $0 \le \lambda^k \le \cos(\frac{\pi}{n/k+1})$.

We also extend previous results obtained by Greenbaum at al. [2] about the polynomial numerical hull $\mathcal{H}_k(J_\lambda)$ of degree k for the Jordan block J_λ. It is known that $\mathcal{H}_k(J_\lambda)$ is a circle around λ with radius $r_{k,n}$. When k divides n, we show that

$$r_{k,n} = \left[\cos\left(\frac{\pi}{n/k+1}\right)\right]^{1/k}.$$

Summary. For a Jordan block J_λ, we are able to characterize the ideal GMRES related quantities and prove equality of bounds (2) and (3) in the steps k such that k divides n. Our numerical experience indicates that (2) is equal to (3) for each k, if A is a Jordan block. The generalization of our results for each k remains the subject of further work.

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