Backward stability of MGS-GMRES

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16th Householder Symposium

on Numerical Linear Algebra,

Pennsylvania, May 22-27, 2005.

The Major Players

- MGS: "Modified Gram-Schmidt" algorithm:
  $B_j = V_j R_j, \qquad V_j \equiv [v_1, \ldots, v_j],$
  $V_j^T V_j = I_j, \qquad R_j$ upper triangular.

- GMRES: "Generalized Minimum Residual" algorithm to solve $Ax = b, \;\; A \in \mathbf{R}^{n \times n}$.

  Y. Saad & M. H. Schultz, SIAM J. Sci. Statist. Comput., 7 (1986), pp. 856–869.

- Based on the algorithm by W. Arnoldi, Quart. Appl. Math., 9 (1951), pp. 17–29.

The Supporting Cast

- Unit roundoff ϵ . Singular values $\sigma(\cdot)$. Condition $\kappa_2(A) \equiv \sigma_{max}(A)/\sigma_{min}(A)$.
- $\tilde{\gamma}_n \equiv \tilde{c}n\epsilon/(1 - \tilde{c}n\epsilon)$, some $\tilde{c} \geq 1$ (N. Higham, 2002).
- Orthonormal vectors $V_j \equiv [v_1, \ldots, v_j]$.
- The *computed* supposedly orthonormal vectors $\bar{V}_j \equiv [\bar{v}_1, \ldots, \bar{v}_j]$. "Bar" denotes "computed".
- Here we use

$$B_{j+1} \equiv [b, AV_j], \qquad \bar{B}_{j+1} \equiv [b, fl(A\bar{V}_j)],$$

but MGS results apply to *general* B_{j+1}.

MGS-GMRES for $Ax = b, \; A \in \mathbf{R}^{n\times n}$.

Take $\varrho \equiv \|b\|_2, \; v_1 \equiv b/\varrho;$ generate columns of $V_{j+1} \equiv [v_1, \ldots, v_{j+1}]$ via the Arnoldi algorithm:

$$AV_j = V_{j+1}H_{j+1,j}, \qquad V_{j+1}^T V_{j+1} = I_{j+1}. \; *$$

Approximate solution $x_j \equiv V_j y_j$ has residual

$$\begin{aligned} r_j \;&\equiv\; b - Ax_j && = b - AV_j y_j \\ &=\; v_1\varrho - V_{j+1}H_{j+1,j}y_j && = V_{j+1}(e_1\varrho - H_{j+1,j}y_j). \end{aligned}$$

The *minimum* residual is found by taking

$$y_j \equiv \arg\min_y \{\|b - AV_j y\|_2 = \|e_1\varrho - H_{j+1,j}y\|_2\}. \; *$$

* DIFFICULTY: $\bar{V}_{j+1}^T \bar{V}_{j+1} \neq I_{j+1}$.

Stability of MGS-GMRES

For some $k \leq n$, the MGS–GMRES method is backward stable for computing a solution $\bar{x}_k$ to

$$Ax = b, \quad A \in \mathbf{R}^{n \times n}, \quad \sigma_{min}(A) \gg n^2 \epsilon \|A\|_F;$$

as well as intermediate solutions $\bar{y}_j$ to the LLSPs:

$$\min_y \|b - A\bar{V}_j y\|_2, \qquad j = 1, \ldots, k,$$

where $\bar{x}_j \equiv fl(\bar{V}_j \bar{y}_j)$,

ϵ is the unit roundoff.

Proof of Stability – Basics

- The Arnoldi Algorithm is MGS applied to $\bar{B}_{n+1} \equiv [b, fl(A\bar{V}_n)]$.
- MGS applied to *any* B_j is numerically equivalent to Householder QR applied to $\begin{bmatrix} O_j \\ B_j \end{bmatrix}$.

  Charles Sheffield, see Å. Björck & C.C. Paige, SIMAX, 13 (1992), pp. 176–190.
- When MGS is applied to $\bar{B}_j$ to give $\bar{V}_j$, $\kappa_2(\bar{V}_j)$ is *small* until $\bar{B}_j$ is numerically rank deficient!
  L. Giraud and J. Langou,
  IMA J. NA, 22 (2002), pp. 521–528. (M. Arioli).

Proof of Stability – Development

- The MGS–"augmented Householder QR" equivalence and rounding error analysis extends to rank deficient $\bar{B}_j$.
- The variant of MGS-Least Squares used in MGS-GMRES is backward stable.
- The loss of orthogonality in MGS is column scaling independent:

$$\tilde{\kappa}_F(A) \equiv \min_{\text{diagonal } D > 0} \|AD\|_F / \sigma_{min}(AD),$$

MGS on $\bar{B}_j \in \mathbf{R}^{n \times j}$: $\quad j\tilde{\gamma}_n \tilde{\kappa}_F(\bar{B}_j) \leq 1/8 \Rightarrow$

$$\|I - \bar{V}_j^T \bar{V}_j\|_F \leq j^{\frac{1}{2}} \tilde{\gamma}_n \tilde{\kappa}_F(\bar{B}_j).$$

c.f. Åke Björck 1967; Nick Higham 1996, 2002.

Proof of Stability – Philosophy

Although *loss of orthogonality* $\|I - \bar{V}_j^T \bar{V}_j\|_F$
can grow as $\tilde{\kappa}_F(\bar{B}_j), \quad j = 1, 2, \ldots;$
$\kappa_2(\bar{V}_j)$ is much better behaved:

$$j\tilde{\gamma}_n\tilde{\kappa}_F(\bar{B}_j) \leq 1/8 \quad \Rightarrow \; 1 \leq \kappa_2(\bar{V}_j) \leq 4/3.$$

But $\text{rank}(\bar{V}_{n+1}) \leq n$, so $\kappa_2(\bar{V}_{n+1})$ is unbounded.
Let $k \leq n$ be the *last* integer such that $\kappa_2(\bar{V}_k) \leq 4/3$,
then $(k+1)\tilde{\gamma}_n\tilde{\kappa}_F(\bar{B}_{k+1}) > 1/8$, so $\forall$ diagonal $D > 0$

$$\sigma_{min}(\bar{B}_{k+1}D) < 8(k+1)\tilde{\gamma}_n\|\bar{B}_{k+1}D\|_F,$$

showing this singular value must become small!

Proof of Stability – Resolution

- Since $\bar{B}_{k+1} \equiv [b, fl(A\bar{V}_k)]$,
  the last inequality shows that
  for this particular k, and for all $\phi > 0$,

$$\sigma_{min}([b\phi, A\bar{V}_k]) \lesssim \tilde{\gamma}_{kn} \|[b\phi, A\bar{V}_k]\|_F.$$

- This with ideas from C. C. Paige & Z. Strakoš,
  Num. Math. 91 (2002), pp. 93–115,
  allows us to prove we have a small *residual* too.
- The standard Rigal & Gaches approach
  then helps us to prove backward stability.

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