Rank-One Updates in Restarted GMRES

Jens-Peter M. Zemke
zemke@tu-harburg.de

Institut für Numerische Simulation
Technische Universität Hamburg-Harburg

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TUHH
Technische Universität Hamburg-Harburg

Outline

Rank-One Updates

- Updates for GMRES
- Convergence Curves
- Distribution of Eigenvalues

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Sherman-Morrison(-Woodbury)

Theorem (Sherman-Morrison-Woodbury)

Let $A \in \mathbb{R}^{n\times n}$ and $U, V \in \mathbb{R}^{n\times k}$ be given. Suppose that A and $A + UV^T$ are invertible. Then

$$(A + UV^T)^{-1} = A^{-1} - A^{-1}U(I + V^TA^{-1}U)^{-1}V^TA^{-1}. \tag{1}$$

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Corollary (Sherman-Morrison)

Suppose that $k = 1$, $u = U$ and $v = V$. Then

$$(A + uv^T)^{-1} = A^{-1} - \frac{1}{1 + v^TA^{-1}u}A^{-1}uv^TA^{-1}. \quad (2)$$

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Two special rank-one updates; the first update

We are interested in approximate solutions to $Ax = b$ from the KRYLOV space

$$\mathcal{K}(A, b) = \operatorname{span}\{b, Ab, \ldots, A^{k-1}b\}.$$

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Corresponds to preconditioning: $AM\tilde{x} = b$, $\bar{x}_k = M\tilde{x}_k$ with $M = I - dy^T$.

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The Arnoldi decompositions of A and $\tilde{A}$ are given by

$$AQ_k = Q_{k+1}\underline{H}_k, \qquad \tilde{A}Q_k = Q_{k+1}\underline{\tilde{H}}_k, \tag{8}$$

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where $\underline{\tilde{H}}_k = \underline{H}_k - \underline{e}_1 z^T$ with $z = \|b\|Q_k^T y$. Thus, $\tilde{\mathcal{K}} \equiv \mathcal{K}(\tilde{A}, b) = \mathcal{K}$.

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We restrict ourselves to the second choice.

How to choose y?

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Any idea?

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And now for something completely different . . .

Outline

Arioli, Greenbaum, Pták, Strakoš

Theorem ("Any convergence curve is possible")

GMRES on $\hat{A}$ with right hand side b with zero initial guess gives

$$\|\hat{r}_k\| = f_k, \quad 0 \leqslant k \leqslant n-1, \tag{10}$$

if and only if

$$\hat{A} = WR\tilde{H}W^T, \tag{11}$$

R arbitrary nonsingular upper triangular, W orthogonal,

$$W^T b = \begin{pmatrix} \pm\sqrt{f_0^2 - f_1^2} \\ \vdots \\ \pm\sqrt{f_{n-1}^2 - f_n^2} \end{pmatrix} \qquad \tilde{H} = \begin{pmatrix} 0 & \cdots & 0 & 1/(b^T w_n) \\ 1 & & 0 & -(b^T w_1)/(b^T w_1) \\ & \ddots & \vdots & \vdots \\ 0 & & 1 & -(b^T w_{n-1})/(b^T w_1) \end{pmatrix} \tag{12}$$

where $f_n = 0$.

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We sketch the second proof based on the coefficients of y in terms of the Arnoldi basis $\{q_j\}_{j=1}^k$.

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The residual norms are given in terms of sines of angles (cf. Saad, Eiermann/Ernst):

$$\|\tilde{r}_k\| = |\tilde{s}_k \cdot \cdots \cdot \tilde{s}_1| \|b\|. \tag{14}$$

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This implies

$$|\tilde{s}_k| = \frac{\|\tilde{r}_k\|}{\|\tilde{r}_{k-1}\|} = \frac{f_k}{f_{k-1}}. \qquad (15)$$

Jurjen's second proof, cont'd

Jurjen shows by an induction argument that

$$\tilde{s}_k = \frac{\tilde{h}_{k+1,k}^2}{\tilde{h}_{k+1,k}^2 + \left(\sum_{j=1}^{k} \tilde{c}_j \tilde{h}_{jk} \prod_{i=j}^{k-1} (-\tilde{s}_i)\right)^2}. \tag{16}$$

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Since $\underline{\tilde{H}}_k = \underline{H}_k + \underline{e}_1 z^T$,

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We know that $\tilde{h}_{1k} = h_{1k} + z_k = h_{1k} + \|b\| y^T q_k \equiv h_{1k} + \|b\| \alpha_k$.

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Thus, $|\tilde{s}_k| = f_k / f_{k-1}$ when α_k is choosen as

$$\alpha_k^{\pm} = \frac{\pm\sqrt{\frac{1-(f_k/f_{k-1})^2}{(f_k/f_{k-1})^2}}\, h_{k+1,k} - \sum_{j=1}^{k} \tilde{c}_j h_{jk} \prod_{i=j}^{k-1}(-\tilde{s}_j)}{-\|b\| \prod_{i=1}^{k-1}(-\tilde{s}_j)}. \qquad (18)$$

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- In theory it is possible to use a global minimization.
- What about practicability?

Outline

"Any eigenvalue distribution is possible"

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Let the grade of b *be* n. *Let* $\tilde{\Lambda} = \{\tilde{\lambda}_j\}_{j=1}^{n}$, *where multiple* $\tilde{\lambda}_j$ *are allowed. Then a vector* y *exists such that* $\tilde{\Lambda}$ *is the spectrum of* $\tilde{A} = A - by^T$.

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$$\prod_{j=1}^{n}(z - \tilde{\lambda}_j) = \sum_{j=0}^{n} \alpha_j z^j, \qquad \alpha_n = 1. \tag{19}$$

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$$(A - by^T)X = X \begin{pmatrix} 0 & \cdots & 0 & -\alpha_0 \\ 1 & 0 & \cdots & -\alpha_1 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & -\alpha_{n-1} \end{pmatrix}. \tag{20}$$

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Proof (part IV, final part).

Thus, we have to solve the linear system of equations

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for γ. The vector y is given by $X^{-T}\gamma$. □

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Thus, we have to solve the linear system of equations

$$\begin{pmatrix} 1 & \alpha_{n-1} & \cdots & \alpha_1 \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \alpha_{n-1} \\ 0 & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma_n \\ \vdots \\ \gamma_2 \\ \gamma_1 \end{pmatrix} = \begin{pmatrix} \alpha_0 + \beta_0 \\ \alpha_1 + \beta_1 \\ \vdots \\ \alpha_{n-1} + \beta_{n-1} \end{pmatrix} \tag{25}$$

for γ. The vector y is given by $X^{-T}\gamma$. □

Remark

The vector y is given by $y = X(y)^{-T}\gamma(y)$. Reading backwards, we can define $\gamma = \gamma(\alpha, \beta)$ independent of y. But what about X? The columns of X satisfy $x_j = x_j(A, b, \gamma)$ and by inspection X is regular.

Jurjen's proof

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Outline

SHERMOR(m, k)

The algorithm sketched in prescribing residual norms is denoted by SHERMOR(m, k), where

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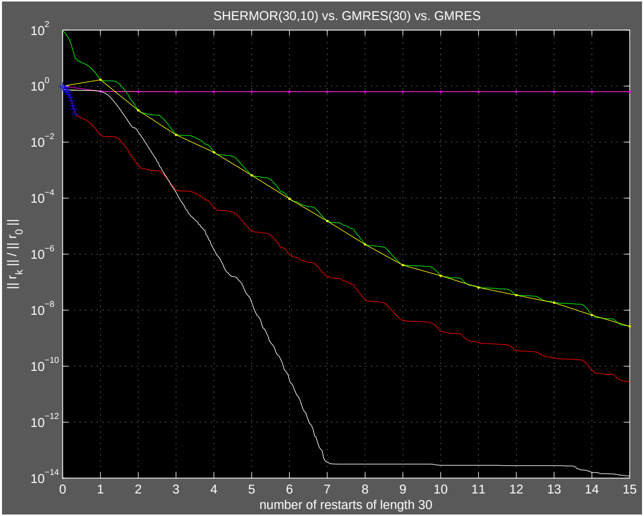
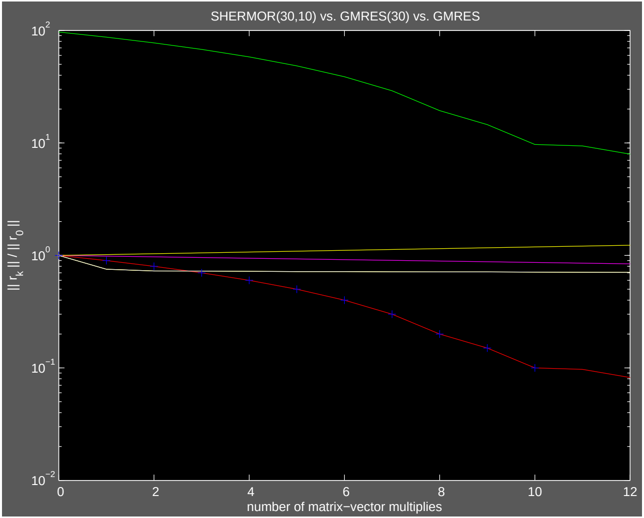
- GMRES(m) is used on $\tilde{A} = A - by^T$ and the result is backtransformed,

$$r_m = \frac{\tilde{r}_m}{1 + y^T \tilde{x}_m}, \qquad x_m = \frac{\tilde{x}_m}{1 + y^T \tilde{x}_m}. \tag{26}$$

SHERMOR(30, 10)



SHERMOR(30, 10) – a closer view



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He proves that if the prescribed slope of convergence is to steep, the method fails when the backtransformation takes place since then $y^T x_m \approx -1$.

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Locally minimizing sines

Jurjen uses the knowledge used in SHERMOR(m, k) to minimize locally the sines to obtain an algorithm named LOCAL(m, k).

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He shows that the local minimization corresponds to the setting

$$y^T\left(x_0, \tilde{q}_1, \ldots, \tilde{q}_k\right) = \frac{1}{\|b\|^2} b^T\left(-r_0, A\tilde{q}_1, \ldots, A\tilde{q}_k\right). \tag{27}$$

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This is an orthogonalization against b, namely, the basis is constructed by setting $r_0^{\text{mod}} = r_0 - b^T r_0 b / \|b\|^2$ and iterating

$$v_k = Aq_k - \sum_{j=1}^{k} h_{jk} q_j - \frac{b^T A q_k}{\|b\|^2} b, \tag{28}$$

where $h_{jk} = q_j^T A q_k$.

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where $h_{jk} = q_j^T A q_k$. The next basis vector is given by $q_{k+1} = v_k / \|v_k\|$.

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Jurjen uses in the implementation the setting $\gamma = y^T d = 0$ and $d = x_0$, such that in case of convergence $Ad \rightarrow b$ and we end up with the first update.

The quantity m is from GMRES(m), the k stands for $k \leqslant m$ local minimizations.

Outline

DEFSHERMOR(m)

We are interested in deflating the smallest Ritz value(s). When the smallest Ritz value θ_k is simple and the left Ritz pair $(\theta_k, \check{s}_k)$ is real, this is achieved by

$$z = (\theta_k - \tilde{\theta}_k)\frac{\check{s}_k}{\check{s}_{1k}} = (\theta_k - \tilde{\theta}_k)\check{\nu}(\theta_k). \tag{29}$$

$$\begin{aligned} \check{s}_k^T(H_k - e_1 z^T) &= \theta_k \check{s}_k^T - (\theta_k - \tilde{\theta}_k)\check{s}_k^T e_1 \frac{\check{s}_k^T}{\check{s}_{1k}} \\ &= \theta_k \check{s}_k^T - (\theta_k - \tilde{\theta}_k)\check{s}_{1k}\frac{\check{s}_k^T}{\check{s}_{1k}} = \tilde{\theta}_k \check{s}_k^T \end{aligned} \tag{30}$$

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Jurjen gives another, more complicated proof that works for all Ritz values.

A new deflation inside DEFSHERMOR(m, k)

```
    shift = [2 2 0.01];       % these are Jurjen's shifts .. how to choose?
    zzz = zeros(RESTART,1);   % initializing zzz
    eone = eye(RESTART,1);    % the first standard unit vector
%
    [W,D] = eig((He(1:RESTART,1:RESTART)-eone*zzz')');
    [theta,index] = sort(diag(D));
    OldEigenvalues = theta
    W = W(:,index);
%
    ell = 1;
%
    while ell < 4
         if isreal(theta(1))
            zzz = zzz+(theta(1)-shift(ell))*W(:,1)/W(1,1);
            ell = ell+1;
         else
            disp('not yet implemented');
            zzz = zzz+rand(RESTART,1);
         end
%
         [W,D] = eig((He(1:RESTART,1:RESTART)-eone*zzz')');
         [theta,index] = sort(diag(D));
         ChangedEigenvalues = theta
         W = W(:,index);
     end
%
     NewEigenvalues = theta
     yy = V*zzz/nnr0;
```

Jurjen vs. Jens $:-)$

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These eigenvector changes might give a computational feasible way to prescribe stably a change in a couple of eigenvalues.

At least, the changes are trivially restricted to (all) the left eigenvectors and only the right eigenvectors corresponding to the changed eigenvalues.

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The resulting algorithm is denoted by DEFSHERMORN($m, 1$).

Variants for deflation of smallest conjugate complex eigenvalues using a real y are also included in both the algorithms DEFSHERMOR(m) and DEFSHERMORN($m, 1$).

Outline

Global minimization

Jurjen shows that in theory when $x_0 \neq 0$ with the right choice it is possible to achieve a minimization over a $2k$-dimensional space.

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This space is given by $\mathcal{K}_k(A, b) \cup A\mathcal{K}_k(A, r_0)$.

SHERMOR$(30, 10)$ – an even closer view