

Lecture 14: Krylov subspace methods for least squares problems



School of Mathematical Sciences, Xiamen University

1. Conjugate gradient for least squares problems (CGLS)

- The stable way to implement CG for the normal equations is called as CGLS.

Algorithm: CGLS for $\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{Ax}\|_2$

```
 $\mathbf{r}_0 = \mathbf{b} - \mathbf{Ax}_0, \quad \mathbf{p}_0 = \mathbf{A}^* \mathbf{r}_0;$   
for  $j = 1, 2, 3, \dots,$   
     $\alpha_j = \|\mathbf{A}^* \mathbf{r}_{j-1}\|_2^2 / \|\mathbf{Ap}_{j-1}\|_2^2;$   
     $\mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1};$   
     $\mathbf{r}_j = \mathbf{r}_{j-1} - \alpha_j \mathbf{Ap}_{j-1};$   
     $\beta_j = \|\mathbf{A}^* \mathbf{r}_j\|_2^2 / \|\mathbf{A}^* \mathbf{r}_{j-1}\|_2^2;$   
     $\mathbf{p}_j = \mathbf{A}^* \mathbf{r}_j + \beta_j \mathbf{p}_{j-1};$   
end
```

- CGLS (also called CGNR) is mathematically equivalent to LSQR, which is based on Golub–Kahan bidiagonalization for $[\mathbf{b} \quad \mathbf{A}]$.

2. Householder bidiagonalization

$$\begin{array}{ccc}
 \begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix} & \xrightarrow{\mathbf{U}_1^* \cdot} & \begin{bmatrix} \times & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \\ 0 & \times & \times & \times \end{bmatrix} & \xrightarrow{\cdot \mathbf{V}_1} & \begin{bmatrix} \times & \times & 0 & 0 \\ & \times & \times & \times \\ & \times & \times & \times \\ & \times & \times & \times \\ & \times & \times & \times \\ & \times & \times & \times \end{bmatrix} \\
 \mathbf{A} & & \mathbf{U}_1^* \mathbf{A} & & \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1 \\
 \\
 & \xrightarrow{\mathbf{U}_2^* \cdot} & \begin{bmatrix} \times & \times & & \\ & \times & \times & \times \\ & 0 & \times & \times \\ & 0 & \times & \times \\ & 0 & \times & \times \\ & 0 & \times & \times \end{bmatrix} & \xrightarrow{\cdot \mathbf{V}_2} & \begin{bmatrix} \times & \times & & \\ & \times & \times & 0 \\ & & \times & \times \\ & & \times & \times \\ & & \times & \times \\ & & \times & \times \end{bmatrix} \\
 & & \mathbf{U}_2^* \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1 & & \mathbf{U}_2^* \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1 \mathbf{V}_2
 \end{array}$$

Proposition 1 (Case $m \geq n$)

Every matrix $\mathbf{A} \in \mathbb{C}^{m \times n}$ has a bidiagonal decomposition:

$$\mathbf{A} = \mathbf{U} \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix} \mathbf{V}^* = \mathbf{U} \begin{bmatrix} \beta_1 & \alpha_1 & & & \\ & \beta_2 & \ddots & & \\ & & \ddots & \alpha_{n-1} & \\ & & & \beta_n & \end{bmatrix} \mathbf{V}^*,$$

where $\mathbf{B} \in \mathbb{R}^{n \times n}$ is bidiagonal, $\alpha_i \geq 0$, $\beta_i \geq 0$, $\mathbf{U} \in \mathbb{C}^{m \times m}$ is unitary, and

$$\mathbf{V} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q} \end{bmatrix} \in \mathbb{C}^{n \times n}$$

is unitary.

- Note that in this proposition and in the rest of this lecture we do not consider the stability issue.

- **Another** bidiagonalization algorithm: Note that

$$\mathbf{A}^* \mathbf{U}_n = \mathbf{V} \mathbf{B}^*, \quad \mathbf{A} \mathbf{V} = \mathbf{U}_n \mathbf{B},$$

i.e.,

$$\mathbf{A}^* \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_n \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_n \end{bmatrix} \begin{bmatrix} \beta_1 & & & \\ \alpha_1 & \beta_2 & & \\ & \ddots & \ddots & \\ & & \alpha_{n-1} & \beta_n \end{bmatrix}$$

and

$$\mathbf{A} \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_n \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_n \end{bmatrix} \begin{bmatrix} \beta_1 & \alpha_1 & & \\ & \beta_2 & \ddots & \\ & & \ddots & \alpha_{n-1} \\ & & & \beta_n \end{bmatrix}.$$

Equating column i on both sides, we get

$$\mathbf{A}^* \mathbf{u}_i = \beta_i \mathbf{v}_i + \alpha_i \mathbf{v}_{i+1}, \quad 1 \leq i \leq n-1;$$

and

$$\mathbf{A} \mathbf{v}_i = \alpha_{i-1} \mathbf{u}_{i-1} + \beta_i \mathbf{u}_i, \quad 2 \leq i \leq n.$$

Algorithm: Golub–Kahan bidiagonalization for \mathbf{A}

$$\beta_1 = \|\mathbf{a}_1\|_2, \quad \mathbf{u}_1 = \mathbf{a}_1/\beta_1, \quad \mathbf{v}_1 = \mathbf{e}_1$$

for $i = 1, 2, 3, \dots,$

$$\mathbf{v}_{i+1} = \mathbf{A}^* \mathbf{u}_i - \beta_i \mathbf{v}_i$$

$$\alpha_i = \|\mathbf{v}_{i+1}\|_2$$

$$\mathbf{v}_{i+1} = \mathbf{v}_{i+1}/\alpha_i$$

$$\mathbf{u}_{i+1} = \mathbf{A} \mathbf{v}_{i+1} - \alpha_i \mathbf{u}_i$$

$$\beta_{i+1} = \|\mathbf{u}_{i+1}\|_2$$

$$\mathbf{u}_{i+1} = \mathbf{u}_{i+1}/\beta_{i+1}$$

end

3. LSQR

- LSQR is based on Golub–Kahan bidiagonalization for $\begin{bmatrix} \mathbf{b} & \mathbf{A} \end{bmatrix}$:

$$\begin{aligned} \mathbf{U}^* \begin{bmatrix} \mathbf{b} & \mathbf{A} \end{bmatrix} \mathbf{V} &= \begin{bmatrix} \mathbf{U}^* \mathbf{b} & \mathbf{U}^* \mathbf{A} \mathbf{Q} \end{bmatrix} = \begin{bmatrix} \beta_1 \mathbf{e}_1 & \tilde{\mathbf{B}} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \\ &= \left[\begin{array}{c|cccc} \beta_1 & \alpha_1 & & & \\ & \beta_2 & \ddots & & \\ & & \ddots & \alpha_n & \\ & & & \beta_{n+1} & \end{array} \right]. \end{aligned}$$

We can write the least squares problem as

$$\min_{\mathbf{x} \in \mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2 = \min_{\mathbf{x} \in \mathbb{C}^n} \left\| \begin{bmatrix} \mathbf{b} & \mathbf{A} \end{bmatrix} \begin{bmatrix} 1 \\ -\mathbf{x} \end{bmatrix} \right\|_2 = \min_{\mathbf{y} \in \mathbb{C}^n} \|\beta_1 \mathbf{e}_1 - \tilde{\mathbf{B}}\mathbf{y}\|_2.$$

Algorithm: Golub–Kahan bidiagonalization for $[\mathbf{b} \ \mathbf{A}]$

$$\beta_1 = \|\mathbf{b}\|_2, \quad \mathbf{u}_1 = \mathbf{b}/\beta_1, \quad \mathbf{q}_0 = \mathbf{0}$$

for $i = 1, 2, 3, \dots$,

$$\mathbf{q}_i = \mathbf{A}^* \mathbf{u}_i - \beta_i \mathbf{q}_{i-1},$$

$$\alpha_i = \|\mathbf{q}_i\|_2$$

$$\mathbf{q}_i = \mathbf{q}_i / \alpha_i$$

$$\mathbf{u}_{i+1} = \mathbf{A} \mathbf{q}_i - \alpha_i \mathbf{u}_i$$

$$\beta_{i+1} = \|\mathbf{u}_{i+1}\|_2$$

$$\mathbf{u}_{i+1} = \mathbf{u}_{i+1} / \beta_{i+1}$$

end

Proposition 2

Assume that all α_i and β_i for $1 \leq i \leq k$ in the above algorithm are nonzero. Then the sets $\{\mathbf{u}_i\}_{i=1}^k$ and $\{\mathbf{q}_i\}_{i=1}^k$ are orthonormal bases for $\mathcal{K}_k(\mathbf{A}\mathbf{A}^, \mathbf{b})$ and $\mathcal{K}_k(\mathbf{A}^*\mathbf{A}, \mathbf{A}^*\mathbf{b})$, respectively.*

The proof is left as an exercise.

- Define the matrices

$$\mathbf{U}_k = [\mathbf{u}_1 \quad \mathbf{u}_2 \quad \cdots \quad \mathbf{u}_k], \quad \mathbf{Q}_k = [\mathbf{q}_1 \quad \mathbf{q}_2 \quad \cdots \quad \mathbf{q}_k],$$

and

$$\tilde{\mathbf{B}}_{k+1} = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \ddots & & \\ & \ddots & \alpha_k & \\ & & \beta_{k+1} & \end{bmatrix} \in \mathbb{C}^{(k+1) \times k}.$$

We have

$$\mathbf{A}\mathbf{Q}_k = \mathbf{U}_{k+1}\tilde{\mathbf{B}}_{k+1}.$$

Assume that we want to find the best approximate solution in the subspace, $\mathcal{K}_k(\mathbf{A}^*\mathbf{A}, \mathbf{A}^*\mathbf{b}) = \text{range}(\mathbf{Q}_k)$, that is

$$\begin{aligned} \min_{\mathbf{y} \in \mathbb{C}^k} \|\mathbf{b} - \mathbf{A}\mathbf{Q}_k\mathbf{y}\|_2 &= \min_{\mathbf{y} \in \mathbb{C}^k} \|\mathbf{b} - \mathbf{U}_{k+1}\tilde{\mathbf{B}}_{k+1}\mathbf{y}\|_2 \\ &= \min_{\mathbf{y} \in \mathbb{C}^k} \|\beta_1\mathbf{e}_1 - \tilde{\mathbf{B}}_{k+1}\mathbf{y}\|_2. \end{aligned}$$

- The least squares problem with bidiagonal structure can be solved using a sequence of Givens rotations. Consider the matrix

$$\begin{bmatrix} \tilde{\mathbf{B}}_{k+1} & \beta_1 \mathbf{e}_1 \end{bmatrix} = \begin{bmatrix} \alpha_1 & & & & & \beta_1 \\ \beta_2 & \alpha_2 & & & & 0 \\ & \beta_3 & \alpha_3 & & & 0 \\ & & \ddots & \ddots & & \vdots \\ & & & \beta_k & \alpha_k & 0 \\ & & & & \beta_{k+1} & 0 \end{bmatrix}.$$

In the first step we zero β_2 by using a Givens rotation:

$$\begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_1 & & & & \gamma_1 \\ 0 & \hat{\alpha}_2 & & & & \hat{\gamma}_2 \\ & \beta_3 & \alpha_3 & & & 0 \\ & & \ddots & \ddots & & \vdots \\ & & & \beta_k & \alpha_k & 0 \\ & & & & \beta_{k+1} & 0 \end{bmatrix}.$$

In the next step, we zero β_3 by using a Givens rotation:

$$\begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_1 & & & & \gamma_1 \\ 0 & \hat{\alpha}_2 & \hat{\beta}_2 & & & \gamma_2 \\ & 0 & \hat{\alpha}_3 & & & \hat{\gamma}_3 \\ & & \beta_4 & \ddots & & \vdots \\ & & & \ddots & \alpha_k & 0 \\ & & & & \beta_{k+1} & 0 \end{bmatrix}.$$

The final result after k steps is

$$\begin{bmatrix} \hat{\alpha}_1 & \hat{\beta}_1 & & & & \gamma_1 \\ & \hat{\alpha}_2 & \hat{\beta}_2 & & & \gamma_2 \\ & & \ddots & \ddots & & \vdots \\ & & & \ddots & \hat{\beta}_{k-1} & \gamma_{k-1} \\ & & & & \hat{\alpha}_k & \gamma_k \\ & & & & & \hat{\gamma}_{k+1} \end{bmatrix} := \begin{bmatrix} \hat{\mathbf{B}}_k & \gamma_k \\ \mathbf{0} & \hat{\gamma}_{k+1} \end{bmatrix}.$$

Actually, we have the QR factorization for $\begin{bmatrix} \tilde{\mathbf{B}}_{k+1} & \beta_1 \mathbf{e}_1 \end{bmatrix}$:

$$\begin{bmatrix} \tilde{\mathbf{B}}_{k+1} & \beta_1 \mathbf{e}_1 \end{bmatrix} = \hat{\mathbf{Q}} \begin{bmatrix} \hat{\mathbf{B}}_k & \gamma_k \\ \mathbf{0} & \hat{\gamma}_{k+1} \end{bmatrix},$$

i.e.,

$$\tilde{\mathbf{B}}_{k+1} = \hat{\mathbf{Q}} \begin{bmatrix} \hat{\mathbf{B}}_k \\ \mathbf{0} \end{bmatrix}, \quad \text{and} \quad \beta_1 \mathbf{e}_1 = \hat{\mathbf{Q}} \begin{bmatrix} \gamma_k \\ \hat{\gamma}_{k+1} \end{bmatrix}.$$

Then we have

$$\arg \min_{\mathbf{y} \in \mathbb{C}^k} \|\beta_1 \mathbf{e}_1 - \tilde{\mathbf{B}}_{k+1} \mathbf{y}\|_2 = \hat{\mathbf{B}}_k^{-1} \gamma_k$$

and

$$\min_{\mathbf{y} \in \mathbb{C}^k} \|\beta_1 \mathbf{e}_1 - \tilde{\mathbf{B}}_{k+1} \mathbf{y}\|_2 = |\hat{\gamma}_{k+1}|.$$

Define the matrix $\mathbf{W}_k := \mathbf{Q}_k \hat{\mathbf{B}}_k^{-1} = [\mathbf{w}_1 \ \cdots \ \mathbf{w}_k]$, we have

$$\mathbf{Q}_k = \mathbf{W}_k \hat{\mathbf{B}}_k,$$

which implies $\mathbf{w}_k = (\mathbf{q}_k - \hat{\beta}_{k-1} \mathbf{w}_{k-1}) / \hat{\alpha}_k$. We have the recurrence

$$\begin{aligned} \mathbf{x}_k &= \mathbf{W}_k \gamma_k = [\mathbf{W}_{k-1} \ \mathbf{w}_k] \begin{bmatrix} \gamma_{k-1} \\ \gamma_k \end{bmatrix} \\ &= \mathbf{W}_{k-1} \gamma_{k-1} + \gamma_k \mathbf{w}_k \\ &= \mathbf{x}_{k-1} + \gamma_k \mathbf{w}_k. \end{aligned}$$

- C. C. Paige and M. A. Saunders.

LSQR: An algorithm for sparse linear equations and sparse least squares.

ACM Trans. Math. Software, 8(1):43–71, 1982.

4. Other methods

- D. C.-L. Fong and M. Saunders.
LSMR: An iterative algorithm for sparse least-squares problems.
SIAM J. Sci. Comput., 33(5):2950–2971, 2011.
- R. Estrin, D. Orban, and M. A. Saunders.
LSLQ: An iterative method for linear least-squares with an error minimization property.
SIAM J. Matrix Anal. Appl., 40(1):254–275, 2019.
- R. Estrin, D. Orban, and M. A. Saunders.
LNLQ: An iterative method for least-norm problems with an error minimization property.
SIAM J. Matrix Anal. Appl., 40(3):1102–1124, 2019.
- Craig’s method (also called CGNE): E. J. Craig. 1955
The N -step iteration procedures. J. Math. and Phys., 34:64–73.