Lecture 14: Krylov subspace methods for least squares problems

School of Mathematical Sciences, Xiamen University

1. Conjugate gradient for least squares problems (CGLS)

- CGLS is an implementation of CG for the normal equations.

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

$$
\begin{aligned}
&\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0, \quad \mathbf{p}_0 = \mathbf{A}^*\mathbf{r}_0;\\
&\textbf{for } j = 1, 2, 3, \ldots,\\
&\qquad \alpha_j = \|\mathbf{A}^*\mathbf{r}_{j-1}\|_2^2 / \|\mathbf{A}\mathbf{p}_{j-1}\|_2^2;\\
&\qquad \mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1};\\
&\qquad \mathbf{r}_j = \mathbf{r}_{j-1} - \alpha_j \mathbf{A}\mathbf{p}_{j-1};\\
&\qquad \beta_j = \|\mathbf{A}^*\mathbf{r}_j\|_2^2 / \|\mathbf{A}^*\mathbf{r}_{j-1}\|_2^2;\\
&\qquad \mathbf{p}_j = \mathbf{A}^*\mathbf{r}_j + \beta_j \mathbf{p}_{j-1};\\
&\textbf{end}
\end{aligned}
$$

- Assume that $\mathbf{A}$ has full column rank. We have

$$
\begin{aligned}
\mathbf{x}_j &= \underset{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}^*\mathbf{A}, \mathbf{A}^*\mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{A}^\dagger \mathbf{b} - \mathbf{x}\|_{\mathbf{A}^*\mathbf{A}}\\
&= \underset{\mathbf{x} \in \mathbf{x}_0 + \mathcal{K}_j(\mathbf{A}^*\mathbf{A}, \mathbf{A}^*\mathbf{r}_0)}{\operatorname{argmin}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2.
\end{aligned}
$$

2. Householder bidiagonalization

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

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

$$
\mathbf{U}_4^*\mathbf{U}_3^*\mathbf{U}_2^*\mathbf{U}_1^*\mathbf{A}\mathbf{V}_1\mathbf{V}_2 = \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{A} = \mathbf{U}_1\mathbf{U}_2\mathbf{U}_3\mathbf{U}_4 \begin{bmatrix} \mathbf{B} \\ \mathbf{0} \end{bmatrix} (\mathbf{V}_1\mathbf{V}_2)^*.
$$

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*

$$\mathbf{V} = \begin{bmatrix}1 & \mathbf{0}\\ \mathbf{0} & \mathbf{Q}\end{bmatrix} \in \mathbb{C}^{n\times n}$$

is unitary.

- Exercise: Prove Proposition 1.

- Golub–Kahan bidiagonalization: Note that

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

i.e.,

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

and

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

Equating column i on both sides, we get

$$\mathbf{A}\mathbf{v}_1 = \beta_1 \mathbf{u}_1, \qquad \mathbf{A}\mathbf{v}_i = \alpha_{i-1}\mathbf{u}_{i-1} + \beta_i \mathbf{u}_i, \quad 2 \le i \le n,$$

and

$$\mathbf{A}^*\mathbf{u}_i = \beta_i \mathbf{v}_i + \alpha_i \mathbf{v}_{i+1}, \quad 1 \le i \le n-1, \qquad \mathbf{A}^*\mathbf{u}_n = \beta_n \mathbf{v}_n.$$

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

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

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

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

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

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

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

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

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

end

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3. LSQR

- Consider Householder bidiagonalization of $\begin{bmatrix}\mathbf{b} & \mathbf{A}\end{bmatrix}$:

$$\mathbf{U}^* \begin{bmatrix}\mathbf{b} & \mathbf{A}\end{bmatrix} \mathbf{V} = \begin{bmatrix}\mathbf{U}^*\mathbf{b} & \mathbf{U}^*\mathbf{A}\mathbf{Q}\end{bmatrix} = \begin{bmatrix}\beta_1\mathbf{e}_1 & \widetilde{\mathbf{B}} \\ \mathbf{0} & \mathbf{0}\end{bmatrix}$$

$$= \left[\begin{array}{c|cccc} \beta_1 & \alpha_1 & & & \\ & \beta_2 & \ddots & & \\ & & \ddots & \alpha_n & \\ & & & \beta_{n+1} & \\ \hline & & & & \\ & & & & \end{array}\right].$$

Using $\mathbf{y} := \mathbf{Q}^*\mathbf{x}$, we can write the least squares problem as

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

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

Algorithm: Golub–Kahan bidiagonalization for $\begin{bmatrix} \mathbf{b} & \mathbf{A} \end{bmatrix}$

$$
\begin{aligned}
&\mathbf{q}_0 = \mathbf{0}, \quad \beta_1 = \|\mathbf{b}\|_2, \quad \mathbf{u}_1 = \mathbf{b}/\beta_1 \\
&\textbf{for } i = 1, 2, 3, \ldots, \\
&\qquad \mathbf{q}_i = \mathbf{A}^*\mathbf{u}_i - \beta_i \mathbf{q}_{i-1}, \\
&\qquad \alpha_i = \|\mathbf{q}_i\|_2 \\
&\qquad \mathbf{q}_i = \mathbf{q}_i/\alpha_i \\
&\qquad \mathbf{u}_{i+1} = \mathbf{A}\mathbf{q}_i - \alpha_i \mathbf{u}_i \\
&\qquad \beta_{i+1} = \|\mathbf{u}_{i+1}\|_2 \\
&\qquad \mathbf{u}_{i+1} = \mathbf{u}_{i+1}/\beta_{i+1} \\
&\textbf{end}
\end{aligned}
$$

Proposition 2

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

- Exercise: Prove Proposition 2.

- Define the matrices

$$\mathbf{U}_j = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_j \end{bmatrix}, \qquad \mathbf{Q}_j = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_j \end{bmatrix},$$

and

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

We have

$$\mathbf{A}\mathbf{Q}_j = \mathbf{U}_{j+1}\widetilde{\mathbf{B}}_{j+1}.$$

At step j, LSQR seeks the best approximate solution $\mathbf{x}_j = \mathbf{Q}_j\mathbf{y}_j$ in $\mathcal{K}_j(\mathbf{A}^*\mathbf{A}, \mathbf{A}^*\mathbf{b})$, where $\mathbf{y}_j$ solves

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

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

$$\begin{bmatrix} \widetilde{\mathbf{B}}_{j+1} & \beta_1 \mathbf{e}_1 \end{bmatrix} = \begin{bmatrix} \alpha_1 & & & & & \beta_1 \\ \beta_2 & \alpha_2 & & & & 0 \\ & \beta_3 & \alpha_3 & & & 0 \\ & & \ddots & \ddots & & \vdots \\ & & & \beta_j & \alpha_j & 0 \\ & & & & \beta_{j+1} & 0 \end{bmatrix}.$$

In the first step we zero β_2 by using a Givens rotation $\mathbf{G}_1$:

$$\mathbf{G}_1 \begin{bmatrix} \widetilde{\mathbf{B}}_{j+1} & \beta_1 \mathbf{e}_1 \end{bmatrix} = \begin{bmatrix} \widehat{\alpha}_1 & \widehat{\beta}_1 & & & & \gamma_1 \\ 0 & \widetilde{\alpha}_2 & & & & \widehat{\gamma}_2 \\ & \beta_3 & \alpha_3 & & & 0 \\ & & \ddots & \ddots & & \vdots \\ & & & \beta_j & \alpha_j & 0 \\ & & & & \beta_{j+1} & 0 \end{bmatrix}.$$

In the next step, we zero β_3 by using a Givens rotation $\mathbf{G}_2$:

$$\mathbf{G}_2\mathbf{G}_1\begin{bmatrix}\widetilde{\mathbf{B}}_{j+1} & \beta_1\mathbf{e}_1\end{bmatrix} = \begin{bmatrix} \widehat{\alpha}_1 & \widehat{\beta}_1 & & & & \gamma_1 \\ 0 & \widehat{\alpha}_2 & \widehat{\beta}_2 & & & \gamma_2 \\ & 0 & \widetilde{\alpha}_3 & & & \widehat{\gamma}_3 \\ & & \beta_4 & \ddots & & \vdots \\ & & & \ddots & \alpha_j & 0 \\ & & & & \beta_{j+1} & 0 \end{bmatrix}.$$

The final result after j steps is $\mathbf{G}_j\cdots\mathbf{G}_2\mathbf{G}_1\begin{bmatrix}\widetilde{\mathbf{B}}_{j+1} & \beta_1\mathbf{e}_1\end{bmatrix}$:

$$\begin{bmatrix} \widehat{\alpha}_1 & \widehat{\beta}_1 & & & & \gamma_1 \\ & \widehat{\alpha}_2 & \widehat{\beta}_2 & & & \gamma_2 \\ & & \ddots & \ddots & & \vdots \\ & & & \ddots & \widehat{\beta}_{j-1} & \gamma_{j-1} \\ & & & & \widehat{\alpha}_j & \gamma_j \\ & & & & & \widehat{\gamma}_{j+1} \end{bmatrix} := \begin{bmatrix} \widehat{\mathbf{B}}_j & \boldsymbol{\gamma}_j \\ \mathbf{0} & \widehat{\gamma}_{j+1} \end{bmatrix}.$$

Define $\widehat{\mathbf{Q}} := \mathbf{G}_1^\top \mathbf{G}_2^\top \cdots \mathbf{G}_j^\top$. We obtain the QR factorization:

$$\begin{bmatrix} \widetilde{\mathbf{B}}_{j+1} & \beta_1 \mathbf{e}_1 \end{bmatrix} = \widehat{\mathbf{Q}} \begin{bmatrix} \widehat{\mathbf{B}}_j & \boldsymbol{\gamma}_j \\ \mathbf{0} & \widehat{\gamma}_{j+1} \end{bmatrix},$$

which implies

$$\widetilde{\mathbf{B}}_{j+1} = \widehat{\mathbf{Q}} \begin{bmatrix} \widehat{\mathbf{B}}_j \\ \mathbf{0} \end{bmatrix} \quad \text{and} \quad \beta_1 \mathbf{e}_1 = \widehat{\mathbf{Q}} \begin{bmatrix} \boldsymbol{\gamma}_j \\ \widehat{\gamma}_{j+1} \end{bmatrix}.$$

Thus we have

$$\mathbf{y}_j = \arg\min_{\mathbf{y} \in \mathbb{C}^j} \|\beta_1 \mathbf{e}_1 - \widetilde{\mathbf{B}}_{j+1} \mathbf{y}\|_2 = \widehat{\mathbf{B}}_j^{-1} \boldsymbol{\gamma}_j$$

and

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

- Define the matrix

$$\mathbf{W}_j := \mathbf{Q}_j \widehat{\mathbf{B}}_j^{-1} = \begin{bmatrix} \mathbf{w}_1 & \mathbf{w}_2 & \cdots & \mathbf{w}_j \end{bmatrix}.$$

We have

$$\mathbf{Q}_j = \mathbf{W}_j \widehat{\mathbf{B}}_j,$$

which implies $\mathbf{w}_j = (\mathbf{q}_j - \widehat{\beta}_{j-1}\mathbf{w}_{j-1})/\widehat{\alpha}_j$. We have the recurrence

$$\begin{aligned}\mathbf{x}_j &= \mathbf{Q}_j \widehat{\mathbf{B}}_j^{-1} \boldsymbol{\gamma}_j = \mathbf{W}_j \boldsymbol{\gamma}_j = \begin{bmatrix} \mathbf{W}_{j-1} & \mathbf{w}_j \end{bmatrix} \begin{bmatrix} \boldsymbol{\gamma}_{j-1} \\ \gamma_j \end{bmatrix} \\ &= \mathbf{W}_{j-1}\boldsymbol{\gamma}_{j-1} + \gamma_j \mathbf{w}_j \\ &= \mathbf{x}_{j-1} + \gamma_j \mathbf{w}_j.\end{aligned}$$

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4. Other methods

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