Lecture 14: Krylov subspace methods for least squares problems

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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 $\min_{\mathbf{x}} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2$

$\quad \mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0, \quad \mathbf{p}_0 = \mathbf{A}^* \mathbf{r}_0;$

$\quad$ **for** $j = 1, 2, 3, \ldots,$

$\quad\quad \alpha_j = \|\mathbf{A}^* \mathbf{r}_{j-1}\|_2^2 / \|\mathbf{A}\mathbf{p}_{j-1}\|_2^2;$

$\quad\quad \mathbf{x}_j = \mathbf{x}_{j-1} + \alpha_j \mathbf{p}_{j-1};$

$\quad\quad \mathbf{r}_j = \mathbf{r}_{j-1} - \alpha_j \mathbf{A}\mathbf{p}_{j-1};$

$\quad\quad \beta_j = \|\mathbf{A}^* \mathbf{r}_j\|_2^2 / \|\mathbf{A}^* \mathbf{r}_{j-1}\|_2^2;$

$\quad\quad \mathbf{p}_j = \mathbf{A}^* \mathbf{r}_j + \beta_j \mathbf{p}_{j-1};$

$\quad$ **end**

- CGLS (also called CGNR) is mathematically equivalent to LSQR, which is based on Golub–Kahan bidiagonalization.

2. Householder bidiagonalization

$$
\begin{bmatrix} \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \\ \times & \times & \times & \times \end{bmatrix}
\quad \overset{\mathbf{U}_1^* \cdot}{\longrightarrow} \quad
\begin{bmatrix} \mathbf{\times} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \mathbf{0} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \mathbf{0} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \mathbf{0} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \mathbf{0} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ \mathbf{0} & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix}
\quad \overset{\cdot \mathbf{V}_1}{\longrightarrow} \quad
\begin{bmatrix} \times & \mathbf{\times} & \mathbf{0} & \mathbf{0} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \end{bmatrix}
$$

$$
\mathbf{A} \qquad\qquad \mathbf{U}_1^* \mathbf{A} \qquad\qquad \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1
$$

$$
\overset{\mathbf{U}_2^* \cdot}{\longrightarrow}
\begin{bmatrix} \times & \times & & \\ & \mathbf{\times} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{0} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{0} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{0} & \mathbf{\times} & \mathbf{\times} \\ & \mathbf{0} & \mathbf{\times} & \mathbf{\times} \end{bmatrix}
\quad \overset{\cdot \mathbf{V}_2}{\longrightarrow} \quad
\begin{bmatrix} \times & \times & & \\ & \times & \mathbf{\times} & \mathbf{0} \\ & & \mathbf{\times} & \mathbf{\times} \\ & & \mathbf{\times} & \mathbf{\times} \\ & & \mathbf{\times} & \mathbf{\times} \\ & & \mathbf{\times} & \mathbf{\times} \end{bmatrix}
$$

$$
\mathbf{U}_2^* \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1 \qquad\qquad \mathbf{U}_2^* \mathbf{U}_1^* \mathbf{A} \mathbf{V}_1 \mathbf{V}_2
$$

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.

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

- **Another** bidiagonalization algorithm: Note that

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

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

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

and

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

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

$\quad \beta_1 = \|\mathbf{a}_1\|_2, \quad \mathbf{u}_1 = \mathbf{a}_1/\beta_1, \quad \mathbf{v}_1 = \mathbf{e}_1$
$\quad$**for** $i = 1, 2, 3, \ldots,$
$\qquad \mathbf{v}_{i+1} = \mathbf{A}^*\mathbf{u}_i - \beta_i\mathbf{v}_i$
$\qquad \alpha_i = \|\mathbf{v}_{i+1}\|_2$
$\qquad \mathbf{v}_{i+1} = \mathbf{v}_{i+1}/\alpha_i$
$\qquad \mathbf{u}_{i+1} = \mathbf{A}\mathbf{v}_{i+1} - \alpha_i\mathbf{u}_i$
$\qquad \beta_{i+1} = \|\mathbf{u}_{i+1}\|_2$
$\qquad \mathbf{u}_{i+1} = \mathbf{u}_{i+1}/\beta_{i+1}$
$\quad$**end**

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3. LSQR

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

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

$$= \begin{bmatrix} \beta_1 & \alpha_1 & & & \\ & \beta_2 & \ddots & & \\ & & \ddots & \alpha_n & \\ & & & \beta_{n+1} & \\ & & & & \\ & & & & \end{bmatrix}.$$

We can write the least squares problem as

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

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

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

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

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

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

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

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

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

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

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

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

and

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

We have

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

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

$$\min_{\mathbf{y} \in \mathbb{C}^k} \|\mathbf{b} - \mathbf{A}\mathbf{Q}_k\mathbf{y}\|_2 = \min_{\mathbf{y} \in \mathbb{C}^k} \|\mathbf{b} - \mathbf{U}_{k+1}\widetilde{\mathbf{B}}_{k+1}\mathbf{y}\|_2$$

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

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

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

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

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

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

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

The final result after k steps is

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

Actually, we have the QR factorization for $\left[\widetilde{\mathbf{B}}_{k+1} \quad \beta_1\mathbf{e}_1\right]$:

$$\left[\widetilde{\mathbf{B}}_{k+1} \quad \beta_1\mathbf{e}_1\right] = \widehat{\mathbf{Q}} \begin{bmatrix} \widehat{\mathbf{B}}_k & \boldsymbol{\gamma}_k \\ \mathbf{0} & \widehat{\gamma}_{k+1} \end{bmatrix},$$

i.e.,

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

Then we have

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

and

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

Define the matrix $\mathbf{W}_k := \mathbf{Q}_k \widehat{\mathbf{B}}_k^{-1} = \begin{bmatrix} \mathbf{w}_1 & \cdots & \mathbf{w}_k \end{bmatrix}$, we have

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

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

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

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4. Other methods

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