Modified Gram-Schmidt

MATH 6610 Lecture 12

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Trefethen & Bau: Lecture 8

Orthogonalization

Output

The main goal of orthogonalization:

Given $\{a_j\}_{j=1}^n \subset \mathbb{C}^m$, compute $\{q_j\}_{j=1}^n$ such that:

Input

$$\langle q_j, q_k \rangle = \delta_{j,k}, \qquad \text{span}\{a_1, \ldots, a_n\} = \text{span}\{q_1, \ldots, q_n\}$$

$\text{span}\{a_1, \ldots a_j\} = \text{span}\{q_1, \ldots q_j\}, \quad 1 \le j \le n.$

Orthogonalization

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Any algorithm to accomplish this (e.g., Gram-Schmidt) implies:

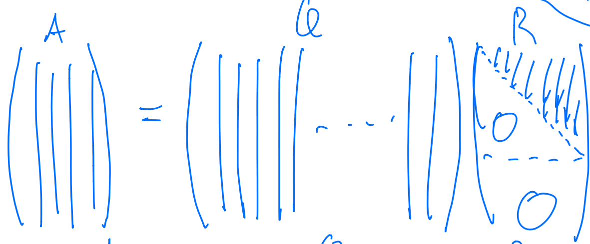
$$A = QR, \quad A = \begin{pmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{pmatrix}, \quad Q = \begin{pmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{pmatrix},$$

with R upper triangular. (Q has orthonormal columns)

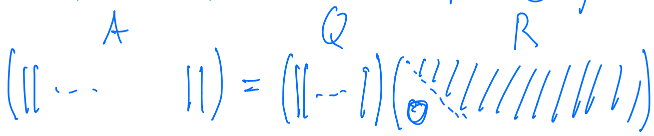
Recall: this generalizes. So if $A \in \mathbb{C}^{m \times n}$ matrix:

$\Longrightarrow$ $A = QR$, $Q \in \mathbb{C}^{m \times m}$ unitary

$R \in \mathbb{C}^{m \times n}$ is upper triangular.



diagonal elements of R might be nonzero



"QR decomposition"

Gram-Schmidt

The orthogonalization performed by Gram-Schmidt:

$$u_j = \underline{a_j} - \underline{P_{j-1} a_j}, \qquad q_j = \frac{u_j}{\|u_j\|_2},$$

with P_{j-1} the orthogonal projector onto $\operatorname{span}\{q_1, \ldots, q_{j-1}\}$.

$$A = \begin{pmatrix} | & & | \\ a_1 & \cdots & a_n \\ | & & | \end{pmatrix} \qquad P_j = Q_j Q_j^*, \qquad Q_j = \begin{pmatrix} | & & | \\ q_1 & \cdots & q_j \\ | & & | \end{pmatrix}$$

Note: $P_{j-1} a_j = \sum_{k=1}^{j-1} q_k \cdot (q_k^* a_j)$

Gram-Schmidt

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It turns out that this is an unstable algorithm. ☹

"Modified" Gram-Schmidt

$P_{j-1} = Q_{j-1} Q_{j-1}^*$ ✓

$$u_j = a_j - P_{j-1} a_j, \qquad q_j = \frac{u_j}{\|u_j\|},$$

The cause of numerical instability is that, if a_j is nearly parallel to $\mathrm{span}\{q_1, \ldots, q_{j-1}\}$, this projection step can produce numerically incorrect results.

(We saw this in a code demo)

Problem: $\{q_j\}$ are not orthonormal.

Problem: a_j is orthogonalized against $\{q_k\}_{k=1}^{j-1}$ "all at once" (apply P_{j-1})

Fix: project out q_k "one at a time"!

“Modified” Gram-Schmidt

$$u_j = a_j - P_{j-1} a_j, \qquad\qquad q_j = \frac{u_j}{\|u_j\|},$$

The cause of numerical instability is that, if a_j is nearly parallel to $\mathrm{span}\{q_1, \ldots, q_{j-1}\}$, this projection step can produce numerically incorrect results.

This problem can be fixed with a “modified” version of Gram-Schmidt, which essentially does

$$\begin{aligned}
& u_1 = a_j \\
& \texttt{For } k = 1, \ldots, j-1 \\
& \qquad u_{k+1} = u_k - q_k q_k^* u_k \\
& q_j = \frac{u_j}{\|u_j\|}.
\end{aligned}$$

Thus, the projections are computed “one at a time”.