Modified Gram-Schmidt

MATH 6610 Lecture 12

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Trefethen & Bau: Lecture 8

Orthogonalization

The main goal of orthogonalization:

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

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

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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.

Gram-Schmidt

The orthogonalization performed by Gram-Schmidt:

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

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

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It turns out that this is an unstable algorithm. ☹

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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.

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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”.