Blocked Lanczos Procedure

Recall: BLAS 3 operations great
BLAS 2 operations good but much slower than BLAS3

Let \( b \) be a block size
Let \( A \) be a \( n \times n \) and hermitian matrix
Let \( Q \) be an \( n \times \) given, ON matrix
we seek matrices

\[
Q = \begin{bmatrix}
q_1 & q_2 & \cdots
\end{bmatrix} \quad \Leftarrow \text{unitary}
\]

\[
T = \begin{bmatrix}
t_{11} & t_{12} & 0 & \cdots \\
0 & t_{22} & t_{23} & \cdots \\
0 & 0 & t_{33} & \cdots \\
0 & 0 & \cdots & 0
\end{bmatrix} \quad \Leftarrow \text{block tridiagonal each block size } b \times b
\]

We want \( A = QTQ^* \)
\[\iff AQ = QT \]  (1)

First block col of (1): \( AQ_1 = Q_1 T_{11} + Q_2 T_{21} \)
multiply by \( Q_1^* \) \( Q_1^* AQ_1 = Q_1^* Q_1 T_{11} + Q_1^* Q_2 T_{21} \)
\[Q_1^* AQ_1 = I_b T_{11} + 0 T_{21}\]

\[T_{11} = Q_1^* AQ_1\]

\[Q_2 T_{21} = AQ_1 - Q_1 T_{11}\]
\([Q_2, T_{21}] = qr(AQ_1 - Q_1 T_{11}) \Leftarrow \text{non-pivoted}\)
and \( T_{21}' = T_{12} \)

Second block of (2):
\[AQ_2 = Q_1 T_{12} + Q_2 T_{22} + Q_3 T_{32}\]
\[T_{22} = Q_2^* AQ_2\]
\[Q_3 T_{32} = AQ_2 - Q_1 T_{12} - Q_2 T_{22} \Leftarrow QR factorization\]
Convergence of Lanczos

Set $T_k = T(1 : k, 1 : k)$. Let $b$ be the starting vector of Lanczos iteration $q_1 = \frac{b}{\|b\|}$.

Idea: evals of $T_k$ converge to $k$ evals of $A$ (largest ones first)

Set $p^*(\lambda) = det(T_k - \lambda I)$ so $p^*$ is the characteristic polynomial of $T_k$

Recall: $\lambda$ is an eval of $T_k \iff p^*(\lambda) = 0$

Set $P^\infty_k$ is the set of "monic" polynomials of degree $k$

Then $\|p^*(A)b\| \leq \|p(A)b\| \forall p \in P^\infty_k$

Consider the evd of $A$, $A = UDU^*$

Then $A^t = UDU^*$

so for any polynomial $p$ we have $p(A) = U p(D) U^*$

$\|p(A)b\| = \|U p(D) U^*b\| = \| p(D)b' \|$, $b' = U^*b$

\[
\begin{bmatrix}
p(\lambda_1)b'_1 \\
p(\lambda_2)b'_2 \\
\vdots \\
p(\lambda_n)b'_n
\end{bmatrix}
\]

We expect the zeros of $p^*$ to "hit" the dominant evals of $A$

Arnoldi Procedure

Let $A$ be an $n \times n$ general matrix

Let $b$ be a starting vector and set $q_1 = \frac{b}{\|b\|}$

Set $K_k(A, b) = span \{b, Ab, A^2b, ..., A^{k-1}b\}$

We will build an ON set $\{q_j\}_{j=1}^n$ such that $\{q_j\}_{j=1}^n$ is an ON basis for $K_k(A, b)$

We formalize this as seeking a factorization $A = QH Q^*$

where $Q = \begin{bmatrix} | & | & | \\
q_1 & q_2 & ... & q_n \\
| & | & |
\end{bmatrix}$ is unitary

and where $H$ is a Hessenberg matrix
\[
H = \begin{bmatrix}
h_{11} & h_{12} & h_{13} & \cdots \\
h_{21} & h_{22} & h_{23} & \cdots \\
0 & h_{32} & h_{33} & \cdots \\
| & 0 & & 0
\end{bmatrix}
\]

(we cannot get a tridiagonal since \( A \) is not hermitian)

(1) \( AQ = QH \) (2)

First col of (2) = \( Aq_1 = q_1 h_{11} + q_2 h_{21} \)

\[h_{11} = q_1^* A q_1\]

\[q_2 h_{21} = A q_1 - q_1 h_{11} \quad \leftarrow \text{determines } q_2, q_1\]

Second col of (2):

**** note \( H \) is not symmetric

\[A q_2 = q_1 h_{12} + q_2 h_{22} + q_3 h_{32}\] (3)

\[q_1^* \times (3) \Rightarrow h_{12} = q_1^* A q_2\]

\[q_2^* \times (3) \Rightarrow h_{22} = q_2^* A q_2\]

\[q_3 h_{32} = A q_2 - q_1 h_{12} - q_2 h_{22} \rightarrow q_3, h_{32}\]

The kth Step:

\[A q_k = \sum_{i=1}^{k} q_i h_{ik} + q_{k+1} h_{k+1,k}\]

\( \rightarrow h_{ik} = q_i^* A q_k \quad \text{for } i = 1, 2, ..., k\)

\( h_{k+1,k} q_{k+1} = A q_k - \sum_{i=1}^{k} h_{ik} - q_i \rightarrow h_{k+1,k} \text{ and } q_{k+1}\)

Some comments: in its "pure" form Arnoldi’s procedure is more work than Lanczos

- It requires more memory since all \( q \) vectors must be stored
- Stabilized Lanczos also requires a lot of storage
- Restarting is a common tool to deal with both memory problems and operation cos of Arnoldi
- Arnoldi converges more slowly, and the theory is less sharp