Class Notes from Monday, February 22nd

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 hermition matrix

Let Q be an $n \times b$ given, ON matrix

we seek matrices

$$Q = \begin{bmatrix} | & | & \\ q_1 & q_2 & ... \\ | & | & \end{bmatrix} \quad \Leftarrow \textit{unitary}$$

$$T = \begin{bmatrix} t_{11} & t_{12} & 0 & ... \\ t_{21} & t_{22} & t_{23} & ... \\ t_{33} & ... & . & \\ 0 & ... & & . \end{bmatrix} \quad \Leftarrow \textit{block tridiagonal each block size } b \times b$$

We want $A = QTQ^*$

$\iff \quad AQ = QT \quad (1)$

First block col of (1) : $\;AQ_1 = Q_1\, T_{11} + Q_2\, T_{21}$

multiyply by $Q_1^* \;\rightarrow\; Q_1^*AQ_1 = Q_1^*Q_1\, T_{11} + Q_1^*Q_2\, T_{21}$

$Q_1^*AQ_1 = I_b\, T_{11} + 0\, T_2 1$

$$T_{11} = Q_1^*AQ_1$$

$\Rightarrow \quad Q_2T_{21} = AQ_1 - Q_1T_{11}$

$[Q_2, T_{21}] = qr(AQ_1 - Q_1T_{11}) \Leftarrow \; non-pivoted$

and $T_{21}^* = T_{12}$

Second block of (2):

$AQ_2 = Q_1T_{12} + Q_2T_{22} + Q_3T_{32}$

$T_{22} = Q_2^*AQ_2$

$Q_3T_{32} = AQ_2 - Q_1T_{12} - Q_2T_{22} \quad \leftarrow \; QR\ factorization$

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

Set P_k^∞ = set of "monic" polynomials of degree k

$$\left\{p : p(z) = z^k + C_{k-1}z^{k-1} + ... + C_1 z + C_0\right\}$$

Then $\left\|p^*(A)b\right\| \leq \left\|p(A)b\right\| \ \forall \ p \ \in \ P_k^\infty$

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

then $A^i = UD^iU^*$

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

$\left\|p(A)b\right\| = \left\|Up(D)U^*b\right\| = \left\|p(D)b'\right\|, \quad b' = U^*b$

$$= \left\| \begin{bmatrix} p(\lambda_1)b'_1 \\ p(\lambda_1)b'_2 \\ . \\ . \\ . \\ p(\lambda_n)b'_n \end{bmatrix} \right\|$$

.

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

We will build an ON set $\{q_1\}_{j=1}^n$ such that $\left\{q_j\right\}_{j=1}^n$ is an ON basis for $K_k(A, b)$

We formalize this as seeking a fatorization $A = QHQ^*$

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

and where H is a Hessenberg matrix

$$H = \begin{bmatrix} h_{11} & h_{12} & h_{13} & — \\ h_{21} & h_{22} & h_{23} & — \\ 0 & h_{32} & h_{33} & — \\ | & 0 & & \\ & & 0 & \end{bmatrix}$$

(we cannot get a tridiagonal since A is not hermition)

(1) $\Leftrightarrow \quad AQ = QH$ (2)

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

$h_{11} = q_1^* A q_1$

$q_2 h_{21} = Aq_1 - q_1 h_{11} \ \leftarrow$ determines q_2, q_1

Second col of (2):

**** note H is not symmetric

$Aq_2 = q_1 h_{12} + q_2 h_{22} + q_3 h_{32}(3)$

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

$q_2^* \ \times \ (3) \quad \Rightarrow \quad h_{22} = q_2^* A q_2$

$q_3 h_{32} = Aq_2 - q_1 h_{12} - q_2 h_{22} \quad \rightarrow \quad q_3, h_{32}$

<u>The kth Step:</u>

$Aq_k = \sum_{i=1}^{k} \ q_i h_{ik} + q_{k+1} h_{k+1,k}$

$\rightarrow \ h_{ik} = q_i^* A q_k$ for $i = 1, 2, ..., k$

$\rightarrow \ h_{k+1,k} q_{k+1} = Aq_k - \sum_{i=1}^{k} \ h_{ik} - q_i \ \rightarrow h_{k+1,k}$ and q_{k+1}

<u>Some comments:</u> in its "pure" form Arnoldi's procedure is more work then Lanczos

– It requires more memory since all q vectors must be stored

– Stabalized 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