Lanczos Iteration

This section is a repeat of the end of class on Wednesday, February 17. Let $\mathbf{A}$ be a $n \times n$ matrix with $\mathbf{A} = \mathbf{A}^*$. Let $\vec{q}_1 \in \mathbb{R}^n$ is a starting vector such that $\|\mathbf{q}_1\| = 1$. We seek a factorization

$$\mathbf{A} = \mathbf{QTQ}^* \tag{1}$$

$\mathbf{Q}$ should be unitary with the first column of $\mathbf{Q} = \vec{q}_1$ and $\mathbf{T}$ should be tridiagonal

1. Iteration Process

1.1. **Note.** λ is a an eigenvalue of $\mathbf{A}$ if and only if λ is an eigenvalue of $\mathbf{T}$. Also, we typically stop after k steps

$$\mathbf{A} \approx \mathbf{Q}(\,:, 1 : k)\,\mathbf{T}(\,1 : k, 1 : k)\,\mathbf{Q}(\,:, 1 : k)^*$$

1.2. **Iteration.** Multiply 1 by $\mathbf{Q}$ from the right:

$$\mathbf{AQ} = \mathbf{QT} \tag{2}$$

Looking at the first column of 2

$$\mathbf{A}\vec{q}_1 = \vec{q}_1 t_{1,1} + \vec{q}_2 t_{2,1}$$

$$\vec{q}_1^*\mathbf{A}\vec{q}_1 = \vec{q}_1^*\vec{q}_1 t_{1,1} + \vec{q}_1^*\vec{q}_2 t_{2,1}$$

Since Q is orthonormal, $\vec{q}_1^*\vec{q}_2 = 0$ and $\vec{q}_1^*\vec{q}_1 = 1$

$$t_{1,1} = \vec{q}_1^*\mathbf{A}\vec{q}_1$$

$$t_{2,1}\vec{q}_2 = \mathbf{A}\vec{q}_1 - t_{1,1}\vec{q}_1$$

Set $\vec{r}_1 = \mathbf{A}\vec{q}_1 - t_{1,1}\vec{q}_1$

$$t_{2,1} = \|\vec{r}_1\|$$

$$\vec{q}_2 = \frac{\vec{r}_1}{t_{2,1}}$$

$\mathbf{T}$ is symmetric so $t_{2,1} = t_{1,2}$ Looking at the second column of 2

$$\mathbf{A}\vec{q}_2 = \vec{q}_1 t_{1,2} + \vec{q}_2 t_{2,2} + \vec{q}_3 t_{3,2}$$

The left hand side of the equation, and the first two terms of the right hand side of the equation are known. This leaves $\vec{q}_3 t_{3,2}$ as the only unknown

$$\vec{q}_2^*\mathbf{A}\vec{q}_2 = t_{2,2}$$

$$\vec{r}_2 = \vec{q}_3 t_{3,2} = \mathbf{A}\vec{q}_2 - t_{1,2}\vec{q}_1 - t_{2,2}\vec{q}_2$$

$$t_{3,2} = \|\vec{r}_2\|$$

$$\vec{q}_3 = \frac{\vec{r}_2}{t_{3,2}}$$

Looking at the k^{th} step,

$$\mathbf{A}\vec{q}_k = \vec{q}_{k-1} t_{k-1,k} + \vec{q}_k t_{k,k} + \vec{q}_{k+1} t_{k+1,k}$$

$$t_{k,k} = \vec{q}_k^*\mathbf{A}\vec{q}_k$$

$$\vec{r}_k = \mathbf{A}\vec{q}_k - t_{k-1,k}\vec{q}_{k-1} - t_{k,k}\vec{q}_k$$

$$t_{k+1,k} = \|\vec{r}_k\|$$

$$\vec{q}_{k+1} = \frac{\vec{r}_k}{t_{k+1,k}}$$

1.3. **Lanczos Iteration as a function.** The inputs to the LANCZOS Iteration are as follows: $\mathbf{A}$ and $\vec{q}_1$ such that $\|\vec{q}_1\| = 1$

$$t_{1,1} = \vec{q}_1^* \mathbf{A} \vec{q}_1$$
$$\vec{r}_1 = \mathbf{A}\vec{q}_1 - t_{1,1}\vec{q}_1$$

for j = 2, 3, . . . , n

$$t_{j-1,j} = \|\vec{r}_{j-1}\|$$
$$\vec{q}_j = \frac{\vec{r}_{j-1}}{t_{j-1,j}}$$
$$t_{j,j} = \vec{q}_j^* \mathbf{A} \vec{q}_j$$
$$\vec{r}_j = \mathbf{A}\vec{q}_j - t_{j-1,j}\vec{q}_{j-1} - t_{j,j}\vec{q}_j$$

end

1.4. **Remarks about Q. Claim** For any k, $\{\vec{q}_j\}_{j=1}^k$ is an Orthonormal basis for $Span\{\vec{q}_1, \mathbf{A}\vec{q}_1, \dots, \mathbf{A}^{k-1}\vec{q}_1\}$ **Sketch of the Proof** Obviously true for k = 1. **k = 2**

$$\vec{q}_2 = \frac{1}{t_{2,1}}(\mathbf{A}\vec{q}_1 - t_{1,1}\vec{q}_1) \in Span\{\vec{q}_1, \mathbf{A}\vec{q}_1\}$$

Note $Span\{\vec{q}_1, \mathbf{A}\vec{q}_1\}$ has dimension 2 **k = 3**

$$\vec{q}_3 = \frac{1}{t_{3,2}}(\mathbf{A}\vec{q}_2 - t_{2,1}\vec{q}_1 - t_{2,2}\vec{q}_2) \in Span\{\vec{q}_1, \vec{q}_2, \mathbf{A}\vec{q}_1\} \subseteq Span\{\vec{q}_1, \mathbf{A}\vec{q}_1, \mathbf{A}^2\vec{q}_1\}$$

Induction can be used to complete the proof

1.5. **Invariant Subspaces.** What if $\vec{r}_k = 0$ at some step k. Then $\mathbf{A}\vec{q}_k = \vec{q}_{k-1}t_{k-1,k} + \vec{q}_k t_{k,k}$. Set $V = Span\{\vec{q}_1, \vec{q}_2, \dots, \vec{q}_k\}$. Then V is an invariant subspace of $\mathbf{A}$. Suppose $\vec{v} \in V \iff \vec{v} = \sum_{j=1}^k c_j \vec{q}_j$

$$\mathbf{A}\vec{v} = \sum_{j=1}^{k} c_j \mathbf{A}\vec{q}_j = c_k \mathbf{A}\vec{q}_k + \sum_{j=1}^{k-1} c_j \mathbf{A}\vec{q}_j$$

$\mathbf{A}\vec{q}_k \in Span\{\vec{q}_{k+1}, \vec{q}_k\} \subseteq V$ and $\sum_{j=1}^{k-1} c_j \mathbf{A}\vec{q}_j \in V$, so $\mathbf{A}\vec{v} \in V$ We see that $\vec{q}_1$ lies in an invariant subspace of $\mathbf{A}$. Suppose $rank(\mathbf{A}) = p$. Suppose $\vec{g}$ is a Gaussian vector and set $\vec{q}_1 = \frac{\vec{g}}{\|\vec{g}\|}$. Let $\{\vec{v}_j\}_{j=1}^p$ be the eigenvectors of $\mathbf{A}$ with eigenvalues λ_j so $\lambda_j \neq 0$

$$\vec{q}_1 = \frac{1}{\|\vec{g}\|} \sum_{j=1}^{p} c_j \vec{v}_j$$

All coefficients c_j are Gaussian random numbers. But, if you should happen to find $\vec{r}_k = 0$, then you found an invariant subspace which is very nice because now

$$\mathbf{A} = \mathbf{QTQ}^* = [\,\mathbf{Q}_k \mathbf{Q}_k] \begin{bmatrix} \mathbf{T}_{LL} & 0 \\ 0 & \mathbf{T}_{RR} \end{bmatrix} \begin{bmatrix} \mathbf{Q}_L^* \\ \mathbf{Q}_L^* \end{bmatrix} = \mathbf{Q}_L \mathbf{T}_{LL} \mathbf{Q}_L^* + \mathbf{Q}_R \mathbf{T}_{RR} \mathbf{Q}_R^*$$

The eigenvalues of $\mathbf{T}_{LL}$ are all eigenvalues of $\mathbf{A}$. Pick $\vec{q}_{k+1}$ as a random vector that is orthongonal to $\vec{q}_1, \vec{q}_2, \dots, \vec{q}_k$ and proceed.

$$\vec{g} = randn(n, 1)$$
$$\vec{r} = \vec{g} - \sum_{j=1}^{k} (\vec{q}_j^* \vec{g})\, \vec{q}_j$$
$$\vec{q}_{k+1} = \frac{\vec{r}}{\|\vec{r}\|}$$

If all you want are eigenvalues (not eigenvectors) , then you only need to store $\mathbf{T}$ and the last two q-vectors

1.6. **Stability.** The Lanczos procedure is unstable. $t_{j-1,j}$ can be very small. The round-off errors will cause the sequence $\{\vec{q}_j\}_{j=1}^{k}$ to lose orthogonality as k increases. To fix this, one can store all $\{\vec{q}_j\}$ and explicitly re-orthonormalize. Once you compute $\vec{r}_j$, do

$$\vec{r}_k \leftarrow \vec{r}_k - \sum_{k=1}^{j-1} (\,\vec{r}_k \vec{q}_j)\vec{q}_j$$