Supplementary Derivations for the Lanczos-Algorithm Lecture

Spectral representation

The eigenvalues and eigenvectors satisfy

$$\sum_{j=1}^{n} A_{ij} q_j^{(\alpha)} = \lambda_\alpha q_i^{(\alpha)} = \sum_{\beta=1}^{n} q_i^{(\alpha)} \left(\lambda_\beta \delta_{\beta\alpha}\right), \tag{1}$$

where $\delta_{\beta\alpha} = 1 \ (\alpha = \beta); \ 0 \ (\alpha \neq \beta)$. Define an orthogonal matrix $\mathbf{Q}$ such that its α-th column is the α-th eigenvector $\mathbf{q}^{(\alpha)}$, i.e., $\mathbf{Q} = [\mathbf{q}^{(1)}\mathbf{q}^{(2)}\cdots\mathbf{q}^{(n)}]$, and a diagonal matrix Λ such that $\Lambda_{\beta\alpha} = \lambda_\beta \delta_{\beta\alpha}$, and Eq. (1) is reduced to a matrix equation,

$$\mathbf{AQ} = \mathbf{Q}\Lambda . \tag{2}$$

From the orthonormality of the eigenvector set,

$$\left(\mathbf{Q}^T\mathbf{Q}\right)_{\alpha\beta} = \sum_{i=1}^{n} Q_{i\alpha} Q_{i\beta} = \sum_{i=1}^{n} q_i^{(\alpha)} q_i^{(\beta)} = \mathbf{q}^{(\alpha)} \bullet \mathbf{q}^{(\beta)} = \delta_{\alpha\beta}, \tag{3}$$

where $\mathbf{Q}^T$ is the transpose of $\mathbf{Q}$. Therefore,

$$\mathbf{Q}^T\mathbf{Q} = \mathbf{I}, \tag{4}$$

where the identity matrix is defined as $\mathbf{I}_{\alpha\beta} = \delta_{\alpha\beta}$. Multiplying $\mathbf{Q}^T$ from the left, then, Eq. (2) becomes

$$\mathbf{Q}^T\mathbf{AQ} = \Lambda . \tag{5}$$

Variational principle: The best approximation to $\mathbf{q}^{(1)}$ is whatever the vector that makes $\rho(\mathbf{x}; \mathbf{A})$ the smallest.

Once $\mathbf{q}^{(1)}$ is found, the best approximation to $\mathbf{q}^{(2)}$ is whatever the vector $\{\mathbf{x} \mid \mathbf{x} \bullet \mathbf{q}^{(1)} = 0\}$ that makes $\rho(\mathbf{x}; \mathbf{A})$ the smallest, and so on.

Gram-Schmidt orthogonalization

For a set of un-orthonormalized vectors $\{\mathbf{s}_1, \ldots, \mathbf{s}_n\}$, suppose that the first $i-1$ vectors have been orthonormalized to form $\{\mathbf{q}_1, \ldots, \mathbf{q}_{i-1}\}$, and consider

$$\mathbf{q}_i' \leftarrow \mathbf{s}_i - \sum_{j=1}^{i-1} \mathbf{q}_j \left(\mathbf{q}_j \bullet \mathbf{s}_i\right); \quad \mathbf{q}_i \leftarrow \mathbf{q}_i' / \left|\mathbf{q}'\right|_i . \tag{6}$$

Then

$$\begin{aligned}
\mathbf{q}_{j(<i)} \bullet \mathbf{q}_i' &= \mathbf{q}_j \bullet \left[\mathbf{s}_i - \sum_{k=1}^{i-1} \mathbf{q}_k \left(\mathbf{q}_k \bullet \mathbf{s}_i\right)\right] \\
&= \mathbf{q}_j \bullet \mathbf{s}_i - \sum_{k=1}^{i-1} \left(\mathbf{q}_j \bullet \mathbf{q}_k\right)\left(\mathbf{q}_k \bullet \mathbf{s}_i\right) \\
&= \mathbf{q}_j \bullet \mathbf{s}_i - \sum_{k=1}^{i-1} \delta_{jk} \left(\mathbf{q}_k \bullet \mathbf{s}_i\right) = 0
\end{aligned}$$

i.e., the modified vector is orthogonal to all the low-lying vectors $\mathbf{q}_j$.

Lanczos recursion formula

From the tridiagonality,

$$\mathbf{A}\mathbf{q}_i = a\mathbf{q}_{i-1} + b\mathbf{q}_i + c\mathbf{q}_{i+1} \,. \tag{7}$$

$\mathbf{q}_i^T \times$ (7)

$$\mathbf{q}_i^T\mathbf{A}\mathbf{q}_i = b\mathbf{q}_i^T\mathbf{q}_i = b$$

$$\therefore b = \alpha_i = \mathbf{q}_i^T\mathbf{A}\mathbf{q}_i \tag{8}$$

$\mathbf{q}_{i-1}^T \times$ (7)

$$\mathbf{q}_{i-1}^T\mathbf{A}\mathbf{q}_i = a\mathbf{q}_{i-1}^T\mathbf{q}_{i-1} = a$$

$$\therefore a = \mathbf{q}_{i-1}^T\mathbf{A}\mathbf{q}_i = \mathbf{q}_i^T\mathbf{A}\mathbf{q}_{i-1}(\text{real}) = \beta_{i-1} \quad (i \geq 2) \tag{9}$$

$\mathbf{q}_{i+1}^T \times$ (7)

$$\mathbf{q}_{i+1}^T\mathbf{A}\mathbf{q}_i = c\mathbf{q}_{i+1}^T\mathbf{q}_{i+1} = c$$

$$\therefore c = \mathbf{q}_{i+1}^T\mathbf{A}\mathbf{q}_i = \beta_i \tag{10}$$

Lanczos algorithm (last step)

$$\|\mathbf{r}_i\| = \|\beta_i\mathbf{q}_{i+1}\| = \beta_i\|\mathbf{q}_{i+1}\| = \beta_i$$