Supplementary Derivations for the Lanczos-Algorithm Lecture

Spectral representation

The eigenvalues and eigenvectors satisfy

\[ \sum_{j=1}^{n} A_{ij} q_j^{(\alpha)} = \lambda_{\alpha} q_i^{(\alpha)} = \sum_{\beta=1}^{n} q_i^{(\alpha)} (\lambda_{\rho} \delta_{\beta\alpha}), \]

where \( \delta_{\beta\alpha} = 1 \ (\alpha = \beta); \ 0 \ (\alpha \neq \beta). \)

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

\[ AQ = QA \Lambda. \]  

From the orthonormality of the eigenvector set,

\[ (Q^T Q)_{\alpha\beta} = \sum_{i=1}^{n} Q_{i\alpha} Q_{i\beta} = \sum_{i=1}^{n} q_i^{(\alpha)} q_i^{(\beta)} = q^{(\alpha)} \cdot q^{(\beta)} = \delta_{\alpha\beta}, \]

where \( Q^T \) is the transpose of \( Q \). Therefore,

\[ Q^T Q = I, \]

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

\[ Q^T AQ = \Lambda. \]

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

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

Gram-Schmidt orthogonalization

For a set of un-orthonormalized vectors \( \{s_1, \ldots, s_n\} \), suppose that the first \( i-1 \) vectors have been orthonormalized to form \( \{q_1, \ldots, q_{i-1}\} \), and consider

\[ q_i' \leftarrow s_i - \sum_{j=1}^{i-1} q_j (q_j \cdot s_i); \quad q_i \leftarrow q_i' / |q_i'|. \]

Then

\[ q_j(\langle i \rangle) \cdot q_i' = q_j \cdot \left[ s_i - \sum_{k=1}^{i-1} q_k (q_k \cdot s_i) \right] \]

\[ = q_j \cdot s_i - \sum_{k=1}^{i-1} (q_j \cdot q_k)(q_k \cdot s_i) \]

\[ = q_j \cdot s_i - \sum_{k=1}^{i-1} \delta_{jk} (q_k \cdot s_i) = 0 \]

i.e., the modified vector is orthogonal to all the low-lying vectors \( q_j \).
Lanczos recursion formula

From the tridiagonality,

\[ Aq_i = aq_{i-1} + bq_i + cq_{i+1}. \]  
\( Aq_i = aq_{i-1} + bq_i + cq_{i+1}. \)  
\( 7 \)

\[ q_i^T \times (7) \]

\[ q_i^T Aq_i = b q_i^T q_i = b \]
\[ \therefore b = q_i^T Aq_i \]  
\( 8 \)

\[ q_{i-1}^T \times (7) \]

\[ q_{i-1}^T Aq_i = a q_{i-1}^T q_{i-1} = a \]
\[ \therefore a = q_{i-1}^T Aq_i = q_i^T Aq_{i-1} \text{(real)} = \beta_{i-1} \quad (i \geq 2) \]  
\( 9 \)

\[ q_{i+1}^T \times (7) \]

\[ q_{i+1}^T Aq_i = c q_{i+1}^T q_{i+1} = c \]
\[ \therefore c = q_{i+1}^T Aq_i = \beta_i \]  
\( 10 \)

Lanczos algorithm (last step)

\[ ||r_i|| = ||\beta_i q_{i+1}|| = \beta_i ||q_{i+1}|| = \beta_i \]