Found at: http://www.met.rdg.ac.uk/~ross/Documents/Lanczos.pdf

Lanczos method for hermitian and non-hermitian operators

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1. Hermitian operators

1. Generate Krylov subspace basis members

N must be the normalization factor, not a count.

$H|v_i\rangle = \beta_{i-1}|v_{i-1}\rangle + \alpha_i|v_i\rangle + \beta_i|v_{i+1}\rangle$

$$\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\mathbf{O}\vec{\psi}_n - \sum_{j=1}^{n}\alpha_{jn}\vec{\psi}_j\right). \qquad (A)$$

2. Impose orthogonality of subspace basis

$\langle v_1|H|v_3\rangle = \langle v_1|\beta_2|v_2\rangle + \langle v_1|\alpha_3|v_3\rangle + \langle v_1|\beta_3|v_4\rangle$

$= \langle v_1|\beta_3|v_4\rangle$

Applying H the other direction

$\langle v_1|H|v_3\rangle = \langle v_1|\alpha_1|v_3\rangle + \langle v_2|\beta_1|v_3\rangle = 0$

apply inductively

Orthogonality is mathematically guarenteed, but numerically drifts off and must be enforced.

$$\vec{\psi}_i^{\dagger}\vec{\psi}_j = \delta_{ij}, \qquad (B)$$

Eq. (B) into Eq. (A):
$$\vec{\psi}_i^{\dagger}\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\vec{\psi}_i^{\dagger}\mathbf{O}\vec{\psi}_n - \sum_{j=1}^{n}\alpha_{jn}\vec{\psi}_i^{\dagger}\vec{\psi}_j\right), \qquad (C)$$

$$\delta_{i,n+1} = \frac{1}{N_{n+1}}\left(O_{in} - \sum_{j=1}^{n}\alpha_{jn}\delta_{ij}\right), \qquad (D)$$

where
$$O_{in} \equiv \vec{\psi}_i^{\dagger}\mathbf{O}\vec{\psi}_n. \qquad (E)$$

3. Choose $i < n + 1$

Eq. (D):
$$0 = \frac{1}{N_{n+1}}(O_{in} - \alpha_{in}), \qquad (F)$$

$$\alpha_{in} = O_{in}. \qquad (G)$$

4. Choose $i = n + 1$

Eq. (D):
$$1 = \frac{1}{N_{n+1}}(O_{n+1,n} - 0), \qquad (H)$$

$$N_{n+1} = O_{n+1,n}. \qquad (I)$$

5. Insert Eqs. (G) and (I) back into Eq. (D)

$$O_{n+1,n}\delta_{i,n+1} = O_{in} - \sum_{j=1}^{n}O_{jn}\delta_{ij}. \qquad (J)$$

To prove that the matrix elements of $\mathbf{O}$ in the $\vec{\psi}$ basis form a tridiagonal matrix, consider Eq. (J) for matrix element (i, n),

(i) $i > n + 1$:

$$0 = O_{in}, \qquad (K)$$

(ii) $i = n + 1$:

$$O_{n+1,n} = O_{n+1,n}, \qquad (L)$$

(iii) $i = n$:

$$0 = O_{nn} - O_{nn}, \qquad (M)$$

(iv) $i = n - 1$:

$$0 = O_{n-1,n} - O_{n-1,n}, \tag{N}$$

(v) $i < n - 1$:

$$\text{use hermitian property: } O_{in} = O^*_{ni} \ (= 0 \ \text{from Eq. (K)}). \tag{O}$$

Eq. (A) is then,

$$\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\mathbf{O}\vec{\psi}_n - O_{nn}\vec{\psi}_n - O_{n-1,n}\vec{\psi}_{n-1}\right). \tag{P}$$

2. Non-hermitian operators

1. Generate Krylov subspace basis members and their duals

ψ_1 = random unit vector

should ψ^1 be the same?

$$\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\mathbf{O}\vec{\psi}_n - \sum_{j=1}^{n} \alpha_{jn}\vec{\psi}_j\right), \tag{A1}$$

$$\vec{\psi}^{n+1} = \frac{1}{N^{n+1}}\left(\mathbf{O}^\dagger\vec{\psi}^n - \sum_{j=1}^{n} \beta_{jn}\vec{\psi}^j\right). \tag{A2}$$

2. Impose bi-orthogonality of subspace basis

$$\vec{\psi}^{i\dagger}\vec{\psi}_j = \delta_{ij}, \tag{B1}$$

$$\vec{\psi}_i^\dagger\vec{\psi}^j = \delta_{ij}, \tag{B2}$$

$$\text{Eq. (B1) into Eq. (A1): } \vec{\psi}^{i\dagger}\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\vec{\psi}^{i\dagger}\mathbf{O}\vec{\psi}_n - \sum_{j=1}^{n} \alpha_{jn}\vec{\psi}^{i\dagger}\vec{\psi}_j\right), \tag{C1}$$

$$\delta_{i,n+1} = \frac{1}{N_{n+1}}\left(O_{in} - \sum_{j=1}^{n} \alpha_{jn}\delta_{ij}\right), \tag{D1}$$

$$\text{where } O_{in} \equiv \vec{\psi}^{i\dagger}\mathbf{O}\vec{\psi}_n, \tag{E1}$$

$$\text{Eq. (B2) into Eq. (A2): } \vec{\psi}_i^\dagger\vec{\psi}^{n+1} = \frac{1}{N^{n+1}}\left(\vec{\psi}_i^\dagger\mathbf{O}^\dagger\vec{\psi}^n - \sum_{j=1}^{n} \beta_{jn}\vec{\psi}_i^\dagger\vec{\psi}^j\right), \tag{C2}$$

$$\delta_{i,n+1} = \frac{1}{N^{n+1}}\left(O^\dagger_{in} - \sum_{j=1}^{n} \beta_{jn}\delta_{ij}\right), \tag{D2}$$

$$\text{where } O^\dagger_{in} \equiv \vec{\psi}_i^\dagger\mathbf{O}^\dagger\vec{\psi}^n. \tag{E2}$$

3. Choose $i < n + 1$

$$\text{Eq. (D1): } 0 = \frac{1}{N_{n+1}}\left(O_{in} - \alpha_{in}\right), \tag{F1}$$

$$\alpha_{in} = O_{in}, \tag{G1}$$

$$\text{Eq. (D2): } 0 = \frac{1}{N^{n+1}}\left(O^\dagger_{in} - \beta_{in}\right), \tag{F2}$$

$$\beta_{in} = O^\dagger_{in}. \tag{G2}$$

$$\text{Eqs. (G1), (G2): } \alpha_{in} = \beta^*_{ni} \tag{G3}$$

4. Choose $i = n + 1$

$$\text{Eq. (D1):}\ \ 1 = \frac{1}{N_{n+1}}\left(O_{n+1,n} - 0\right), \tag{H1}$$

$$N_{n+1} = O_{n+1,n}, \tag{I1}$$

$$\text{Eq. (D2):}\ \ 1 = \frac{1}{N^{n+1}}\left(O^{\dagger}_{n+1,n} - 0\right), \tag{H2}$$

$$N^{n+1} = O^{\dagger}_{n+1,n}. \tag{I2}$$

5. Insert Eqs. (G1), (G2) and (I1), (I2) back into Eqs. (D1), (D2)

$$O_{n+1,n}\delta_{i,n+1} = O_{in} - \sum_{j=1}^{n} O_{jn}\delta_{ij}, \tag{J1}$$

$$O^{\dagger}_{n+1,n}\delta_{i,n+1} = O^{\dagger}_{in} - \sum_{j=1}^{n} O^{\dagger}_{jn}\delta_{ij}. \tag{J2}$$

To prove that the matrix elements of $\mathbf{O}$ in the $\vec{\psi}$ basis and of $\mathbf{O}^{\dagger}$ in the dual of the $\vec{\psi}$ basis form tridiagonal matrices, consider Eqs. (J1), (J2) for matrix elements $(i,\ n)$,

(i) $i > n + 1$

$$0 = O_{in}, \tag{K1}$$

$$0 = O^{\dagger}_{in}. \tag{K2}$$

(ii) $i = n + 1$

$$O_{n+1,n} = O_{n+1,n}, \tag{L1}$$

$$O^{\dagger}_{n+1,n} = O^{\dagger}_{n+1,n}. \tag{L2}$$

(iii) $i = n$

$$0 = O_{nn} - O_{nn}, \tag{M1}$$

$$0 = O^{\dagger}_{nn} - O^{\dagger}_{nn}. \tag{M2}$$

(iv) $i = n - 1$

$$0 = O_{n-1,n} - O_{n-1,n} \tag{N1}$$

$$0 = O^{\dagger}_{n-1,n} - O^{\dagger}_{n-1,n}. \tag{N2}$$

(v) $i < n - 1$

$$\text{use general property: } O_{in} = O^{\dagger\,*}_{ni}\ \ (= 0 \text{ from Eq. (K2)}), \tag{O1}$$

$$\text{use general property: } O^{\dagger}_{in} = O^{*}_{ni}\ \ (= 0 \text{ from Eq. (K1)}). \tag{O2}$$

Eqs. (A1) and (A2) are then,

$$\vec{\psi}_{n+1} = \frac{1}{N_{n+1}}\left(\mathbf{O}\vec{\psi}_n - O_{nn}\vec{\psi}_n - O_{n-1,n}\vec{\psi}_{n-1}\right), \tag{P1}$$

$$\vec{\psi}^{\,n+1} = \frac{1}{N^{n+1}}\left(\mathbf{O}^{\dagger}\vec{\psi}^{\,n} - O^{\dagger}_{nn}\vec{\psi}^{\,n} - O^{\dagger}_{n-1,n}\vec{\psi}^{\,n-1}\right). \tag{P2}$$