Diagonalizing Large Matrices: the Lánczos method

- the Lánczos method converts an arbitrary matrix to tridiagonal form
- finding the eigenvalues of a tridiagonal matrix is easier than that of a normal matrix
- construction of the matrix proceeds iteratively

- assume H is the Hamiltonian matrix
  - select some vector $|\psi_0\rangle$ randomly
  - a precondition for finding the ground state is that $|\psi_0\rangle$ includes ~~ground~~ a component ~~which~~ of the ground state

$$|\psi_0\rangle = \sum_i |E_i\rangle\langle E_i|\psi_0\rangle$$

$\Downarrow$ most likely will be the case if $|\psi_0\rangle$ is chosen randomly

- then: $$|\psi_1\rangle = H|\psi_0\rangle - \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}|\psi_0\rangle$$

$$\langle\psi_0|\psi_1\rangle = \langle\psi_0|H|\psi_0\rangle - \langle\psi_0|H|\psi_0\rangle = 0$$

$\Rightarrow |\psi_0\rangle$ $|\psi_1\rangle$ are orthogonal

$$|\psi_2\rangle = H|\psi_1\rangle - \frac{\langle\psi_1|H|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle}|\psi_1\rangle - \frac{\langle\psi_1|\psi_1\rangle}{\langle\psi_0|\psi_0\rangle}|\psi_0\rangle$$

$$\langle\psi_1|\psi_2\rangle = \langle\psi_1|H|\psi_1\rangle - \langle\psi_1|H|\psi_1\rangle - \frac{\langle\psi_1|\psi_1\rangle}{\langle\psi_0|\psi_0\rangle}\langle\psi_1|\psi_0\rangle = 0$$

orthogonal

$$\langle\psi_0|\psi_2\rangle = \langle\psi_0|H|\psi_1\rangle - \frac{\langle\psi_1|H|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle}\langle\psi_0|\psi_1\rangle^{0} - \langle\psi_1|\psi_1\rangle$$

$$= \langle\psi_0|H^2|\psi_0\rangle - \frac{\langle\psi_0|H|\psi_0\rangle\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}$$

$$- \left[\langle\psi_0|H - \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}\langle\psi_0|\right]\left[H|\psi_0\rangle - \frac{\langle\psi_0|H|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}|\psi_0\rangle\right]$$

$$= \langle\psi_0|H^2|\psi_0\rangle - \left[\frac{\langle\psi_0|H|\psi_0\rangle^2}{\langle\psi_0|\psi_0\rangle}\right]^2$$

$$- \left[\langle\psi_0|H^2|\psi_0\rangle - 2\frac{\langle\psi_0|H|\psi_0\rangle^2}{\langle\psi_0|\psi_0\rangle} + \frac{\langle\psi_0|H|\psi_0\rangle^2}{\langle\psi_0|\psi_0\rangle}\right]$$

$$= 0$$

$\Rightarrow |\psi_0\rangle, |\psi_1\rangle, |\psi_2\rangle$ are orthogonal

in general: $|\psi_{i+1}\rangle = H|\psi_i\rangle - a_i|\psi_i\rangle - b_i^2|\psi_{i-1}\rangle$

$$a_i = \frac{\langle\psi_i|H|\psi_i\rangle}{\langle\psi_i|\psi_i\rangle} \qquad b_i^2 = \frac{\langle\psi_i|\psi_i\rangle}{\langle\psi_{i-1}|\psi_{i-1}\rangle}$$

in this basis one can show that the Hamiltonian becomes

$$\begin{pmatrix} a_0 & b_1 & 0 & 0 & \\ b_1 & a_1 & b_2 & 0 & \\ 0 & b_2 & a_2 & \ddots & \\ 0 & 0 & \ddots & & \end{pmatrix} \Rightarrow \text{tridiagonal}$$

- to diagonalize one can use packages
  (LAPACK, essl, etc.)

- diagonalizing tridiagonal matrices is significantly more efficient than general matrices, ~~and~~ computational time is saved, and larger matrices can be diagonalized

- example: consider power method to find ~~lowest~~ largest eigenvalue of a matrix $\bar{\bar{H}}$

- choose a random vector $|v\rangle$

$$|v\rangle = \sum_i |i\rangle\langle i|\vec{v}\rangle$$

- keep multiplying it by the matrix → multiply a large number of times

$$\bar{\bar{H}}^K |\vec{v}\rangle = \bar{\bar{H}}^K \sum_i |i\rangle\langle i|\vec{v}\rangle$$

if $|i\rangle$ is the eigenbasis of $\bar{\bar{H}}$ we have

$$\bar{\bar{H}}^K |\vec{v}\rangle = \sum_i H_i^K |i\rangle\langle i|\vec{v}\rangle$$

⇒ upon multiplying K times ⇒ $\bar{\bar{H}}^K|\vec{v}\rangle$ will be dominated by a contribution from the largest eigenvalue of $\bar{\bar{H}}$

$$\vec{M}^K |\vec{v}\rangle = \mu_N^K |N\rangle\langle N|\vec{v}\rangle$$

μ_N - largest eigenvalue

- One can also find the second largest eigenvalue by orthogonalizing at each multiplication to $|N\rangle$,

⇒ ~~choose random~~

⇒ after calculating μ_N and $|N\rangle$ choose another random vector $|\vec{v}'\rangle$

$$|\vec{v}'\rangle \rightarrow \underbrace{|\vec{v}'\rangle - |N\rangle\langle N|\vec{v}'\rangle}_{\text{orthogonalization}} = |\vec{v}'\rangle$$

$$\vec{M}^K |\vec{v}'\rangle = \mu_{N-1}^K |N-1\rangle\langle N-1|\vec{v}'\rangle$$

where μ_{N-1} is the second largest eigenvalue

- in this case, due to numerical error, it is advantageous to orthogonalize at every step
- one can also obtain second, third, etc. but it is progressively less stable
- inverting the matrix one can also obtain the lowest, second lowest, etc. eigenvalue

- consider multiplying by a regular matrix

$$\left(\vec{M}\right)|\vec{v}\rangle \Rightarrow v_i' = \sum_j M_{ij} v_j$$

if matrix has dimension $N \Rightarrow N^2$ operations

- if matrix is tridiagonal

$$\vec{M}_T |\vec{v}\rangle \Rightarrow v_i' = b_{i-1} v_{i-1} + a_{i-1} v_{i-1} + b_i v_i$$

$3N$ operations

for large N makes a big difference