
- Fast way for finding extremal eigenvalues of \(H\), \(N \times N\) matrix
- Input: algorithm for computing \(H(\psi)\) for any vector \(\psi\), \(N\)-component vector

We seek extremal value of \(E[\psi] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \tag{1}\)

Extremal value: \(E_0 = \min E[\psi]\), with \(E[\psi_0] = E_0\). \tag{2}

Functional gradient: \(\frac{\delta E[\psi]}{\delta \psi} = \frac{H(\psi) - E[\psi] \psi}{\langle \psi | \psi \rangle} \equiv 1 \psi_0 \tag{3}\)

gives direction of steepest ascent of functional from the point \(\psi\). Moving in opposite direction will thus have \(E[\psi - \alpha \psi_0] < E[\psi]\) for small, positive \(\alpha\). \tag{4}

To find optimal choice for \(\alpha\), minimize \(E[\psi - \alpha \psi_0]\) \(\text{w.r.t. the "variable parameter" } \alpha\)

in the space \(K_2 = \text{span } \{1\psi, 1\psi_0\} = \text{span } \{1\psi, H1\psi\} \tag{5}\)

First basis vector: \(1\psi_0 = \frac{1\psi}{\sqrt{\langle 1\psi | 1\psi \rangle}} \tag{6}\) \(1\psi\): random initial state

Second basis vector:
Orthogonalize: \(1\psi_1 = H(\psi_0) - 1\psi_0 \langle \psi_0 | H \psi_0 \rangle \tag{7}\)

Normalize: \(1\psi_1 = \frac{1\psi_1}{\sqrt{\langle 1\psi_1 | 1\psi_1 \rangle}} \tag{8}\)

Define \(a_0 \equiv \langle 1\psi_0 | H | 1\psi_0 \rangle\) and \(b_1 = \langle 1\psi_1 | 1\psi_0 \rangle\). \(\text{then} \tag{9}\)

\(H1\psi_0 = b_1 \psi_0 + a_0 1\psi_0 \tag{10}\)

hence \(b_1 = \langle 1\psi_1 | H | 1\psi_0 \rangle \tag{11}\)
In space $K_2$, $H$ has the representation

$$H_{K_2} = \begin{pmatrix} a_0 & b_1 \\ b_1 & a_2 \end{pmatrix}, \quad \text{with } a_2 = \langle v_1 | H | v_2 \rangle$$

Finding ground state of $H_{K_2}$, say $| \Psi_2 \rangle$, yields optimal choice of $\{ \Psi \}$

Now we could iterate: use $| \Psi_2 \rangle$ as starting point for another optimization step. Convergence is rapid.

Monitor quality of result by computing the residual

$$r[\Psi] = \left\| (H - E[\Psi] \psi) \right\|^2 = \langle \psi | H^2 | \psi \rangle - E[\Psi]^2,$$

and stopping when it dips below some threshold.

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**Krylov space**

After $L$ steps, starting from $|v_0\rangle$, resulting vector will lie in

$$K_L (|v_0\rangle) = \text{span} \{ |v_0\rangle, H |v_0\rangle, H^2 |v_0\rangle, \ldots, H^L |v_0\rangle \}$$

$$= \text{"Krylov space of } H \text{ on } |v_0\rangle\text{" (dimension } L+1)$$

Instead of repeatedly minimizing in $2 \times 2$ subspaces, we could first construct $K_L$, then compute its ground state. (This is faster, since it avoids having $L$ simultaneous variational parameters instead of $L$ separate ones.) To do this, iteratively construct a "Krylov basis" for $K_L$.
Krylov basis:

At step $k$: \( b_k \ket{v_i} = \ket{v_{i+1}} = H \ket{v_i} - a_n \ket{v_n} \) (normalization)

Third vector: \( b_3 \ket{v_2} = \ket{v_3} = H \ket{v_2} - \frac{1}{\alpha_i} \sum_{i=0}^{2} \beta_i \ket{v_i} \)

where \( \alpha_i = \bra{v_i} H \ket{v_n} \), \( \beta_i = \bra{v_i} v_i \ket{v_n} = \bra{v_i} H \ket{v_{n-1}} \)

Note that \( \bra{v_2} H \ket{v_0} = 0 \), since \( H \ket{v_0} \in \text{span} \{ \ket{v_0}, \ket{v_1} \} \)

Fourth vector: \( b_4 \ket{v_3} = \ket{v_4} = H \ket{v_3} - \frac{2}{\alpha_2} \sum_{i=0}^{2} \beta_i \ket{v_i} \bra{v_i} H \ket{v_2} \)

where \( \alpha_i = \bra{v_i} H \ket{v_n} \), \( \beta_i = \bra{v_i} v_i \ket{v_n} = \bra{v_i} H \ket{v_{n-1}} \)

Note: there is no contribution from \( \ket{v_2} \), due to (5) !

\[ \Rightarrow \] Two-term recursion scheme! Need to store only 3 vectors at a time!

\[
\begin{align*}
    b_{n+1} \ket{v_{n+1}} &= \ket{v_{n+1}} = H \ket{v_n} - \sum_{i=0}^{n-1} \beta_i \ket{v_i} \bra{v_i} H \ket{v_n} \\
    &= H \ket{v_n} - a_n \ket{v_n} - b_n \ket{v_{n-1}}
\end{align*}
\]

If \( b_{n+1} = 0 \), pick an arbitrary \( \ket{v_{n+1}} \) orthogonal to all \( \{ \ket{v_0} \to \ket{v_n} \} \).

Always: \( \bra{v_{n+1}} H \ket{v_i} = 0 \) \( \forall i = 0, \ldots, n-1 \)

Since \( H \ket{v_i} \in \text{span} \{ \ket{v_0}, \ket{v_1}, \ldots, \ket{v_{n-1}} \} \)

Rearranging: \( H \ket{v_n} = b_n \ket{v_{n-1}} + a_n \ket{v_n} + b_{n+1} \ket{v_{n+1}} \)

Hence, in \( K_n \), \( H \) has

\[
H_{K_n} = \begin{bmatrix}
    a_0 & b_1 & 0 & \cdots & 0 \\
    b_1 & a_1 & b_2 & \cdots & 0 \\
    0 & b_2 & a_2 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & \cdots & a_{L-1} & b_L \\
    0 & 0 & 0 & \cdots & b_L & a_L
\end{bmatrix}
\]
Ground state of $H_{kk'}$: \( \psi^\text{g}_{k} (\psi^\text{g}_{k'})^j = \lambda^j_k \psi^\text{g}_{k} \) \( \text{[estimates in } K_{L} \text{ for } E_{g}. \) \( \text{[can be constructed on the fly, one term at a time, by restarting the Lanczos iteration from } \psi_0 \text{]}

Then \( \psi^\text{g}_{k} \) = \( \sum_{j=0}^{\infty} (\psi^\text{g}_{k})_j \psi^\text{g}_{j} \) is estimate in \( K_{L} \) for \( \psi_{g} \).

Convergence is exponential, with a rate \( \sim \left[ \text{gap to first excited state} \right]^{-1/2} \).

**Summary**:

1. Start with arbitrary \( \psi_{0} \)

2. Abbreviated initial iteration step:
   
   (i) \( |\tilde{\psi}_0\rangle = H |\psi_0\rangle \)

   (ii) \( a_0 = \langle \tilde{\psi}_0 | \psi_0 \rangle \)

   (iii) \( |\tilde{\psi}_0\rangle = |\tilde{\psi}_0\rangle - a_0 |\psi_0\rangle \)

3. General iteration step, for \( n \geq 1 \):

   (i) \( b_n = \sqrt{\langle \tilde{\psi}_n | \tilde{\psi}_{n+1} \rangle} \)

   (ii) \( a_{n+1} \) s.t. \( |\tilde{\psi}_{n+1}\rangle = b_n |\tilde{\psi}_{n+1}\rangle \)

   The post \( |\tilde{\psi}_{n+1}\rangle \) as arbitrary vector with \( \langle \tilde{\psi}_{n+1} | \psi_{n+1} \rangle \), that is orthogonal to all \( |\tilde{\psi}_0\rangle, \ldots, |\tilde{\psi}_{n}\rangle \).

   (iii) \( |\tilde{\psi}_{n+1}\rangle = H |\tilde{\psi}_{n+1}\rangle \)

   (iv) \( a_{n+1} = \langle \tilde{\psi}_{n+1} | \psi_{n+1} \rangle \)

   (v) \( |\tilde{\psi}_{n+1}\rangle = |\tilde{\psi}_{n+1}\rangle - a_{n+1} |\psi_{n+1}\rangle - b_n |\psi_{n}\rangle \)

   and back to 3 (i).

There are other ways of organizing this iteration loop, but this one shown here is numerically the most stable [Paige 1972].
3. DMRG: Excited states

Suppose we have MPS ground state: \( |\Gamma\rangle = \prod \gamma_i \langle \tilde{\sigma} | \) (i)

We can now construct excited states, if desired, by repeating a DMRG sweep in the space orthogonal to \(|\Gamma\rangle\).

Extremize: \( \langle \psi|H|\psi\rangle = \lambda_1 \langle \psi|H|\psi\rangle - \lambda_2 \langle \psi|\tilde{\sigma}^z|\psi\rangle \) (ii)

Lagrangian multipliers ensure \( \langle \psi|\psi\rangle = 1 \), \( \langle \psi|\tilde{\sigma}^z|\psi\rangle = 0 \) (iii)

\[ \sum_{M} \left[ \begin{array}{c} \psi_{1} \\ \vdots \\ \psi_{M} \end{array} \right] = \lambda_1 \left[ \begin{array}{c} \psi_{1} \\ \vdots \\ \psi_{M} \end{array} \right] - \lambda_2 \left[ \begin{array}{c} \psi_{1} \\ \vdots \\ \psi_{M} \end{array} \right] \]

\[ \lambda_1 \left[ \begin{array}{c} \psi_{1} \\ \vdots \\ \psi_{M} \end{array} \right] - \lambda_2 \left[ \begin{array}{c} \psi_{1} \\ \vdots \\ \psi_{M} \end{array} \right] = 0 \] (iv)

\[ G = \psi_{1} \psi_{M} \] (v)

\[ G^\mu = \psi_{1} \psi_{M} = \sum_{m_{1},\ldots,m_{k}} \langle m_{1} \ldots m_{k} | \alpha_{e_{1}} \ldots \alpha_{e_{k}} \rangle \delta_{e_{1} \cdots e_{k}} \langle m_{1} \ldots m_{k} | \alpha_{e_{1}} \ldots \alpha_{e_{k}} \rangle \] (vi)

\[ G^\mu = G_{m_{1},e_{1},\ldots,e_{k},m_{k}} \] (vii)

\[ G^\mu = (m_{1},e_{1},\ldots,e_{k},m_{k}) \] (viii)

\[ L R = m_{1,6} a_{e_{1}} a_{e_{6}} \]

\[ R L = m_{1,6} a_{e_{1}} a_{e_{6}} \] (ix)

\[ L^{(e-1)} = L^{(e)} \]

\[ R^{(e)} = R^{(e+1)} \] (x)
So, we have to solve:

\[ H_{\mu}\lambda_{\mu} = \lambda, \quad N_{\mu}\lambda_{\mu} + 2l_{\mu} \lambda_{\mu}, \quad M^{x}_{\mu} \lambda_{\mu} = 0 \]  

in mixed-canonical basis

Bracket notation for coefficients, \( (M) \leftrightarrow M_{\mu} \), \( (l) \leftrightarrow l_{\mu} \).

and matrix elements, \( \hat{H} \leftrightarrow H_{\mu}\lambda_{\mu} \).

in mixed-canonical basis for site \( k \):

\[ \hat{H}(M) = \lambda, \quad I_{\mu} + \lambda_{\mu} l_{\mu} \]  

Define projector onto subspace orthogonal to \( 1g \):

\[ \hat{P}_{g} = 1 - 1g \langle 1g \rangle \]

\[ \hat{P}_{g} \hat{H}(\hat{P}_{g}^{} + l_{\mu} \langle 1g \rangle I_{\mu})M = \lambda, \quad \hat{P}_{g} IM + \hat{P}_{g} 1g = 0 \]

\[ \hat{P}_{g} \hat{H} \hat{P}_{g} IM = \lambda, \quad \hat{P}_{g} IM \]

This is simply an eigenvalue problem in orthogonal subspace of \( 1g \), with Hamiltonian \( \hat{P}_{g} \hat{H} \).

Can be solved using straightforward extension of Lanczos:

During Lanczos iteration, construct orthogonal Krylov subspace:

1. \( |v_{0}\rangle = \) random initial state \( \rightarrow |v_{0}\rangle = \hat{P}_{g} |v_{0}\rangle \)

2. \( |v_{n+1}\rangle = \hat{P}_{g} H |v_{n}\rangle - a_{n} |v_{n}\rangle - b_{n} |v_{n-1}\rangle \)

etc. Here \( |l_{\mu}\rangle \) always refers to the representation of \( l_{\mu} \) in the local basis of the site that is being optimized.
Why not simply use excited states in $K_e$?

Because numerical noise can cause the $|v_n\rangle$ to be not exactly orthogonal, hence for $i\neq n-2$,
$$<v_n|v_i\rangle \approx 10^{-16} \text{ rather than 0.}$$

This leads to spawning multiple copies of eigenvectors ("ghost states"). For ground state, variational principle ensures that the loss of orthogonality does not become a severe problem. But for excited states, it is.

To prevent this, explicit reorthogonalization is needed at each step, as indicated above.

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**Block-Lanczos for $M$ lowest eigenstates**

**Standard Lanczos:** unit action of $H$ as:

$$H|v_0\rangle = a_0|v_0\rangle + b_1|v_1\rangle \quad \Rightarrow \quad \begin{pmatrix} a_0 & b_1 \\ b_1 & a_1 & b_2 \\ b_2 & b_3 & \ddots \end{pmatrix}$$

**Block-Lanczos:** start with set of $M$ orthogonal vectors, $|v_0^{(i)}\rangle, i = 1, \ldots, M$

and unit action of $H$ as:

$$H|v_0^{(i)}\rangle = a_i^{(i)}|v_0^{(i)}\rangle + b_i^{(i)}|v_1^{(i)}\rangle \quad \text{with} \quad <v_0^{(i)}|v_1^{(i)}\rangle = 0, \quad <v_i^{(i)}|v_0^{(j)}\rangle = \delta_{ij}.$$
4. Two-site update

If one encodes symmetries (will be discussed in a later lecture),
then "one-site update" (discussed above) can get stuck:
if you start in wrong symmetry sector, you stay there, because
one-site update offers no way of enlarging (Hilbert space during
varational search) to explore other symmetry sectors. Cure:

Two-site update:

\[ \frac{\partial}{\partial \eta(x)} \frac{\partial}{\partial \eta(y)} \begin{pmatrix} \lambda_1 & \lambda_2 \\ \lambda_3 & \lambda_4 \end{pmatrix} \]

Represent \(|\psi\rangle\) in mixed canonical two-site basis:

\[ |\psi\rangle = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 | \sigma \rangle \langle \sigma | \qquad (1) \]

\[ \langle \mu | \psi \rangle = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \qquad (2) \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]

\[ = \sum_{\sigma, \sigma_0, \sigma_1, \sigma_2} \langle \sigma_0 \sigma_1 | \sigma \rangle \langle \sigma_0 \sigma_1 | \sigma \rangle \sum_{\sigma_0, \sigma_1, \sigma_2} A^\sigma_0 A^\sigma_1 \langle \mu | \sigma \rangle \langle \mu | \sigma \rangle \]
They find lowest eigenvector of

\[ \langle \mu | \varphi | \mu \rangle = \lambda | \varphi \rangle \]

Updated ground state:

\[ | \varphi \rangle = \sum \mathcal{A} \mathcal{A}^{-1} M \mathcal{A}^{-1} \mathcal{A} \mathcal{A}^{-1} M \mathcal{A}^{-1} \]

Key point: \( S \) is \( Dd \times Dd \), explores larger state space (more quantum numbers).

Truncate basis update:

\[ | \varphi \rangle = \sum \mathcal{A} \mathcal{A}^{-1} M \mathcal{A}^{-1} \mathcal{A} \mathcal{A}^{-1} M \mathcal{A}^{-1} \]

Optimize in next iteration.