Lanczos Method

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1 Limitations of Full Hamiltonian Construction

For small spin systems, we can explicitly construct the Hamiltonian matrix of the Transverse Field Ising Model (TFIM) using Kronecker (tensor) products of the Pauli matrices:

$$H = -J \sum_{i=1}^{N-1} \sigma_x^{(i)} \sigma_x^{(i+1)} - h \sum_{i=1}^{N} \sigma_z^{(i)}.$$

For a system of N spins, the Hilbert space dimension is 2^N,
so the Hamiltonian is a $2^N \times 2^N$ matrix.

- For $N = 8$: matrix size $= 256 \times 256$ (manageable)
- For $N = 12$: matrix size $= 4096 \times 4096$ (large but still possible)
- For $N = 20$: matrix size $= 1,048,576 \times 1,048,576$ (impossible to diagonalize)

This exponential growth makes **exact diagonalization** computationally prohibitive for large systems.

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2 What Do We Really Need?

In most physical situations, we don't need the *entire spectrum* of eigenvalues and eigenvectors.
We're usually interested in just: - The **ground state energy** - Maybe the **first few low-lying excited states**

So rather than diagonalizing the full matrix, we can try to find the **lowest eigenvalues** efficiently.

3 The Power Method Intuition

Before understanding the Lanczos algorithm, it is helpful to start with a simpler idea — the Power Method. It shows how repeated action of a matrix (or Hamiltonian) can amplify one particular eigenstate.

Let an arbitrary normalized state be written as a superposition of the eigenstates of H:

$$|\psi_0\rangle = \sum_n c_n |E_n\rangle, \tag{1}$$

where

$$H|E_n\rangle = E_n|E_n\rangle, \quad E_0 \leq E_1 \leq E_2 \leq \cdots \tag{2}$$

Now apply H repeatedly on $|\psi_0\rangle$:

$$H^k|\psi_0\rangle = \sum_n c_n E_n^k |E_n\rangle. \tag{3}$$

If the eigenvalues are positive and ordered such that $|E_0| < |E_1| < \cdots$, then after many applications, the component corresponding to the largest $|E_n|$ dominates, because E_n^k grows fastest for that term:

$$\lim_{k\to\infty} \frac{H^k|\psi_0\rangle}{|H^k|\psi_0\rangle|} \to |E_{\max}\rangle. \tag{4}$$

Hence, repeated action of H naturally projects the state onto the eigenvector associated with the largest eigenvalue.

3.1 To find Ground States

In most physical systems, we are actually interested in the ground state, which corresponds to the smallest eigenvalue, not the largest.

To use the power method in this case, we shift the Hamiltonian by a constant λ:

$$H' = \lambda I - H. \tag{5}$$

Now, the largest eigenvalue of H' corresponds to the lowest eigenvalue of H. By applying the power method (or, more efficiently, the Lanczos method) to H', we make the ground state dominate the evolution.

In practice, λ is chosen such that all eigenvalues of H' are positive.

3.2 From Power Method to Krylov Subspace

The Krylov subspace used in the Lanczos algorithm is the space spanned by repeated applications of H on an initial trial state:

$$\mathcal{K}_m(H, |\psi_0\rangle) = \text{span}|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, \ldots, H^{m-1}|\psi_0\rangle. \tag{6}$$

The Power Method gives the basic intuition: by acting repeatedly with H, we enhance the contribution of the dominant eigenstate. The Lanczos algorithm refines this idea by: Orthogonalizing the successive vectors (using a three-term recurrence relation), and representing H in this orthonormal Krylov basis, where it becomes a tridiagonal matrix.

3.2.1 Construction of Orthonormal Krylov Space

Start with a trial state, say $|\psi_0\rangle$.

Example:

- 1st basis state

$$|\phi_0\rangle = \frac{|\psi_0\rangle}{\tilde{N}_0}, \quad \tilde{N}_0 = \langle\psi_0|\psi_0\rangle \tag{7}$$

- 2nd basis state

$$|\phi_1\rangle = \frac{H|\phi_0\rangle - h_{00}|\phi_0\rangle}{\tilde{N}_1} \tag{8}$$

- and so on

$$\vdots \tag{9}$$

- n^{th} basis state

$$|\phi_{n+1}\rangle = \frac{H|\phi_n\rangle - h_{nn}|\phi_n\rangle - h_{n-1,n}|\phi_{n-1}\rangle}{\tilde{N}_{n+1}} \tag{10}$$

- In all cases above : $h_{ij} = \langle\phi_i|H|\phi_j\rangle$

3.2.2 Tridiagonal Representation of the Hamiltonian

In this orthonormal Krylov basis, the Hamiltonian takes a tridiagonal form:

$$T = \begin{pmatrix} h_{00} & h_{01} & 0 & \cdots & \\ h_{10} & h_{11} & h_{12} & 0 & \cdots \\ 0 & h_{21} & h_{22} & h_{23} & \cdots \\ \vdots & \ddots & \ddots & \ddots & \end{pmatrix}.$$

Diagonalizing this small tridiagonal matrix yields very accurate approximations to the lowest eigenvalues of the full Hamiltonian — allowing us to extract the ground state energy efficiently, even for very large systems.

3.2.3 Extracting the Ground State Energy

Finally, we diagonalize this small tridiagonal matrix T:

$$Tv = \tilde{E}v.$$

- The lowest eigenvalue $\tilde{E}_0$ gives an excellent approximation to the **ground state energy** of the full Hamiltonian.

- The corresponding eigenvector v_0 gives the coefficients to reconstruct the approximate **ground state wavefunction** in the original space.

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4 Summary

Step	Concept	Description
1	Build Krylov subspace	Apply H repeatedly on a random state
2	Orthonormalize	Use the Lanczos recurrence relation
3	Tridiagonalize	Represent H as a small $m \times m$ matrix
4	Diagonalize	Extract low-energy eigenvalues

This approach — the **Lanczos method** — allows us to find ground state energies for systems where full diagonalization is completely infeasible.

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