Mathematics 15: The Lanczos Algorithm

The states of a spin-half may be represented in terms of a basis of two states: Either down or up, which can be represented by 0 or 1. A state of a system composed of many spins may then be represented by a sequence of bits, which can be constituted into a number which labels a particular state.

The Hamiltonians are represented for this basis in 'Maths12', but since the number of states scales like 2^N with N the number of spins, a matrix involves 2^{2N} elements which soon becomes larger than the maximum number of numbers permitted in the computer, of order $1,000,000 \sim 2^{20}$, and so naively we can deal with only 10 spins. Dealing with this problem effectively is equivalent to squeezing the calculation into a 'small space' on the computer.

The Lanczos algorithm allows us to partially diagonalise a matrix using only a couple of vectors and the ability to *apply* the matrix by multiplication only. This then allows us to reach a system size of about 20 spins. Extracting any additional symmetries can push this number up to about 24 (extracting S^z_{total}) or 26 (also extracting translational invariance) or 32 (also extracting S_{total}).

Lanczos involves the construction of a new basis by sequential applications of the Hamiltonian combined with Gram-Schmidt orthogonalisation. An initial state, $\mid \psi >$ say, is selected. The selection of this state *can* cause problems (see on). The next state is constructed by applying H to the previous state and then orthonormalising with *all* previous states:

$$\mid n+1 > H_{n+1,n} = H \mid n > - \sum_{m=1}^{n} \mid m > H_{m,n}$$

where $H_{m,n}$ are chosen to ensure that $< m \mid n+1 >= 0$ for $m \leq n$ and $H_{n+1,n}$ is chosen to ensure that $< n+1 \mid n+1 >= 1$. The orthogonalisation enforces:

$$H_{m,n} =< m \mid H \mid n >$$

and the normalisation enforces:

$$\mid H_{n+1,n} \mid^2 = \parallel H \mid n > - \sum_{m=1}^{n} \mid m > H_{m,n} \parallel^2$$

If H is *hermitian*, then $H_{m,n}$ is *tri-diagonal*. It is this result that makes the theory so useful for the computer.

$$H \mid n >= \sum_{m=1}^{n+1} \mid m > H_{m,n}$$

by construction, and so:

$$H_{m,n} =< m \mid H \mid n >= 0 \qquad m > n+1$$

which leads to:

$$H_{m,n} =< m \mid H \mid n >=< n \mid H^\dagger \mid m >^* =< n \mid H \mid m >^* = 0 \quad n > m+1 \quad m < n-1$$

so:

$$H \mid n>=\mid n+1> H_{n+1,n}+ \mid n> H_{n,n}+ \mid n-1> H_{n-1,n}$$

is tri-diagonal.

To use this result on the computer, we require *two* 'vectors' (of components) and the ability to *apply* the Hamiltonian, ie to construct its matrix elements on demand. We start out at 'square one':

Vector 1	Vector 2
$-\mid n-1> H_{n-1,n}$	$\mid n>$

and then we apply the Hamiltonian to the second vector, adding the result to the first, yielding:

Vector 1	Vector 2
$-\mid n-1> H_{n-1,n}+H \mid n>$	$\mid n>$

we then determine the Hamiltonian matrix elements in the new basis by overlapping:

$$H_{n,n} =< n \mid \left[-H_{n-1,n} \mid n-1> +H \mid n>\right]$$

$$\mid H_{n+1,n} \mid^2 = \parallel \left[-H_{n-1,n} \mid n-1> +H \mid n>\right] - H_{n,n} \mid n> \parallel^2$$

and we may *choose* $H_{n+1,n}$ to be real and positive. Given $x_n \equiv H_{n,n}$ and $y_n \equiv \mid H_{n+1,n} \mid$, then:

Vector 1	Vector 2
$-y_n \mid n>$	$\mid n+1>= \frac{1}{y_n}\left(\left[-H_{n-1,n} \mid n-1> +H \mid n>\right] - x_n \mid n>\right)$

and we are back at 'square one', advanced by one.

In the new basis, $\{\mid n>\}$, the Hamiltonian matrix is $H_{m,n}$ which can be diagonalised easily for small systems. If we find an eigenvalue and eigenvector:

$$\sum_m H_{n,m} v_m = \epsilon v_n$$

then:

$$\mid \psi >= \sum_n v_m \mid m>$$

is an eigenstate of H, since:

$$H \mid \psi >= \sum_m v_m H \mid m >= \sum_m \sum_n \mid n> H_{n,m} v_m = \sum_n \mid n> v_n \epsilon = \epsilon \mid \psi >$$

and a *second* run through the calculation allows us to create $\mid \psi >$ in a third 'vector' using the v_n and the sequentially constructed $\mid n>$.

Why is this new basis useful? The calculation is equivalent to performing a *variational* calculation on the finite space generated by:

$$\{\mid 1>, H \mid 1>, H^2 \mid 1>, ..., H^n \mid 1>\}$$

at the n'th step. Now if the exact eigenstates of the system are $\mid \tilde{n} >$ with energies ϵ_n then:

$$\mid \psi >=\mid 1 >= \sum_m \mid \tilde{m} >< \tilde{m} \mid \psi >$$

and:

$$\left[\frac{H-\Lambda}{\epsilon_0-\Lambda}\right]^n \mid \psi >= \sum_m \mid \tilde{m} >< \tilde{m} \mid \psi > \left[\frac{\epsilon_m-\Lambda}{\epsilon_0-\Lambda}\right]^n$$

and if:

$$abs\left[\frac{\epsilon_m-\Lambda}{\epsilon_0-\Lambda}\right] < 1$$

for $m > 0$ then as $n \mapsto \infty$

$$\left[\frac{H-\Lambda}{\epsilon_0-\Lambda}\right]^n \mid \psi > \mapsto \mid \tilde{0} >< \tilde{0} \mid \psi >$$

exponentially and is in our subspace. We can find $\mid \tilde{0} >$ with exponential accuracy, provided that:

$$abs\left[\frac{\epsilon_m-\Lambda}{\epsilon_0-\Lambda}\right] < 1$$

Now if ϵ_{max} exists, choose $\Lambda > \epsilon_{max}$ and then $\Lambda - \epsilon_m < \Lambda - \epsilon_0$ and $\epsilon_0 < \epsilon_m$ so unless ϵ_0 is *degenerate* we have exponential convergence, *unless* $< \tilde{0} \mid \psi >= 0$.

We will find the ground-state of our system *exponentially unless* $< \tilde{0} \mid \psi >= 0$.

In fact, the technique provides a sequence of low energy eigenstates which have an overlap with $\mid \psi >$