Title: Summer Undergrad 2020 - Numerical Methods (A) - Lecture 4

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Collection: Summer Undergrad 2020 - Numerical Methods

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Abstract: Exact diagonalization part 2: Continue with finding matrices for N-site Ising model, solve for eigenvalues and eigenstates of model

12:49 PM Wed Jun 3

Note Jun 3, 2020 (2)
Jun 3, 2020 at 12:48 PM

Ising model N sites (cont.)

$$H = -\sum_i \underbrace{\sigma_i^z \sigma_{i+1}^z} - g \cdot \sum_i \sigma_i^x$$

$$Id_0 \otimes Id_1 \otimes \dots \otimes \sigma_i^z \otimes \sigma_{i+1}^z \otimes Id \otimes \dots$$

1 / 2

12:50 PM Wed Jun 3

Ising model N sites (cont.)

$$H = -\sum_i \sigma_i^z \sigma_{i+1}^z - g \cdot \sum_i \sigma_i^x$$

$$Id_0 \otimes Id_1 \otimes \cdots \otimes \sigma_i^z \otimes \sigma_{i+1}^z \otimes Id \otimes \cdots \otimes Id$$

To construct H, we separately construct

ZZ term: $\sum_i \sigma_i^z \sigma_{i+1}^z$

X term: $\sum_i \sigma_i^x$

separately b/c don't need to redo for every "g"

1 / 2

separately b/c don't need to redo for every "g"

Last time:

ZZ term w/ Method 1: Kronecker product

$Id \otimes \sigma_z \otimes \sigma_z \quad (N=3)$

$$(Id \otimes \sigma_z) = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \otimes$$

12:52 PM Wed Jun 3

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ZZ term w/ Method 1: Kronecker product

$Id \otimes \sigma_z \otimes \sigma_z \qquad (N=3)$

$$\left[(Id \otimes \sigma_z) = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \right] \otimes \sigma^z$$

$$\begin{pmatrix} 1 & & & & & & & \\ & -1 & & & & & & \\ & & -1 & & & & & \\ & & & 1 & & & & \\ & & & & 1 & & & \\ & & & & & -1 & & \\ & & & & & & -1 & \\ & & & & & & & 1 \end{pmatrix}$$

Same for $\sigma_z \otimes \sigma_z \otimes Id$,
add them ... .

1 / 3

12:53 PM Wed Jun 3

Method 2: Column-by-column

1st col of matrix is op applied to 1st basis state

$\boxed{\text{step 1}}$ convert basis vector

$$\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \begin{matrix} \\ \\ \\ \leftarrow i \\ \\ \\ \\ \end{matrix}$$

to a list of

2 / 3

12:54 PM Wed Jun 3

$|i\rangle$ basis state

$\boxed{\text{step 1}}$ convert basis vector

$$\begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow i$$

to a list of spins

last time:

$$[\, i // 2^{N-1}, (i // 2^{N-2}) \% 2,$$

$//$: divide & toss remainder

$\%$: mod

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2 / 3

12:54 PM Wed Jun 3

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \leftarrow i$$

to a list of spins

last time:

$$[\, i // 2^{N-1},\ (i // 2^{N-2}) \% 2,\ \ldots,\ i \% 2 \,]$$

divide & toss remainder

mod

eg $[\,0,\ 1,\ 1,\ 0,\ \ldots,\ 0\,]$

$|\uparrow\rangle \quad |\downarrow\rangle \quad |\downarrow\rangle \quad |\uparrow\rangle \quad \ldots \quad |\uparrow\rangle$

12:56 PM Wed Jun 3

$$|\uparrow\rangle\otimes|\downarrow\rangle\otimes|\downarrow\rangle\otimes|\uparrow\rangle\otimes\cdots\otimes|\uparrow\rangle$$

② Apply operator to this basis state

A concrete example (not from Ising model)

$$\mathcal{O} = \mathrm{Id}\otimes\sigma^x\otimes\sigma^z + \sigma^x\otimes\sigma^z\otimes\mathrm{Id}$$

2 / 4

12:57 PM Wed Jun 3

$$\mathcal{O} = Id \otimes \sigma^x \otimes \sigma^z + \sigma^x \otimes \sigma^z \otimes Id$$

basis $|\uparrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle, |\uparrow\downarrow\uparrow\rangle, \ldots, |\downarrow\downarrow\downarrow\rangle$

8 total

matrix: 8×8

col 0 : $i = 0$

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \xrightarrow[\text{step 1}]{} [0, 0, 0]$$

$$\downarrow$$

$$|\uparrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle$$

apply $\mathcal{O}$:

3 / 4

1:00 PM Wed Jun 3

$|\uparrow\rangle \otimes |\uparrow\rangle$

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apply θ: $Id \otimes \sigma^x \otimes \sigma^z |\uparrow\uparrow\uparrow\rangle = |\uparrow\downarrow\uparrow\rangle$

$\sigma^x \otimes \sigma^z \otimes Id\, |\uparrow\uparrow\uparrow\rangle = |\downarrow\uparrow\uparrow\rangle$

$$[0,0,0] \longrightarrow \big((1, [0,1,0]), (1, [1,0,0]) \big)$$

call

$$\theta\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \underset{\text{step1}}{=} \theta\,[0,0,1] = \theta(|\uparrow\uparrow\downarrow\rangle)$$

step 3

3 / 4

1:02 PM Wed Jun 3

$$= \sigma\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \underset{\text{step1}}{=} \sigma[0,0,1] = \sigma(|\uparrow\uparrow\downarrow\rangle)$$

step3 $Id \otimes \sigma^x \otimes \sigma^z |\uparrow\uparrow\downarrow\rangle$

$$= -|\uparrow\downarrow\downarrow\rangle$$

$$(\sigma^x \otimes \sigma^z \otimes Id)|\uparrow\uparrow\downarrow\rangle = |\downarrow\uparrow\downarrow\rangle$$

$$[0,0,1] \longrightarrow \big((-1,[0,1,1]),(1,[1,0,1])\big)$$

step3: convert back to vector repres.

3 / 5

1:04 PM Wed Jun 3

step3: convert back to vector representation.

$$\begin{array}{cccc} & [\,0, & 1, & 0\,] \\ & \uparrow & \uparrow & \uparrow \\ \cdots & 2^2 & 2 & 1 \end{array} = 0\cdot 2^2 + 1\cdot 2 + 0 = 2$$

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

apply step 3 to example:

col 0: $\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \rightarrow$

3 / 5

apply step 3 to example:

col 0:

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \to [0,0,0] \to (1,[0,1,0]),\ (1,[1,0,0])$$

$$\downarrow$$

$$1 \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} + 1 \cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

col 1:

$$\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \to [0,0,1] \to$$

1:06 PM Wed Jun 3

$$1\cdot\begin{pmatrix}0\\0\\1\\0\\0\\0\\0\\0\end{pmatrix} + 1\cdot\begin{pmatrix}0\\0\\0\\0\\1\\0\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\\1\\0\\0\\0\end{pmatrix}$$

$$\underline{\text{col } 1}: \begin{pmatrix}0\\1\\0\\0\\0\\0\\0\\0\end{pmatrix} \to [0,0,1] \to (-1,[0,1,1]),\ (1,[1,0,1])$$

$$\Big\downarrow \text{(step 3)}$$

$$-1\cdot\begin{pmatrix}0\\0\\0\\1\\0\\0\\0\\0\end{pmatrix} + 1\cdot\begin{pmatrix}0\\0\\0\\0\\0\\1\\0\\0\end{pmatrix} = \begin{pmatrix}0\\0\\0\\-1\\0\\1\\0\\0\end{pmatrix}$$

1:12 PM Wed Jun 3

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ZZ coeff

$$\mathrm{Id} \otimes \mathrm{Id} \cdots \otimes \sigma_i^z \otimes \sigma_{i+1}^z \otimes \mathrm{Id} \cdots \otimes \mathrm{Id}$$

$$|s_0 \; s_1 \; \cdots \; s_i \; s_{i+1} \; \cdots \; s_{N-1}\rangle$$

$$|s_0\rangle \otimes |s_1\rangle \otimes \cdots \otimes \underbrace{\sigma^z |s_i\rangle \otimes \sigma^z |s_{i+1}\rangle} \otimes \cdots \otimes |s_{N-1}\rangle$$

$+1 \; \uparrow \qquad +1 \; \uparrow$

$-1 \; \downarrow \qquad -1 \; \downarrow$

4 / 6

1:13 PM Wed Jun 3

$$|s_0\rangle \otimes |s_1\rangle \otimes \dots \otimes \underbrace{\sigma^z |s_i\rangle \otimes \sigma^z |s_{i+1}\rangle} \otimes \dots \otimes |s_{N-1}\rangle$$

$+1$ ↑ $\quad$ $+1$ ↑

-1 ↓ $\quad$ -1 ↓

<u>overall</u> $\quad +1$ if ↑↑, ↓↓

$\qquad\qquad -1$ if ↑↓, ↓↑

we represented

$|\uparrow\rangle \to 0 \qquad 0,0$ or $1,1 \Rightarrow 1$

$|\downarrow\rangle \to 1 \qquad 0,1$ or $1,0 \Rightarrow -1$

$b[j] \quad b[j+1]$

$(-1)^{b[j]+b}$

5 / 6

1:14 PM Wed Jun 3

We represented

$$|\uparrow\rangle \to 0 \qquad 0,0 \text{ or } 1,1 \Rightarrow 1$$

$$|\downarrow\rangle \to 1 \qquad 0,1 \text{ or } 1,0 \Rightarrow -1$$

$b[j]$ $\quad$ $b[j+1]$

$(-1)^{b[j]+b[j+1]}$ works

Method 3:

5 / 6

1:14 PM Wed Jun 3

Method 3: Use some knowledge specific to the operator.

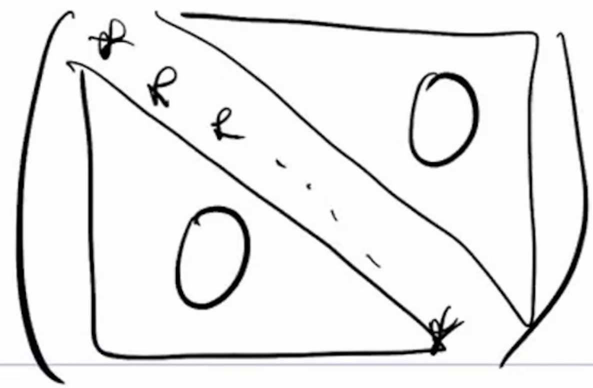
In particular, we know

$$\sum_i \sigma_i^z \sigma_{i+1}^z \text{ is } \underline{\underline{\text{diagonal}}}$$

5 / 7

1:15 PM Wed Jun 3

$\sum_i \sigma_i^z \sigma_{i+1}^z$ is diagonal



But the diagonal elts are just the expectation value of

$$\left\langle \sum_i \sigma_i^z \sigma_{i+1}^z \right\rangle \text{ in}$$

5 / 7

But the diagonal elts are just the expectation value of

$$\left\langle \sum_i \sigma_i^z \sigma_{i+1}^z \right\rangle$$ in each basis state

<u>eg</u> $|\uparrow\uparrow\downarrow\rangle$

$$\langle \sigma_0^z \otimes \sigma_1^z \otimes Id + Id \otimes \sigma_1^z \otimes \sigma_2^z \rangle$$

1:17 PM Wed Jun 3

$\langle \sum_i \sigma_i \sigma_{i+1} \rangle$ in each basis state

eg $|\uparrow\uparrow\downarrow\rangle$

$$\langle \sigma_0^z \otimes \sigma_1^z \otimes Id + Id \otimes \sigma_1^z \otimes \sigma_2^z \rangle$$

$$\underbrace{\langle \sigma_0^z \otimes \sigma^z \otimes Id \rangle}_{(-1)^{\text{spin } 0 + \text{spin } 1}} + \underbrace{\langle Id \otimes \sigma^z \otimes \sigma^z \rangle}_{(-1)^{\text{spin } 1 + \text{spin } 2}}$$

in general $[0, 0, 1, 0, \ldots 1]$

$$\langle \sum_i \sigma^z \sigma^z \rangle \text{ is } \sum_i (-1)^{\text{spin } i + \text{spin } i+1}$$

6 / 7

1:20 PM Wed Jun 3

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in general $[0, 0, 1, 0, \ldots 1]$

$\langle \sum_i \sigma^z \sigma^z \rangle$ is $\sum_i (-1)^{\text{spin } i + \text{spin } i+1}$

step1 convert col index to list of spins

step2 calculate and put it on the diagonal

6 / 7

1:21 PM Wed Jun 3

$\langle \sum_i \sigma^z \sigma^z \rangle$ is $\sum_i (-1)$

step1 convert col index to list of spins

step2 calculate and put it on the diagonal

For 1 spin, the change of basis is given by $\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2} \equiv H$

For N spins, it is $\underbrace{\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}/\sqrt{2} \otimes H \otimes \cdots \otimes H}$

6 / 7