Color Network Document

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目录

由于对本领域并不熟悉，本文档会夹杂中文。

第一章　Basic Topics

1.0.1　NRG and DMRG

Here we will introduce numerical renormalization group and density matrix renormalization group using an example to solve an equation of a single particle.

We will consider solving such an equation in range $x \in [-1, 1]$.

$$\begin{aligned} &\frac{\partial^2}{\partial x^2} f(x) = a f(x), \\ &f(-1) = f(1) = 0, \end{aligned} \tag{1.1}$$

with

$$\frac{\partial^2}{\partial x^2} f(x) \approx \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{\Delta x^2}, \tag{1.2}$$

the discretized version is an eigen-problem

$$\frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & 0 & -1 & 2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix} f = af, \tag{1.3}$$

It can be written as

$$\frac{1}{\Delta x^2} \begin{pmatrix} H_0 & L_0 & 0 & 0 & \dots & 0 & 0 \\ L_0 & H_0 & L_0 & 0 & \dots & 0 & 0 \\ 0 & L_0 & H_0 & L_0 & \dots & 0 & 0 \\ 0 & 0 & L_0 & H_0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_0 & L_0 \\ 0 & 0 & 0 & 0 & \dots & L_0 & H_0 \end{pmatrix} f \approx \frac{1}{\Delta x^2} \begin{pmatrix} H_0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & H_0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & H_0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & H_0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & H_0 \end{pmatrix} = af, \tag{1.4}$$

with

$$H_0 = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}, \quad L_0 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{1.5}$$

The first step is to solve eigen system of H, the two lowest eigen values and eigen vectors are

$$H_0 \begin{pmatrix} \frac{1}{5+\sqrt{5}} & -\frac{1}{5-\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} & \frac{1}{5-\sqrt{5}} \end{pmatrix} = \begin{pmatrix} \dfrac{3-\sqrt{5}}{2} \times \begin{matrix} \frac{1}{5+\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} \end{matrix} & \dfrac{5-\sqrt{5}}{2} \times \begin{matrix} -\frac{1}{5-\sqrt{5}} \\ -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{5-\sqrt{5}} \end{matrix} \end{pmatrix} \tag{1.6}$$

Then, truncate use

$$\begin{aligned} U &= \begin{pmatrix} \frac{1}{5+\sqrt{5}} & -\frac{1}{5-\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} & \frac{1}{5-\sqrt{5}} \end{pmatrix} \\ H' = U^T H_0 U &= \begin{pmatrix} \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \quad L' = U^T L_0 U = \begin{pmatrix} -\frac{1}{(5+\sqrt{5})^2} & -\frac{1}{20} \\ \frac{1}{20} & \frac{1}{(5-\sqrt{5})^2} \end{pmatrix}. \end{aligned} \tag{1.7}$$

Now, we are dealing with a truncated problem

$$\frac{1}{\Delta x^2} \begin{pmatrix} H_1 & L_1 & 0 & 0 & \dots & 0 & 0 \\ L_1 & H_1 & L_1 & 0 & \dots & 0 & 0 \\ 0 & L_1 & H_1 & L_1 & \dots & 0 & 0 \\ 0 & 0 & L_1 & H_1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_1 & L_1 \\ 0 & 0 & 0 & 0 & \dots & L_1 & H_1 \end{pmatrix} f = af, \tag{1.8}$$

with

$$\begin{aligned} H_1 &= \begin{pmatrix} H' & L' \\ L' & H' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 & -\frac{1}{\left(\sqrt{5}+5\right)^2} & \frac{1}{20} \\ 0 & \frac{1}{2} & -\frac{1}{20} & \frac{1}{\left(5-\sqrt{5}\right)^2} \\ -\frac{1}{\left(\sqrt{5}+5\right)^2} & -\frac{1}{20} & \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 \\ \frac{1}{20} & \frac{1}{\left(5-\sqrt{5}\right)^2} & 0 & \frac{1}{2} \end{pmatrix}, \\ L_1 &= \begin{pmatrix} 0 & L' \\ 0 & 0 \end{pmatrix} \end{aligned} \tag{1.9}$$

Again, we solve $H_1 f = af$, the lowest two eigenvalues are 0.067 and 0.026. As a compare, the lowest two eigenvalues of a 16×16 original matrix are 0.135 and 0.034.

第二章　Decompose Methods

2.1　Matrix Decompose

2.1.1　Matrix SVD using Lanczos

The matrix SVD is to decompose

$$t_{i_1,i_2,\ldots,i_m,j_1,j_2,\ldots,j_n} = \sum_{k_l,k_r} V_{i_1,i_2,\ldots,i_m,k_l} S_{k_l,k_r} U_{k_r,j_1,j_2,\ldots,j_n}, \tag{2.1}$$

where

$$\begin{aligned}
&\sum_{k_l} V^*_{I_1,I_2,\ldots,I_m,k_l} V_{i_1,i_2,\ldots,i_m,k_l} = \delta_{(i_m)=(I_m)}, \\
&\sum_{k_r} U^*_{J_1,J_2,\ldots,J_n,k_r} U_{j_1,j_2,\ldots,j_m,k_l} = \delta_{(J_n)=(j_n)}, \\
&S_{k_l \neq k_r} = 0,
\end{aligned} \tag{2.2}$$

One can imagine that, $\{i_n\}$ is ONE combined index of a matrix. Then, it is the normal SVD. Usually, $dim(k)$ is small.

2.1.1.1　Lanczos bidiagonalization

Lanczos bidiagonalization is for such task:

For $A = C^{m\times n}$, find $A \approx UBV^\dagger$ such that B is a bidiagonal matrix

$$B = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 & 0 \\ 0 & \alpha_2 & \beta_2 & 0 & 0 \\ & \ldots & & & \\ 0 & 0 & 0 & \alpha_{k-1} & \beta_{k-1} \\ 0 & 0 & 0 & 0 & \alpha_k \end{pmatrix} \tag{2.3}$$

Note here $||v|| = \sqrt{\sum_i |v_i|^2}$.

Algorithm 1 Lanczos bidiagonalization

$A = C^{m\times n}$

$\mathbf{v}_1$ is an n-vectors satisfying $||\mathbf{v}_1|| = 1$.

for $i = 1$ to k **do**

  if $i > 1$ **then**

    $\mathbf{v}_i = \mathbf{p}/\beta_{i-1}$.

  end if

  $\mathbf{r} = A\mathbf{v}_i - \beta_{i-1}\mathbf{u}_{i-1}$. ▷ $\beta_0 = 0$ and $\mathbf{u}_0 = 0$.

  $\alpha_i = ||\mathbf{r}||$.

  $\mathbf{u}_i = \mathbf{r}/\alpha_i$.

  if $i < k$ **then**

    $\mathbf{p} = A^\dagger\mathbf{u}_i - \alpha_i\mathbf{v}_i$

    $\beta_i = ||\mathbf{p}||$

  end if

end for

It is expected that β approaches zero, if $\beta = 0$, than $A = UTV^\dagger$.

Although the B obtained is not a diagonal matrix, the goal has been archived, and we do not further diagonalize it.