Color Network Document

Ji-Chong Yang

目录

由于对本领域并不熟悉，本文档会夹杂中文。

0.1 Basic Topics

0.1.1 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 $x \in [-1, 1]$.

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

with

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

the discretized version is an eigen-problem

$$\frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 & 0 \\ 0 & -1 & 2 & -1 & \dots & 0 & 0 \\ 0 & 0 & -1 & 2 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 2 & -1 \\ 0 & 0 & 0 & 0 & \dots & -1 & 2 \end{pmatrix} f = a f, \tag{3}$$

It can be written as

$$\frac{1}{\Delta x^2} \begin{pmatrix} H_0 & L_0 & 0 & 0 & \dots & 0 & 0 \\ L_0 & H_0 & L_0 & 0 & \dots & 0 & 0 \\ 0 & L_0 & H_0 & L_0 & \dots & 0 & 0 \\ 0 & 0 & L_0 & H_0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_0 & L_0 \\ 0 & 0 & 0 & 0 & \dots & L_0 & H_0 \end{pmatrix} f \approx \frac{1}{\Delta x^2} \begin{pmatrix} H_0 & 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & H_0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & H_0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & H_0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & H_0 \end{pmatrix} = a f, \tag{4}$$

with

$$H_0 = \begin{pmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{pmatrix}, \quad L_0 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{5}$$

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

$$H_0 \begin{pmatrix} \frac{1}{5+\sqrt{5}} & -\frac{1}{5-\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} & \frac{1}{5-\sqrt{5}} \end{pmatrix} = \left(\frac{3-\sqrt{5}}{2} \times \begin{matrix} \frac{1}{5+\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} \end{matrix} \quad \frac{5-\sqrt{5}}{2} \times \begin{matrix} -\frac{1}{5-\sqrt{5}} \\ -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} \\ \frac{1}{5-\sqrt{5}} \end{matrix} \right) \tag{6}$$

Then, truncate use

$$\begin{gathered} U = \begin{pmatrix} \frac{1}{5+\sqrt{5}} & -\frac{1}{5-\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \\ \frac{1}{5+\sqrt{5}} & \frac{1}{5-\sqrt{5}} \end{pmatrix} \\ H' = U^T H_0 U = \begin{pmatrix} \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \quad L' = U^T L_0 U = \begin{pmatrix} -\frac{1}{(5+\sqrt{5})^2} & -\frac{1}{20} \\ \frac{1}{20} & \frac{1}{(5-\sqrt{5})^2} \end{pmatrix}. \end{gathered} \tag{7}$$

Now, we are dealing with a truncated problem

$$\frac{1}{\Delta x^2} \begin{pmatrix} H_1 & L_1 & 0 & 0 & \dots & 0 & 0 \\ L_1 & H_1 & L_1 & 0 & \dots & 0 & 0 \\ 0 & L_1 & H_1 & L_1 & \dots & 0 & 0 \\ 0 & 0 & L_1 & H_1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & H_1 & L_1 \\ 0 & 0 & 0 & 0 & \dots & L_1 & H_1 \end{pmatrix} f = af, \tag{8}$$

with

$$\begin{gathered} H_1 = \begin{pmatrix} H' & L' \\ L' & H' \end{pmatrix} = \begin{pmatrix} \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 & -\frac{1}{\left(\sqrt{5}+5\right)^2} & \frac{1}{20} \\ 0 & \frac{1}{2} & -\frac{1}{20} & \frac{1}{\left(5-\sqrt{5}\right)^2} \\ -\frac{1}{\left(\sqrt{5}+5\right)^2} & -\frac{1}{20} & \frac{1}{2} - \frac{1}{\sqrt{5}} & 0 \\ \frac{1}{20} & \frac{1}{\left(5-\sqrt{5}\right)^2} & 0 & \frac{1}{2} \end{pmatrix}, \\ L_1 = \begin{pmatrix} 0 & L' \\ 0 & 0 \end{pmatrix} \end{gathered} \tag{9}$$

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.