HW 2 Infinite Potential Well

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$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\,\psi(x)$$

The above equation is the Shrodinger equation. The potential $V = 0$ in the area of interest for the infinite potential well problem. Thus, we could earn exact energy eigenvalues and eigenfunctions analytically which are ...

$$Analytic\ solution:\ \psi_n(x) = \sqrt{\frac{2}{L}}\,sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

We also get the eigenvalues and eigenvectors numerically. The main problem is to handle with second derivatives. We simply use the N by N matrix with ...$\frac{d^2\psi}{dx^2} \simeq \frac{\psi_{i+1}-2\psi_i+\psi_{i-1}}{\Delta x^2}$.

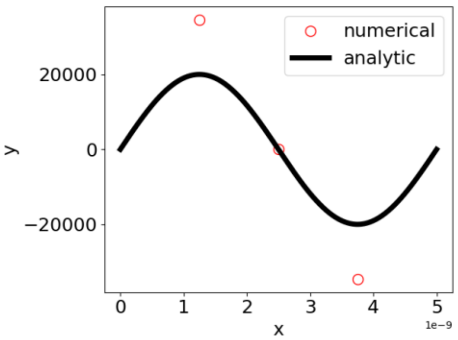
For example if N =3, the numerical shrodinger equation is,

$$Numerical\ representation:\ D\psi = -k^2\psi, \qquad D = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$$

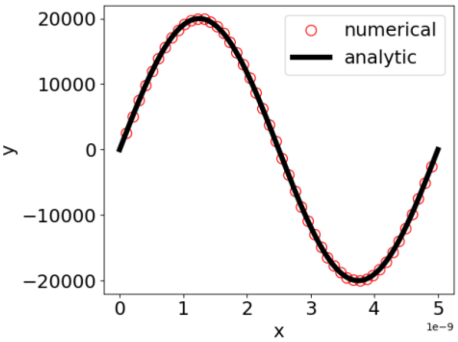
Now the matrix D can make result of energy eigenvalue & eigenvector.

Result 1. Energy eigenvector of $\psi_2(x)$ by N = 5, 50, 500.

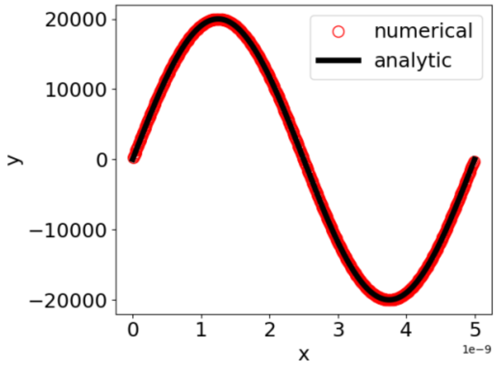
1. N = 5



2. N = 50



3. N = 500



We can see that more N steps makes more accurate result.

Result 2. Energy eigenvalues with N = 5, 50, 500.

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N =  5
Numerical energy =  8.586217948077285e-21
Analytic energy =  1.0592821806131993e-20
N =  50
Numerical energy =  1.0578315395314484e-20
Analytic energy =  1.0592821806131993e-20
N =  500
Numerical energy =  1.0592681851667348e-20
Analytic energy =  1.0592821806131993e-20
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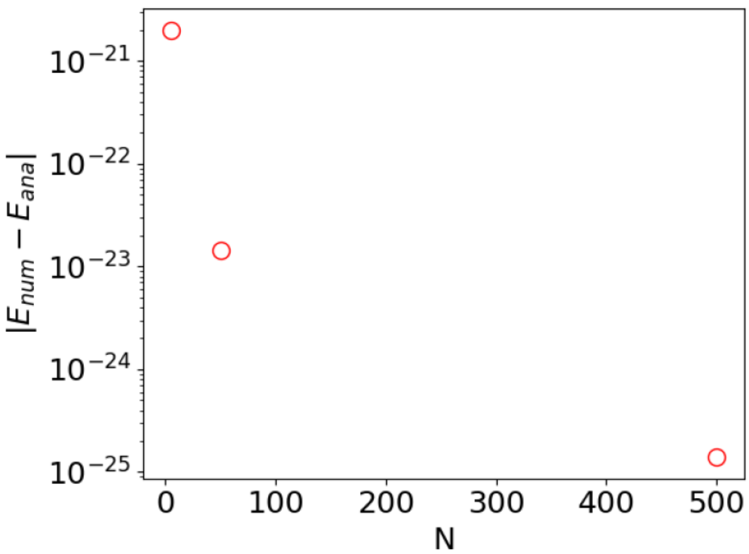
We plot the absolute difference of numerical result and analytical result.



We also found that more N steps makes more accurate result of Energy eigenvalues.