Project: Diagonalization of symmetric tridiagonal matrix (quantum harmonic oscillator problem)

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1 Introduction

In quantum mechanics the energy operator (Hamiltonian) in differential form ($V(\vec{r})$ is interaction potential) is commonly used

$$\widehat{H}(\vec{r}) = -\frac{1}{2}\nabla^2_{\vec{r}} + V(\vec{r}) \tag{1}$$

This operator may act on any function but some of them are special because fullfill the eigenequation of operator

$$\widehat{H}\psi_k = \varepsilon_k \psi_k \tag{2}$$

ψ_k is k-th wave function with eigenenergy ε_k. Our aim is to solve the eigenproblem given in Eq.2 numerically (in most cases it is the only way to find any solution) with finite difference method in one dimension with parabolic confining potential $V(x)$ (quantum harmonic oscillator)

$$\widehat{H}(x) = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2}, \qquad x \in (-\infty, \infty) \tag{3}$$

First, let's limit the range of the computational box $x \in [-x_{max}, x_{max}]$, $x_{max} < \infty$, second, define the number (n) and positions of nodes ($x_i, \quad i = 0, 1, 2, \ldots, n-1$) at which the wave function's values will be determined as well as the distance between neighbouring nodes (Δ)

$$\Delta = \frac{2\, x_{max}}{n-1} \tag{4}$$

$$x \to x_i = -x_{max} + \Delta \cdot i, \quad i = 0, 1, 2, \ldots, n-1 \tag{5}$$

$$\psi^{(k)}(x) \to \psi^{(k)}(x_i) \to \psi^{(k)}_i, \qquad \text{(upper index enumerates the states)} \tag{6}$$

third, replace the second derivative with symmetric three-point finite difference formula

$$\frac{d^2\psi^{(k)}_i}{dx^2} \approx \frac{\psi^{(k)}_{i+1} - 2\psi^{(k)}_i + \psi^{(k)}_{i-1}}{\Delta^2} \qquad \left(+O(\Delta^2)\right) \tag{7}$$

in consequence we get the discretized (algebraic) version of the Hamiltonian (3)

$$\widehat{H}\psi^{(k)} \quad \to \quad H_d\psi^{(k)}_i = -\frac{1}{2}\frac{\psi^{(k)}_{i+1} - 2\psi^{(k)}_i + \psi^{(k)}_{i-1}}{\Delta^2} + \frac{x_i^2}{2}\psi^{(k)}_i \tag{8}$$

In above equation we see that only three neighbouring nodes are explicitly connected, but rewriting it for every i-th node we simply define this eigenproblem in matrix form

$$H_d\vec{\psi}^{(k)} = \varepsilon_k \vec{\psi}^{(k)} \tag{9}$$

for tridiagonal matrix $H_d = [h_{i,j}]$ with non-zero entries defined only for diagonal and sub-(super)diagonal as follows

$$h_{i,i} = \frac{1}{\Delta^2} + \frac{x_i^2}{2} \tag{10}$$

$$h_{i,\pm 1} = -\frac{1}{2\Delta^2} \tag{11}$$

1.1 Analitycal solution

Eigenproblem of harmonic oscillator Hamiltonian has an exact solution, the wave functions are Hermite polynomials ($\mathcal{H}_k$) scaled with Gauss function while the eigenvalues are equally spaced rational numbers

$$\psi^{(k)}(x) = \mathcal{H}_k(x) e^{-\frac{x^2}{2}}, \quad x \in (-\infty, \infty) \tag{12}$$

$$\{\varepsilon_k\} = \left\{ \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \dots \right\} \tag{13}$$

$$\mathcal{H}_0 = 1 \tag{14}$$

$$\mathcal{H}_1 = 2x \tag{15}$$

$$\mathcal{H}_2 = 4x^2 - 2 \tag{16}$$

$$\mathcal{H}_3 = 8x^3 - 12x \tag{17}$$

$$\vdots \tag{18}$$

Three subsequent Hermite polynomials are linked with reccurence formula

$$\mathcal{H}_k(x) = 2x\mathcal{H}_{k-1}(x) - 2(k-1)\mathcal{H}_{k-2}(x), \qquad k = 1, 2, 3, \dots \tag{19}$$

$$\mathcal{H}_{-1}(x) = 0 \quad \& \quad H_0(x) = 1 \quad \leftarrow \text{ starting values} \tag{20}$$

which enables one to recursively calculate value of any polynomial for given point x without the knowledge of its explicit form. We utilize equations (12),(13), (19) and (20) to get the exact solutions with which the numerical solutions would be compared.

2 Practical part

Tasks to do

1. Assume calculation parameters: $n = 100$, $x_{max} = 10$ and determine Δ according to equation (4)
2. Compute diagonal (Eq.10) and subdiagonal (Eq.11) Hamiltonian matrix elements and write them to 1d arrays. Pass these arrays (and other required arguments) to LapackE routine designated for diagonalization of symmetric tridiagonal matrix LAPACKE_dstev(...). Save the computed eigenvalues to file. Normalize the eigenvectors ($\vec{\psi}^{(k)}$) as follows

$$C_k = \int_{-\infty}^{\infty} |\psi^{(k)}(x)|^2 dx \qquad \Longrightarrow \qquad C_k = \sum_{i=0}^{n-1} \left|\psi_i^{(k)}\right|^2 \Delta = \left(\vec{\psi}^{(k)}\right)^T \vec{\psi}^{(k)} \Delta \tag{21}$$

$$\vec{\psi}^{(k)} \leftarrow \frac{\vec{\psi}^{(k)}}{\sqrt{C_k}} \tag{22}$$

   and save them to the file.

3. Calculate the exact eigenvectors using recurrence formulae (19) and (20) at nodes x_i. Normalize these vectors according to (21) and (22), then save them to file.

4. Make a figure showing the energy spectra of eigenvalues obtained from diagonalization and the exact ones (13).

5. At home prepare the report. Besides the energy spectra make separate figures for the following eigenvectors (compare exact and numerical solutions): $\psi^{(1)}$,$\psi^{(2)}$,$\psi^{(3)}$, $\psi^{(15)}$, $\psi^{(20)}$, $\psi^{(30)}$. Repeat calculations for $n = 1000$, make new figures of energy spectra and wave functions. Try to answear to questions:

   - Are the numerical eigenvalues the same as exact ones or not? Which ones are well reproduced? What could be a reason/reasons of observed discrepances. Hint: remind (i) how we approximate the second derivate, and, (ii) how we limit the spatial space (computational box) for numerical solutions.
   - Which eigenvectors obtained from diagonalization are well reconstructed and which are not?
   - Compare generally the results of diagonalization for $n = 100$ and $n = 1000$, which are better and why?

3 Computational hints

In project the diagonalization process of symmetric tridiagonal matrix is conductced by LapackE routine

```
lapack_int LAPACKE_dstev (int matrix_layout, char jobz, lapack_int n,
                          double* d, double* e, double* z, lapack_int LDZ);
```

Arrays d and e keep the diagonal and sub-(super)diagonal elements of Hamiltonian matrix. In array z the routine returns the eigenvectors which are kept in columns (of hypothetical 2D array), depending on the value of **matrix_layout** elements can be encoded in two ways

- **matrix_layout=LAPACK_COL_MAJOR** - whole eigenvectors are placed one after another in z. We get the elements of $\vec{\psi}_i^{(k)}$ (i-node index, k-index of eigenvector) as follows

$$\vec{\psi}_i^{(k)} \leftarrow z[i + k \cdot LDZ], \quad i = 0, 1, 2, \ldots, n-1 \tag{23}$$

- **matrix_layout=LAPACK_ROW_MAJOR** - subsequent elements of array z keep the entries of different eigenvectors, hence n-element-long jumps in array z are required. We get the elements of $\vec{\psi}_i^{(k)}$ as follows

$$\vec{\psi}_i^{(k)} \leftarrow z[i \cdot LDZ + k], \quad i = 0, 1, 2, \ldots, n-1 \tag{24}$$

Evaluation of k-th Hermite plynomial's value at point x can be conducted with following pseudocode encapsulated within the body of separate function

```
initialization: x,k,   a=0, b=1, c=1,    h=0 (returned value)
for i=1 to k by 1 do
    !reccurence formula
        c = 2xb − 2(i − 1)a
```

```
    !save last two values for next iteration
        a=b
        b=c
enddo
!construct solution multiplying c by the Gauss function
        h = c · e^{-x^2/2}
```

This pseudocode is valid for all $k = 0, 1, 2, \ldots$ indices (for $k = 0$ only Gauss function value is returned).

4 Example results

Practical remark: to compare the wave funcations obtained from diagonalization with the exact ones sometimes multiplication of the wave function by a global phase factor $e^{i\pi} = -1$ is needed. It doesn't change the dynamics as well as the solution

$$H\vec{\psi}_k = \varepsilon_k \vec{\psi}_k \quad \Longrightarrow \quad H\left(-\vec{\psi}_k\right) = \varepsilon_k \left(-\vec{\psi}_k\right) \tag{25}$$

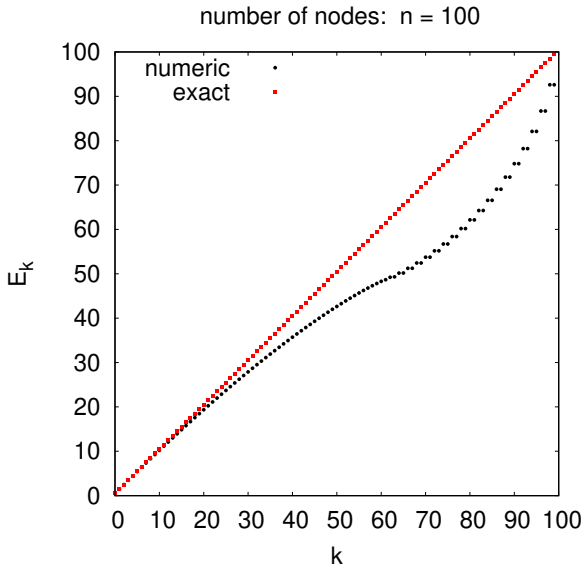

Figure 1: Comparison of exact eigenenergies (red dots) with eigenenergies obtained from diagonalization (black dots) for parameters $x_{max} = 10$ and $n = 100$.

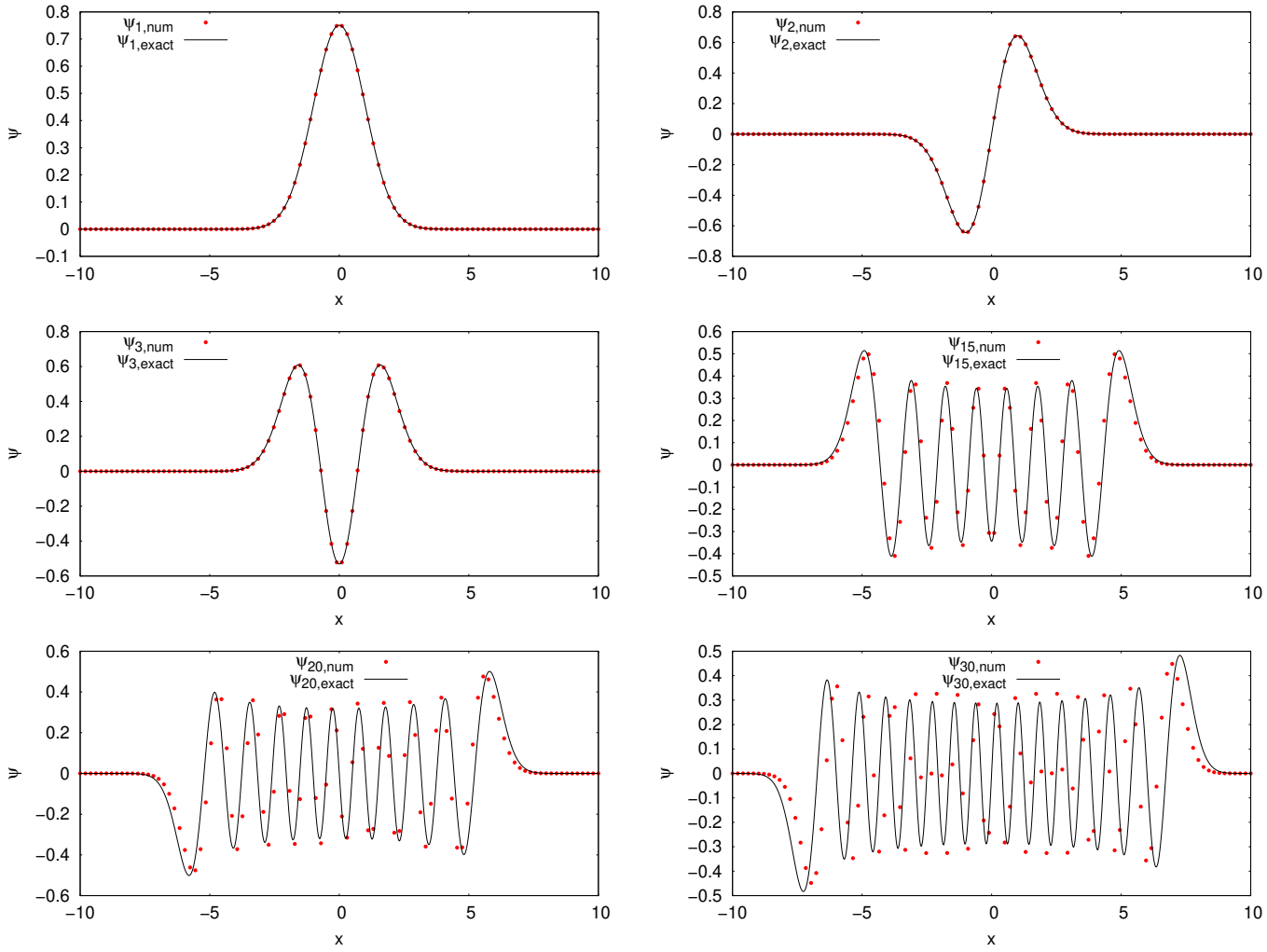

Figure 2: Example wave functions obtained from diagonalization (red points) and analytical solutions (black curve) of harmonic oscillator Hamiltonian for parameters $x_{max} = 10$ and $n = 10$. Indices of states are marked in legends.