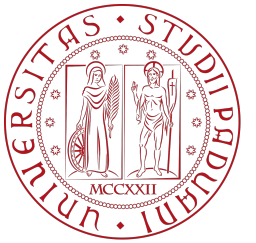

Assignment 4

Continuous-time independent Schrödinger Equation

Quantum Information and Computing

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Eigenproblem

1D Harmonic Oscillator

$$\left[\frac{1}{2}\left(-\nabla_x^2 + \omega^2 x^2\right)\right] |\Psi_k(x_i)\rangle = E_k |\Psi_k(x_i)\rangle$$

Numerical approximation:

- Space discretisation: $dx = \dfrac{b-a}{N}$
- Define potential operator $\hat{V} = \dfrac{\omega x_i^2}{2}$ in matrix form
- Define Kinetic operator $\hat{K} = -\dfrac{1}{2}\hat{\nabla}^2$ via **FINITE DIFFERENCE METHOD**

Second order

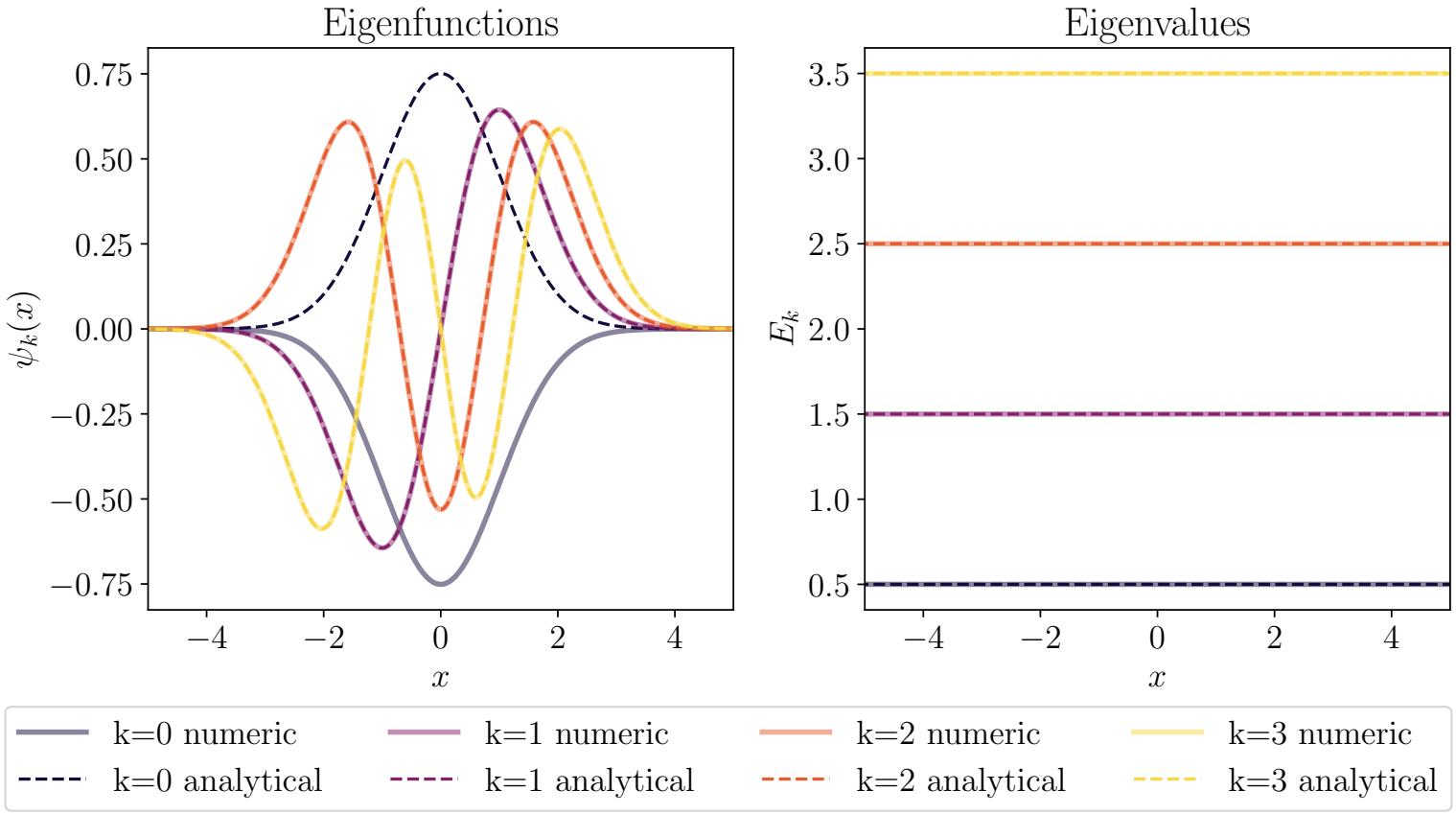
$$\hat{K} = \frac{1}{2dx^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2 \end{pmatrix}$$

Fourth order

$$\hat{K} = \frac{1}{2dx^2}\begin{pmatrix} \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & 0 & \cdots \\ -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \frac{1}{12} & \cdots \\ \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & -\frac{4}{3} & \cdots \\ 0 & \frac{1}{12} & -\frac{4}{3} & \frac{5}{2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Correctness

- Compute **numerically** eigenvalues and eigenvectors by diagonalising $\hat{H} = \hat{K} + \hat{V}$, with: `scipy.sparse.linalg.eigsh`
- Compute analytically eigenvalues and eigenvectors via canonical formulas



From the comparison, numerical and analytical methods are almost perfectly overlapped

Stability and discretisation

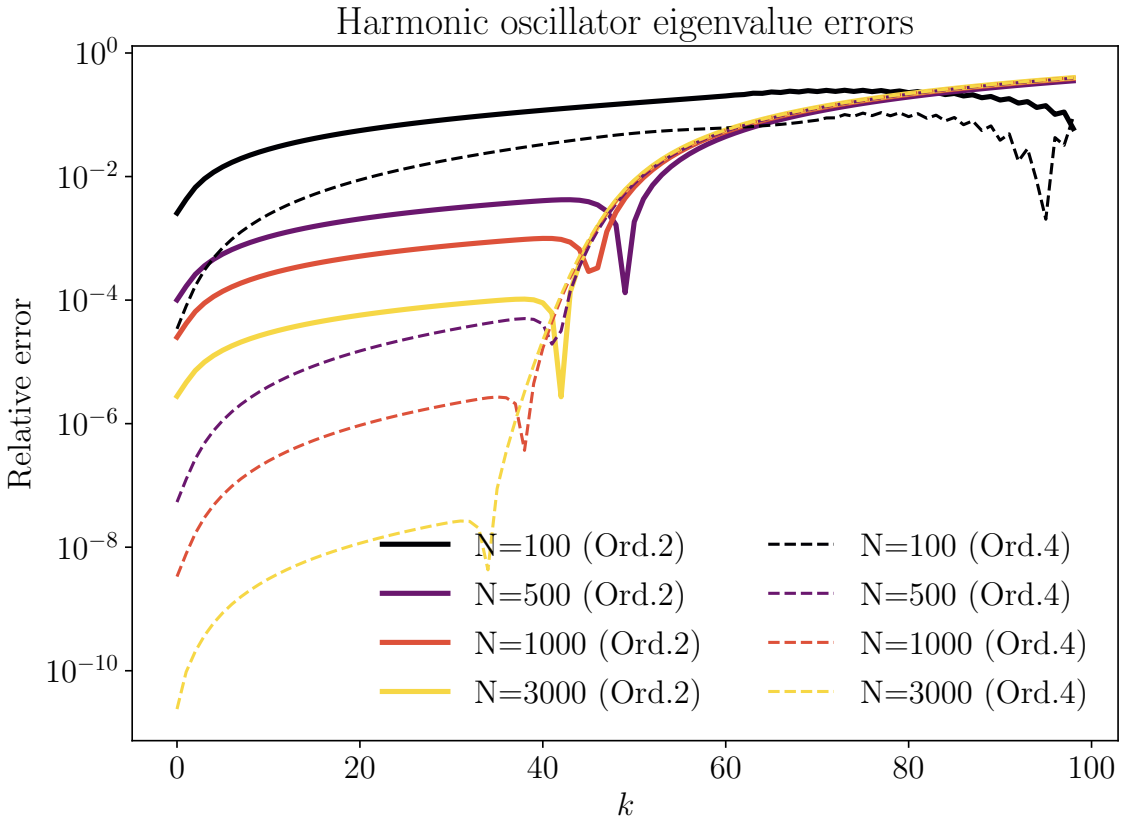
Eigenvalues

Eigenvalues relative error:

$$\epsilon_\lambda = \frac{|\lambda_n - \lambda_a|}{\lambda_a}$$

- Increase k: error increases
- Increase N: error decreases
- Order 4 approximation is better than order 2

Computing eigenvalues beyond the effective grid resolution limit becomes unreliable, as the relative error drastically increases, often approaching $100\,\%\,(10^0)$**.**



Stability and discretisation

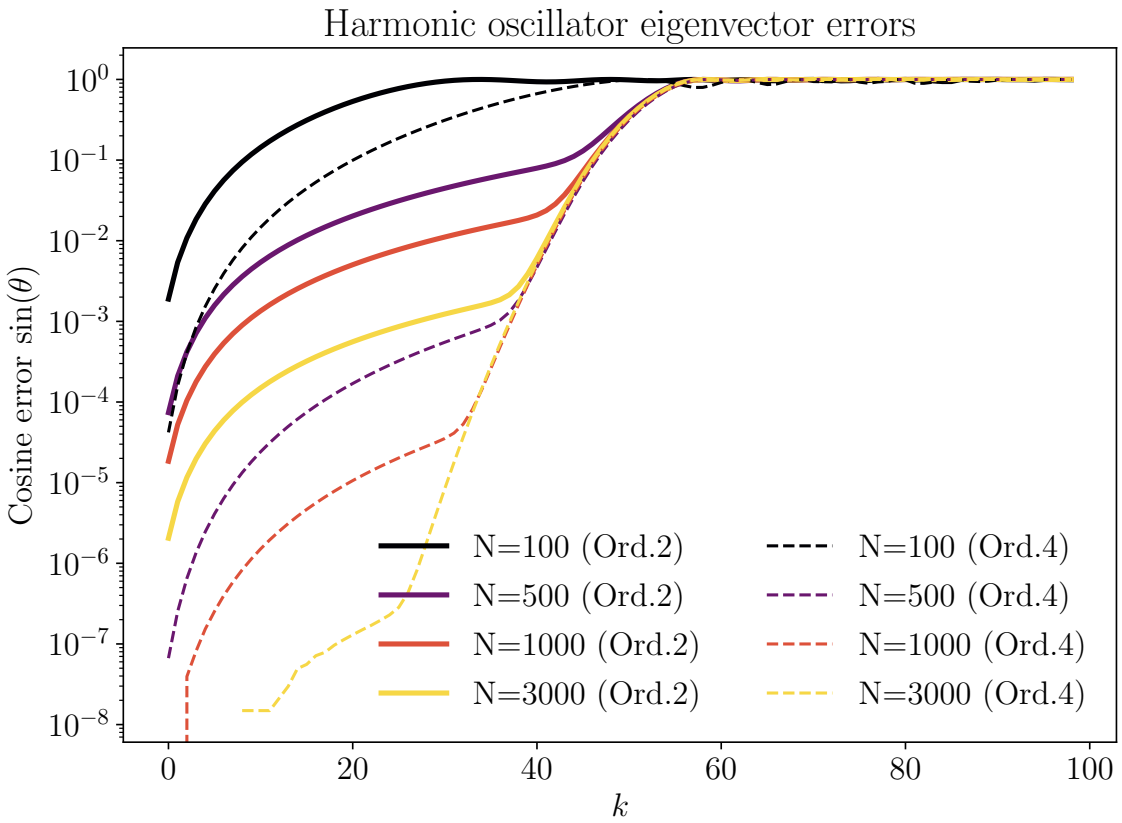
Eigenvectors

Cosine error:

$$d = \sin\theta = \sqrt{1 - \left(\frac{v \cdot w}{||v|| \cdot ||w||}\right)^2}$$

- Low k, $\sin\theta \approx 0$: parallel eigenvectors
- High k, $\sin\theta \approx 1$: orthogonal eigenvectors
- Increasing N the error decreases

Computing too many eigenvectors beyond the resolution limit is meaningless, as they deviate too much from their corresponding analytical value.



Flexibility and Efficiency

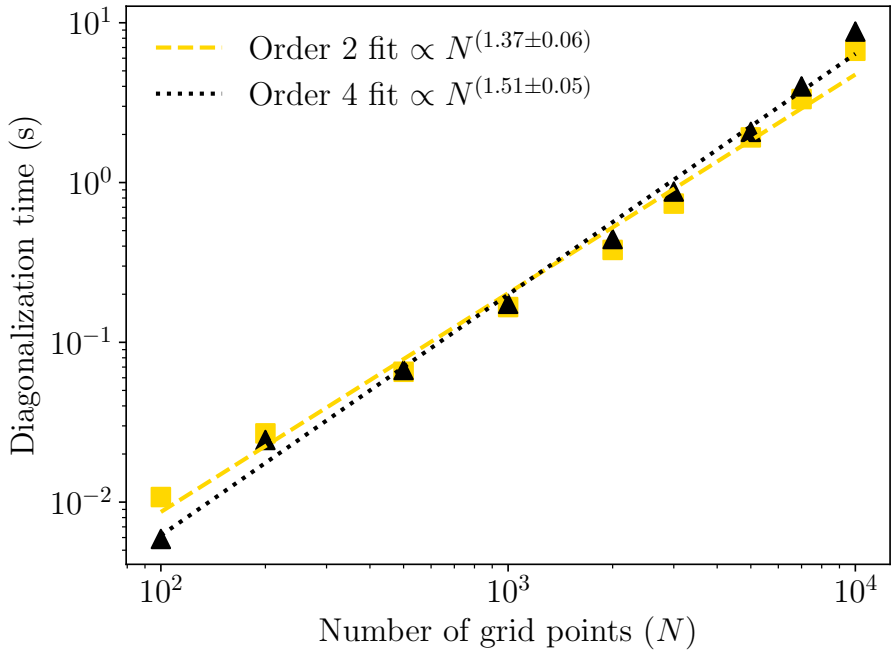
```python
class HarmonicOscillator:
    """
    Harmonic oscillator class handling operators, eigenvalue problems, and error metrics.

    Args:
        a (float): Left boundary of spatial domain.
        b (float): Right boundary of spatial domain.
        npts (int): Number of discretization points.
        m (float): Mass of the particle.
        omega (float): Oscillator frequency.
        hbar (float): Reduced Planck constant.
        derivative_order (int): Finite difference order (2 or 4).
        sparse (bool): Whether to use sparse matrices.
        V_func (callable, optional): Custom potential function.

    Raises:
        AssertionError: If derivative_order is neither 2 nor 4.
    """
```

An `HarmonicOscillator` class has been implemented to store all the methods one can need to solve an harmonic oscillator.

Easy to add new functionalities and create objects in the main program.



Diagonalization time scales as $\approx O(N^{1.5})$ as expected for the diagonalisation algorithm used (ARPACK) in:

`scipy.sparse.linalg.eigsh`