Assignment 4

https://github.com/jchryssanthacopoulos/quantum_information/tree/main/assignment_4

Quantum Information and Computing
AA 2022–23

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Quantum Harmonic Oscillator

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- Goal is to solve 1D Schrodinger equation, $\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$
- Hamiltonian was discretized using finite difference. For $m = \omega = \hbar = 1$, this becomes eigenvalue problem

$$\begin{pmatrix} \frac{x_1^2}{2} + \frac{1}{\Delta x^2} & -\frac{1}{2\Delta x^2} & 0 & \cdots & 0 \\ -\frac{1}{2\Delta x^2} & \frac{x_2^2}{2} + \frac{1}{\Delta x^2} & -\frac{1}{2\Delta x^2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & -\frac{1}{2\Delta x^2} & \frac{x_N^2}{2} + \frac{1}{\Delta x^2} \end{pmatrix} \left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

where $\{x_i\}$ are points between $[-x_{\max}, x_{\max}]$ and $\Delta x = 2x_{\max}/N$

```fortran
! get spacing
dx = (xmax - xmin) / (npoints - 1)

! discretize Hamiltonian
H_off_diag = -1 / (2 * dx ** 2)

do ii = 1, npoints
    x_grid(ii) = xmin + (ii - 1) * dx
    H_diag(ii) = 1 / (dx ** 2) + 0.5 * x_grid(ii) ** 2
end do

! compute eigenvalues and eigenvectors
call dsteqr("I", npoints, H_diag, H_off_diag, eigenvectors, npoints, work, info)

if (info .eq. 0) then
    print *, "Success!"
else
    print *, "Failed to obtain eigenvalues and eigenvectors"
end if
```

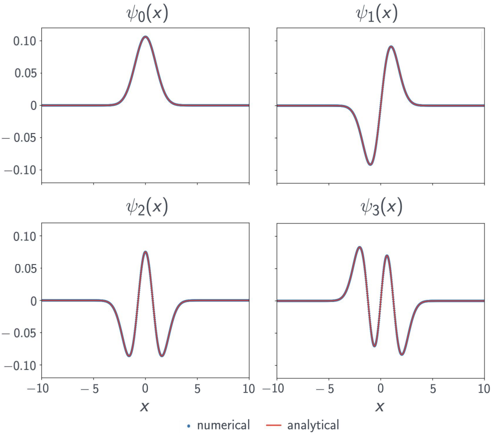
`dsteqr` computes eigenvalues and eigenvectors for tridiagonal matrix, results saved in file

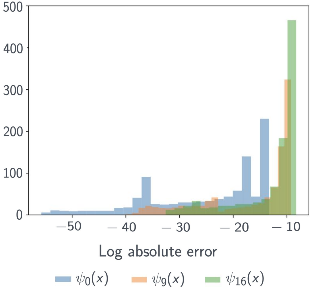
```bash
for N in 100 1000 5000; do
    for xmax in 2.5 5 10 15; do
        echo "Running for N = $N, xmin = -$xmax, xmax = $xmax ..."
        compiled/eigen_schrodinger \
            --output_filename data/solution_$N\_$xmax.txt \
            --npoints $N \
            --xmin -$xmax \
            --xmax $xmax
    done
done
```

Program accepts discretization parameters and output filename, results analyzed in Jupyter notebooks

Eigenfunctions

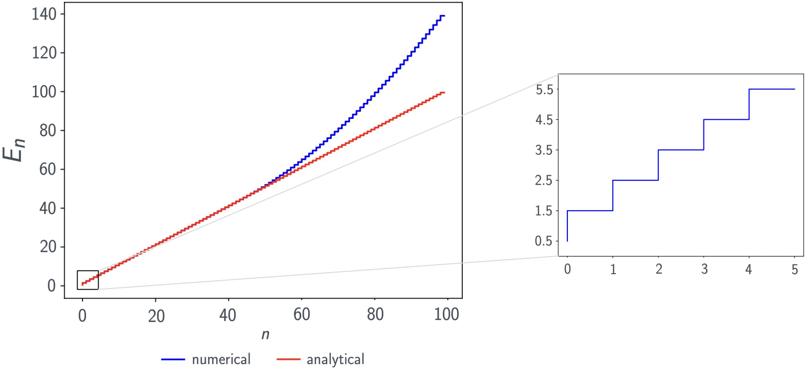
- Eigenfunctions given by $\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{1}{\pi}\right)^{1/4} \exp\left(-x^2/2\right) H_n(x)$
- Good match to expected values using $N = 1000$ and $x_{\text{max}} = 10$, but error increases with n, particularly around edges of domain boundaries





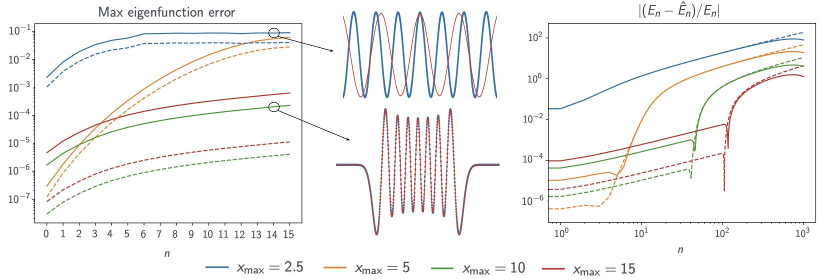
Eigenvalues

- Eigenvalues given by $E_n = n + \frac{1}{2}$
- Good match to expected values, but again, error increases with n



Sensitivity Analysis

- Error decreases as N increases (solid lines are $N = 1000$, dashed lines are $N = 5000$)
- Error decreases as $x_{\max}$ increases, but then increases again. Best overall results found for $x_{\max} = 10$



Self-Rating

- **Correctness.** Results closely match analytical solutions for $n < \mathcal{O}(100)$, but start to diverge for higher values. Loss of acurracy is due to discretizing continuous problem
- **Stability.** Code is stable, and `dsteqr` returns with $\texttt{info} = 0$. Results are reproducible across runs
- **Accurate Discretization.** Accuracy can be improved by making Δx smaller (i.e., increasing N)
- **Flexibility.** Other discretization schemes and potentials can easily be substituted in. It is harder to extend to multidimensional and time-dependent problems
- **Efficiently.** Hamiltonian is tridiagonal, so diagonalization is efficient (e.g., it takes ~ 80 seconds to solve problem with $N = 5000$)