

SciComp Project 1

Weeks 1+2

September 5, 2022

To be handed in Monday September 19 before 12:00 noon

1 Background

Many of you will know the phenomenon that a prism refracts light, i.e. splits it up in different colors, because the refractive index of the prism varies with the frequency ω of light. The underlying property of the molecules forming the material is the frequency dependent polarizability, $\alpha(\omega)$. The polarizability, like many other properties of molecules and materials, can be calculated from the basic laws of physics, here the time-dependent Schrödinger equation.

In the end, the polarizability for a given frequency ω of the incoming light is obtained as the following scalar product of two column vectors \mathbf{z} and \mathbf{x} :

$$\alpha(\omega) = \mathbf{z}^T \mathbf{x} \quad (1)$$

where \mathbf{z} is a vector that can be calculated from the Schrödinger equation, and \mathbf{x} is the solution to the following system of linear equations:

$$(\mathbf{E} - \omega \mathbf{S}) \mathbf{x} = \mathbf{z} \quad (2)$$

Here, \mathbf{E} and \mathbf{S} are two square matrices, and ω is the frequency of the incoming light. Like the column vector \mathbf{z} , the matrices \mathbf{E} and \mathbf{S} are calculated from the Schrödinger equation, which we will not discuss further in this course.

2 Data

In this project we consider the water molecule, H_2O , and its frequency dependent polarizability, $\alpha(\omega)$. It turns out that the matrices \mathbf{E} and \mathbf{S} , and the column vector \mathbf{z} , have a structure that lets us decompose the matrices into submatrices as follows:

$$\mathbf{E} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & \mathbf{A} \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{bmatrix}, \quad \mathbf{z} = \begin{bmatrix} \mathbf{y} \\ -\mathbf{y} \end{bmatrix} \quad (3)$$

The Python-file `watermatrices.py` contains the submatrices \mathbf{A} and \mathbf{B} , and the subvector \mathbf{y} for a water molecule, obtained by an approximate solution to the Schrödinger equation. From this, you can construct the full matrices \mathbf{E} and \mathbf{S} , which in this approximation should be 14×14 .

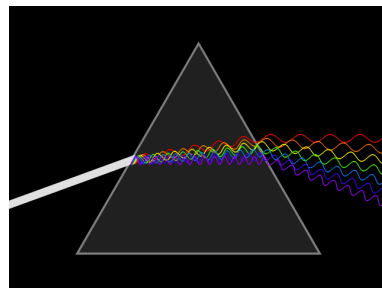


Figure 1: A dispersive prism slows light at different rates depending on the wave-length, causing refraction.

3 Questions for Week 1

- a. (1) Write a small function that computes the condition number of a matrix under the max-norm:

$$\text{cond}_{\infty}(\mathbf{M}) = \|\mathbf{M}\|_{\infty} \|\mathbf{M}^{-1}\|_{\infty}$$

Use a library matrix inversion routine¹ for \mathbf{M}^{-1} , but do program the max-norm yourself using `sum`, `abs`, and `max`. (2) For three frequencies, $\omega = \{0.800, 1.146, 1.400\}$, calculate the condition number for the matrix $\mathbf{E} - \omega\mathbf{S}$. The right-hand-side \mathbf{z} is given with 8 significant digits. How many significant digits could we guarantee in the solution \mathbf{x} if everything else were assumed exact? Why?

- b. (1) For each of the three ω , determine a bound on the relative forward error in the max-norm:

$$\frac{\|\Delta\mathbf{x}\|_{\infty}}{\|\hat{\mathbf{x}}\|_{\infty}} \leq \text{cond}_{\infty}(\mathbf{E} - \omega\mathbf{S}) \frac{\|\delta\omega\mathbf{S}\|_{\infty}}{\|\mathbf{E} - \omega\mathbf{S}\|_{\infty}}$$

for the perturbation that the frequency ω is changed by $\delta\omega = \frac{1}{2} \cdot 10^{-3}$. Recall that $\hat{\mathbf{x}}$ is the *computed* approximate value (known) of the exact \mathbf{x} (unknown), and $\Delta\mathbf{x} \equiv \mathbf{x} - \hat{\mathbf{x}}$. (2) As ω is given with 3 digits after the comma, how many significant digits could we be guarantee in \mathbf{x} if everything else were exact? Why?

- c. Implement three separate functions

1. `L, U = lu_factorize(M)`,² which takes a square matrix \mathbf{M} as input and returns two square matrices: A triangular matrix \mathbf{L} and upper triangular matrix \mathbf{U} such that $\mathbf{M} = \mathbf{L}\mathbf{U}$.
2. `y = forward_substitute(L, z)`, which takes a square lower triangular matrix \mathbf{L} and a vector \mathbf{b} as input, and returns the solution vector \mathbf{y} to $\mathbf{L}\mathbf{y} = \mathbf{b}$.
3. `x = back_substitute(U, y)`, which takes a square upper triangular matrix \mathbf{U} and a vector \mathbf{y} as input, and returns the solution vector \mathbf{x} to $\mathbf{U}\mathbf{x} = \mathbf{y}$.

and test them with the linear equation

$$\begin{bmatrix} 2 & 1 & 1 \\ 4 & 1 & 4 \\ -6 & -5 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 11 \\ 4 \end{bmatrix}$$

You can test your solution against a library routine.³

If you know how, try to use vector operations instead of for-loops where possible (orders of magnitude faster in Python).

- d. Implement a function `alpha = solve_alpha(omega)` for calculating the frequency-dependent polarizability $\alpha(\omega) = \mathbf{z}^T \mathbf{x}$ for water in the given approximation. This routine should solve Equation (2) by LU-factorization using your own three routines from (c). (1) Using your routine, make a table of the polarizabilities for the frequencies given in (a) and their perturbations, i.e. for $\omega = \{0.800 \pm \delta\omega, 1.146 \pm \delta\omega, 1.400 \pm \delta\omega\}$, with $\delta\omega = \frac{1}{2} \cdot 10^{-3}$ as before. (2) Which error-bound is the correct one to understand the variation of the calculated polarizabilities due to the perturbation: (a) or (b) or both? Explain why. (3) Use this bound to derive an upper bound for $\Delta\alpha(\omega) = \alpha(\omega + \delta\omega) - \alpha(\omega)$ of the form $|\Delta\alpha(\omega)| \leq B(\omega)|\delta\omega|$. Do your calculated values fall within this bound?
- e. (1) Compute a table of $\alpha(\omega)$ for 1000 evenly spaced values in the interval $[0.7, 1.5]$ ⁴ using your routine from (d), and plot the values. (2) Can you explain what happens to the linear system of Equation (2) around the frequency $\omega = 1.146307999$, and how is this reflected in $\alpha(\omega)$?

¹E.g. `inv` from `numpy.linalg` for Python. But `inv` is allowed only here.

²If you implement it with pivot, you will be able to solve a wider range of systems. However, it is not required.

³E.g. `numpy.linalg.solve` in Python

⁴Use `linspace` in Python.

4 Questions for Week 2

f. Implement and test the Householder and least-squares routines below.

1. `Q,R = householder_QR_slow(A)`, which takes as input a rectangular matrix \mathbf{M} : $m \times n$ and uses the Householder method to compute its QR decomposition. Check that \mathbf{Q} : $m \times m$ is orthogonal, i.e., $\mathbf{Q}^T \mathbf{Q} = \mathbf{Q} \mathbf{Q}^T = \mathbf{I}$, and that the upper triangular matrix \mathbf{R} : $m \times n$ satisfies $\mathbf{M} = \mathbf{Q} \mathbf{R}$.
2. A more efficient version of (f.1) that doesn't compute the $m \times m$ matrix \mathbf{Q} , but just stores the reflection vectors \mathbf{v} . You can either give it the interface `V,R = householder_fast(A)` or (as is done in practice) let the result be a combined $(m+1) \times n$ matrix \mathbf{VR} , in which the upper $n \times n$ triangle contains \mathbf{R} , and the k th column below the diagonal is \mathbf{v}_k (of length $m-k$).
3. `tilde_x,r = least_squares(A,b)`, which combines this routine with your back-substitution from (c.3) to compute a linear least squares fitting. It should take as input a rectangular $m \times n$ matrix \mathbf{A} and an $m \times 1$ right-hand-side vector \mathbf{b} , returning an $n \times 1$ approximate solution vector $\tilde{\mathbf{x}}$ to $\mathbf{A}\tilde{\mathbf{x}} \simeq \mathbf{b}$ as output, and the residual. If you did not get (f.2) to work, you can just use your solution to (f.1).

You can use the linear system in Heath's Example 3.1 & 3.8 to debug individual steps of your computation. Test your routines against `A1,b1` from `HHexamples.py`, and print the resulting upper triangular \mathbf{R} and solution \mathbf{x} rounded to 3 digit accuracy.

g. We now want to approximate $\alpha(\omega)$ in the interval $[0.7, \omega_p]$ using a polynomial

$$P(\omega) = \sum_{j=0}^n a_j \omega^{2j} \quad (4)$$

(1) Suggest a suitable value of $\omega_p < 1.5$. What makes this choice reasonable? (2) Find the coefficients of the polynomial using your linear least squares routine from (f)⁵, the table computed above, and $n = 4$. (3) Repeat the computation for $n = 6$ and compare the accuracies of the two polynomials: Plot the magnitude of the relative error (in a \log_{10} -scale) of the polynomial approximation as the difference between the $P(\omega)$ and $\alpha(\omega)$ values. (4) How many significant digits does each approximation yield?

h. We would now like to approximate $\alpha(\omega)$ in the entire interval $[0.7, 1.5]$, and choose the *rational* approximating function, which is able to represent singularities:

$$Q(\omega) = \frac{\sum_{j=0}^n a_j \omega^j}{1 + \sum_{j=1}^n b_j \omega^j} \quad (5)$$

(1) Why will this fail with the polynomial approximation of Problem (g)? And why can Eq. (5) do a better job? (2) Find the coefficients a_j and b_j using your linear least squares routine, the table of α -values computed above, and $n = 2$. You need to reformulate the expression as an linear approximation so that you can use a linear least squares fitting. Plot the error of the the rational-function approximation $Q(\omega)$ compared to $\alpha(\omega)$ calculated by Equations (1) and (2).⁶ (2) Repeat the computation for $n = 4$ and compare the accuracies of the two approximations quantitatively. (3) If you look at $\alpha(\omega)$ in the extended interval $\omega \in [-4; 4]$, you will notice that $\alpha(\omega)$ has multiple singularities. Are you able to modify your approximation to accurately approximate the full interval $[-4; 4]$, in particular so that it reproduces the singularities correctly? Explain your solution.

⁵If you could not get your own least squares solver to work, you can use a library version for the remaining problems - but make sure to write clearly that you have done so.

⁶Once you have computed the coefficients \mathbf{a} and \mathbf{b} , be sure to finish the construction of $Q(\omega)$ using Eq. (5), and to use this for the error. It is tempting (but wrong) to just use the linear approximation you used to find \mathbf{a} and \mathbf{b} , but that is linear and hence cannot represent singularities.