Programming Project 1: Frequencies
Computing frequencies and normal modes from the Hessian matrix

Write a script to read in a Hessian matrix, compute the corresponding frequencies and normal modes, and print them to a file in Jmol's `.xyz` format. You should import your `Molecule` class from Project 0 and make use of it in this script.

Extra Files

file name	description
`molecule.xyz`	sample `.xyz` file for H_2O
`hessian.dat`	sample Hessian matrix for H_2O
`project1_answer.xyz`	normal modes and frequencies for H_2O

Equations

Let N be the number of atoms and let m_A and (x_A, y_A, z_A) be the mass and Cartesian coordinates of the A^{th} atom.

$$(\mathbf{H})_{AB} = \frac{\partial^2 E}{\partial X_A \partial X_B} \qquad (X_{3A-2}, X_{3A-1}, X_{3A-0}) = (x_A, y_A, z_A) \qquad \text{for } A \in \{1, \ldots, N\} \tag{1}$$

$$(\tilde{\mathbf{H}})_{AB} = \frac{(\mathbf{H})_{AB}}{\sqrt{M_A M_B}} \qquad (M_{3A-2}, M_{3A-1}, M_{3A-0}) = (m_A, m_A, m_A) \qquad \text{for } A \in \{1, \ldots, N\} \tag{2}$$

$$\tilde{\mathbf{H}}\,\tilde{\boldsymbol{q}}_A = k_A \tilde{\boldsymbol{q}}_A \qquad \text{for } A \in \{1, \ldots, N\} \tag{3}$$

$$(\boldsymbol{q}_A)_B = \frac{(\tilde{\boldsymbol{q}}_A)_B}{\sqrt{M_B}} \qquad \text{for } A, B \in \{1, \ldots, N\} \tag{4}$$

$$k_A \left[\frac{E_h \text{rad}^2}{a_0^2 u}\right] = k_A \left(\frac{E_h[\text{J}]}{a_0[\text{m}]^2 u[kg]}\right) \left[\frac{\text{rad}^2}{\text{s}^2}\right] \qquad \nu_A\,[\text{Hz}] = \frac{1}{2\pi}\left[\frac{\text{cyc}}{\text{rad}}\right] \cdot \sqrt{k_A \left[\frac{\text{rad}^2}{\text{s}^2}\right]} \qquad \tilde{\nu}_A\left[\text{cm}^{-1}\right] = \frac{\nu_A\,[\text{Hz}]}{c\ [\text{cm/s}]} \tag{5}$$

Procedure

Steps 3.–7. should be implemented in a separate `frequencies()` function that takes a `Molecule` object and a `numpy.array` Hessian matrix as arguments.

1. read in the Hessian matrix (defined in equation 1) from `hessian.dat`
2. build a `Molecule` object from `molecule.xyz`
3. build the mass-weighted Hessian matrix (equation 2)
4. compute the eigenvalues (k_A) and eigenvectors ($\tilde{\boldsymbol{q}}_A$) of the mass-weighted Hessian matrix (equation 3)
5. un-mass-weight the eigenvectors (equation 4) to get normal coordinates
6. determine the spatial frequencies $\tilde{\nu}_A$ in cm^{-1} from your force constants k_A, which are in atomic units (equation 5)
7. write the normal modes to a file in `.xyz` format, with frequencies neatly displayed in the comment lines

After you are finished, check your answers against `project1_answer.xyz` and then try visualizing the normal modes in Jmol.

Description of `.xyz` format for normal modes

The file format for visualizing a single normal mode in Jmol is

```
N
COMMENT LINE 1
A1 x1 y1 z1   dx1 dy1 dz1
A2 x2 y2 z2   dx2 dy2 dz2
...
AN xN yN zN   dxN dyN dzN
```

which amounts to a standard `.xyz` geometry file (distance units Å) with the displacement vector for each atom printed next to its Cartesian coordinates. For visualizing multiple motions, this format is simply repeated with an intervening empty line.

```
N
COMMENT LINE 1
A1 x1 y1 z1   dx11 dy11 dz11
A2 x2 y2 z2   dx12 dy12 dz12
...
AN xN yN zN   dx1N dy1N dz1N

N
COMMENT LINE 2
A1 x1 y1 z1   dx21 dy21 dz21
A2 x2 y2 z2   dx22 dy22 dz22
...
AN xN yN zN   dx2N dy2N dz2N

...

N
COMMENT LINE N
A1 x1 y1 z1   dxN1 dyN1 dzN1
A2 x2 y2 z2   dxN2 dyN2 dzN2
...
AN xN yN zN   dxNN dyNN dzNN
```