Exercise

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1. During the Hartree-Fock SCF procedure, we need to diagonalize symmetric matrices several times, i.e., the overlap and the Fock matrices.

   Write a function that can diagonalize a real, symmetric matrix. You can either implement the Jacobi rotations algorithm introduced in the lecture or any other suitable algorithm you know. If you choose to not use the Jacobi rotations, please give a short explanation of the basic algorithm you employ. After diagonalization, please sort the diagonal matrix such that the values on the diagonal are in ascending order. *Don't forget to sort the resulting transformation matrix accordingly.* Consult page 5 of the notes for the algorithm

   Test your algorithm against, for example, the `PDSYEV` Lapack function.

2. The notes introduced suitable closed forms for the important integrals required for the implementation of Hartree-Fock. It is time implement one of these integrals, namely the easiest one: the overlap integrals $S_{\mu\nu}$ (see eq. 31 in the notes and section 2.4.1 and 2.4.2). Please note that we will use contracted basis sets; refer to Section 3.4 of the lecture notes for details of how to obtain the full integrals over the contracted basis functions ψ_μ from the integrals over the individual Gaussian functions ψ_i.

   Before you start, think about suitable data structures to store the definition of basis set in your code and the resulting integrals. Furthermore, you will have to write a small parser to obtain the molecular geometry from file. Make sure to write your code in a modular way, such that each action corresponds to a separate subroutine that is called from the main code.

   The file format for the geometry is as follows. The first line gives the number of atoms in the system. The second line is empty or can contain comments. The subsequent lines give the atomic symbol and the x, y and z coordinates of that atom. Such a file for the case of a water molecule, with coordinates given in units of the Bohr radius, looks like:

```
3

H 1.20 1.43 0.0
H 1.20 -1.43 0.0
O 0.0 0.0 0.0
```

The basis set file is `sto3g.dat`. It contains the STO-3G basis set specification, in Gaussian-code format for H and O. For a description of this format, consult `https://gaussian.com/gen/`and ask any further questions if it is unclear.

There is a list of reference values for different integrals that you can use for testing. These values are found in the `H2O_ref.zip` and `H2_ref.zip` files. These each contain a geometry file and four matrices containing the four integrals within the STO-3G basis, stored as `*.npy` files.

3. Setup a code that can do steps 1, 3, and 4 in page 19 of the notes. The modification is only that in step 3 you only have to evaluate the $S_{\mu\nu}$ values. Print out the result of the diagonalization of $\mathbf{S}$ (eigenvalues and eigenvectors, sorted), and also build and print out the matrix $\mathbf{X}$. Do this for the H2 and H2O molecule.