Exercise Sessions 10–11: Steepest Descent and Conjugate Gradient Methods.

Exercise 1: The Steepest Descent and Conjugate Gradient Methods [10 pts]

1. Implement both the steepest descent (`solve_SD.m`) and the conjugate gradient (`solve_CG.m`) methods to solve user-defined systems of linear equations. The implemented functions should have the form

```
function X=solve_SD(A,b)
X=A/b;
end
```

and

```
function X=solve_CG(A,b)
X=A/b;
end
```

where A is a square matrix and b is a vector. What properties must the matrix A satisfy for the steepest descent and conjugate gradient methods to converge? Make sure that your implementation works properly. Use the provided test script for verifying your implementation.

2. Use both methods to solve the system of linear equations $A1 * x = b1$, defined by the matrix $A1$ and the vector $b1$ contained in the file `Matrices.mat` available on Moodle. Plot the relative error with respect to the exact solution (e.g. obtained using Matlab's $A_1 \backslash b_1$) as a function of the number of iterations. Comment on the convergence trends of both methods and make a connection with the theory.

3. Consider now a larger (50×50) linear system $A2 * x = b2$ defined by matrix $A2$ and vector $b2$ contained in the file `'Matrices.mat'`. Solve the system using the two algorithms (Note: it may take a few minutes for the steepest descent method). Plot the relative error with respect to the exact solution as a function of the number of iterations N_{it}. At which number of iterations do you achieve a convergence compatible with the machine precision? Comment on the result from the point of view of the condition number $\mathcal{K}(A2)$ evaluated using Matlab's `cond` function.

Submit: Matlab functions `solve_SD.m` and `solve_CG.m` each gives [3 pts]. Answers to questions in (2) and (3) give [2 pts] each.

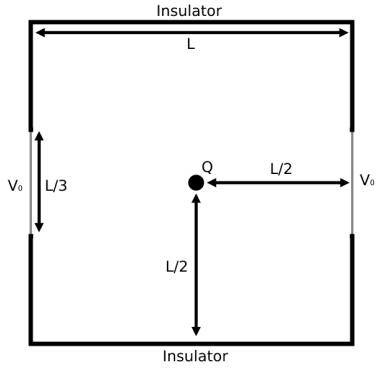
Exercise 2: Discretization of Poisson Equation [8 pts]

The goal of this exercise is to find the electric potential profile in a 2D system using the steepest descent and conjugate gradient algorithms. Assume the system is an empty square of dimensions $L \times L$ with $L = 45$, and there is a charge $Q = 1$ C placed at the centre of the square. Two metallic plates of length $L/3$ are centered on the right and left side of the square, each kept at a potential $V_0 = 1$ V. The remaining sides are insulated, meaning that there is no electric field $\mathbf{E} = -\nabla V$ perpendicular to them. The set-up is shown in the figure below.

In the absence of magnetic fields or currents, the electric potential $V(x, y)$ satisfies the Poisson equation

$$\nabla^2 V(x, y) = \frac{-\rho(x, y)}{\epsilon},$$

as well as the corresponding boundary conditions stated above. For simplicity, assume $\epsilon = 1$.



1. Discretize the problem using an $N \times N$ grid, with $N = 45$. Reformulate it into a system of linear equations, that is $A\mathbf{x} = \mathbf{b}$ (*Hint:* beware of the boundary conditions).
2. Use the steepest descent and conjugate gradient algorithms implemented above to solve the problem numerically. Compare your solution to Matlab's `x = A\b`. Comment on the number of iterations required for the two gradient descent algorithms to converge.
3. Plot the electric potential profile (e.g. using the `imagesc` routine) and the electric field (e.g. using the `quiver` routine). Is it consistent with what you would expect?
4. Implement the Jacobi preconditioning technique. Does it speed up the convergence?

Submit: Your Matlab scripts and answers to each of the points in the report file. Complete answer to each question gives [2 pts].

Exercise 3: The Nonlinear Conjugate Gradient Method [15 pts]

The aim of this exercise is to explore some of the most common molecular geometries by means of a simple potential. Consider an ensemble of N identical atoms interacting with each other by means of a pair-potential

$$E\left(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\right) = \sum_{i \neq j} U_{LJ}\left(|\mathbf{x}_i - \mathbf{x}_j|\right),$$

where $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N$ are the coordinates of atoms and $U_{LJ}(x)$ is the Lennard-Jones (LJ) potential which describes weak van der Waals (dispersion) interaction

$$U_{LJ}(x) = 4\epsilon \left[\left(\frac{\sigma}{x}\right)^{12} - \left(\frac{\sigma}{x}\right)^{6} \right].$$

This model would correspond closely to clusters of inert gas atoms (He, Ne, Ar, etc.) The minima on the potential energy surface described by $E\left(\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\right)$ ($E\left(\{\mathbf{x}_i\}\right)$ for simplicity) correspond to equilibrium configurations of such Lennard-Jones clusters.

1. *Algorithm implementation.* Implement the nonlinear conjugate gradient method for finding the potential surface minima of an ensemble of N atoms interacting by means of the LJ potential. Throughout the rest of the exercise, we assume $\epsilon = \sigma = 1$. For residuals use the numerical gradient of $E\left(\{\mathbf{x}_i\}\right)$. To find a minimum of the function in a given direction use the Newton-Raphson line search method employing Taylor expansion up to the second order.

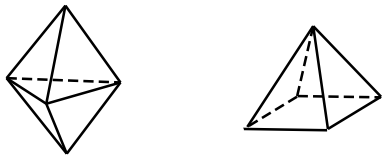
$$E\left(\{\mathbf{x}_i\} + \alpha\mathbf{d}\right) = E\left(\{\mathbf{x}_i\}\right) + \alpha[E'\left(\{\mathbf{x}_i\}\right)]^T\mathbf{d} + \frac{\alpha^2}{2}\mathbf{d}^T E''\left(\{\mathbf{x}_i\}\right)\mathbf{d}$$

Both the vector of gradient $E'\left(\{\mathbf{x}_i\}\right)$ and directional second derivative $\mathbf{d}^T E''\left(\{\mathbf{x}_i\}\right)\mathbf{d}$ can be evaluated numerically.

Hint: The case of $\mathbf{d}^T E''(\{\mathbf{x}_i\})\,\mathbf{d} \leq 0$ should be treated with care. Instead of using the normal expression for α perform a small step (for example, $|\mathbf{d}| = 0.01$) in the direction where potential is smaller along selected search direction $\vec{d}$.

2. *$N = 4$ case.* Consider the case of a cluster composed of 4 atoms. Two distinct configurations are possible: the tetrahedral geometry and the square planar geometry. Locate these two minima by applying your implementation to clusters consisting of 4 atoms and choosing appropriate starting configurations. Discuss the equilibrium structures (you can visualize them with the `visualize_molecule.m` function provided on the course webpage) and the relative stability of the two relaxed geometries. Support your discussion with the calculated values of total energies.

3. *$N = 5$ case.* Consider the case of a cluster composed of 5 atoms. Clusters of 5 atoms can arrange either in a trigonal bipyramid or a square pyramid geometry. Similarly to point (2), locate these two minima and discuss both equilibrium geometries and relative stabilities. Support your discussion with the calculated values of total energies.



trigonal bipyramid square pyramid

4. *$N = 6$ case.* Larger number of particles lead to more diverse possibilities for various configurations. Locate at least two locally stable three-dimensional configurations of 6-atom clusters and discuss their geometry and stability. Which polyhedra do they realize? Support your discussion with the calculated values of total energies.

Grading:

- (5 pts) Plot of the geometries, values of total energies, discussion of the relative stabilities of $N = 5$ configurations
- (5 pts) Plot of the geometries, values of total energies, discussion of the relative stabilities of $N = 5$ configurations.
- (5 pts) Identification of at least two local minima and plot of the corresponding geometries for the $N = 6$ case, values of total energies.

Exercise sessions 12–13: Singular value decomposition.

Exercise 1: Over-defined systema of linear equations [6 pts]

Consider an over-defined system of linear equations

$$\begin{pmatrix} 3 & 2 \\ 4 & 5 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 4 \\ 1 \end{pmatrix}$$

1. Find $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ that minimizes the norm of residual $r(x) = ||Ax - b||$ by computing the Penrose inverse of the matrix A. You can use Matlab's command `pinv`.
2. Illustrate that your solution indeed minimizes the norm of residual $r(x)$ by plotting its magnitude in the vicinity of the solution x. We suggest to use Matlab's command `contour` for this purpose.

Submit: your report as a PDF file as well as your scripts. The points are distributed in the following way:

- [3 pts] for the solution of the system;
- [3 pts] for the plot of the residual.

Exercise 2: Quantum state tomography [24 pts]

Files: `p1.csv, p2.csv, p3.csv`

Quantum state tomography (QST) is a class of methods for reconstructing the quantum mechanical wavefunction, that is both its phase and amplitude from a collection of measurements. The goal of this exercise is to implement a simple tomographic scheme for a two-level system using singular matrix decomposition.

Part A: The density matrix formalism
Consider a single electron (spin-$\frac{1}{2}$), subject to an external magnetic field along the $\hat{z}$ direction. The Hamiltonian is given by

$$\hat{H} = \hbar\Omega\hat{\sigma}_z, \tag{1}$$

where Ω is the angular frequency corresponding to the magnetic field, and $\hat{\sigma}_z$ is the z Pauli matrix. A state $|\psi\rangle = (c_1\ c_2)^T$ has the following time evolution

$$|\psi(t)\rangle = \begin{pmatrix} e^{-i\Omega t}c_1 \\ e^{i\Omega t}c_2 \end{pmatrix}. \tag{2}$$

In order to describe real experiments, it is important to work not only with single quantum states, but also to be able to express a statistical distribution of quantum states. The density matrix formalism is an important tool for that. Consider a statistical mixture of N states $|\psi_n\rangle$, each with probability p_n subject to $\sum_n p_n = 1$. The *density matrix* describing this mixture is defined as

$$\hat{\rho} = \sum_n p_n |\psi_n\rangle \langle\psi_n|. \tag{3}$$

For a pure state $|\psi\rangle$, we have

$$\hat{\rho} = |\psi\rangle \langle\psi|. \tag{4}$$

The statistical average of an operator $\hat{O}$ can be computed using

$$\langle\hat{O}\rangle := \sum_n \langle\psi_n|\hat{O}|\psi_n\rangle = \mathrm{Tr}(\hat{\rho}\hat{O}). \tag{5}$$

1. Diagonalize the two density matrices below. If one of them represents a pure state, give this state. Justify your approach.

$$\hat{\rho}_1 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \hat{\rho}_2 = \frac{1}{2}\begin{pmatrix} 3 & -1 \\ -1 & 1 \end{pmatrix}. \tag{6}$$

2. Not all 2×2 matrices are valid density matrices. In particular, a density matrix must: 1) be hermitian, and 2) have trace one. Any 2×2 matrix can be decomposed as

$$\hat{\rho} = \sum_{n=0}^{3} \rho_n \hat{\sigma}_n \tag{7}$$

for $\rho_n \in \mathbb{C}$, $\hat{\sigma}_0$ the identity matrix, and $\hat{\sigma}_1, \hat{\sigma}_2, \hat{\sigma}_3$ the Pauli matrices. What are the constraints on ρ_n to make $\hat{\rho}$ a valid density matrix, that is fulfilling the two conditions above?

Part B: Simple QST

Our goal is to reconstruct the density matrix $\hat{\rho}$. Consider an observable $\hat{O}$, with eigenvalues and eigenstates λ_1, λ_2, and $|\phi_1\rangle$, $|\phi_2\rangle$, respectively. If this observable is measured, we obtain λ_i with a probability $p_i = \mathrm{Tr}(\hat{\rho}\,|\phi_i\rangle\,\langle\phi_i|)$. By repeating the same experiment sufficient number of times, one can estimate the probabilities p_i, and use them to reconstruct the original state.

However, a single observable generally does not yield enough information to fully reconstruct the density matrix. To generalize this approach, let us assume we have now $M/2$ observables, yielding M projection operators

$$\hat{E}_m := |\phi_m\rangle\,\langle\phi_m|\,. \tag{8}$$

Similarly, let p_m be the probability (known from experiment) associated with $\hat{E}_m$. We now need to solve the following system of equations

$$p_m = \mathrm{Tr}(\hat{\rho}\hat{E}_m)\ \text{, for all } m = 1, \ldots, M. \tag{9}$$

With the decomposition of equation 7, this can be cast in the following matrix equation

$$\vec{p} - \vec{M}_0 = M\vec{\rho}, \tag{10}$$

where

$$\vec{p} = \begin{pmatrix} p_1, & \ldots, & p_M \end{pmatrix}^T, \tag{11}$$

$$\vec{M}_0 = \begin{pmatrix} \frac{1}{2}, & \ldots, & \frac{1}{2} \end{pmatrix}^T, \tag{12}$$

$$\vec{\rho} = \begin{pmatrix} \rho_1 & \rho_2 & \rho_3 \end{pmatrix}^T, \tag{13}$$

$$M = \begin{pmatrix} \mathrm{Tr}(\hat{\sigma}_1\hat{E}_1) & \ldots & \mathrm{Tr}(\hat{\sigma}_3\hat{E}_1) \\ \vdots & \ddots & \vdots \\ \mathrm{Tr}(\hat{\sigma}_1\hat{E}_M) & \ldots & \mathrm{Tr}(\hat{\sigma}_3\hat{E}_M) \end{pmatrix}. \tag{14}$$

Matrix M is called the *measurement matrix*.

1. Consider the following basis of measurement

$$|\phi_1\rangle = |x+\rangle\,, \qquad |\phi_2\rangle = |x-\rangle\,, \tag{15}$$

$$|\phi_3\rangle = |y+\rangle\,, \qquad |\phi_4\rangle = |y-\rangle\,, \tag{16}$$

$$|\phi_5\rangle = |z+\rangle\,, \qquad |\phi_6\rangle = |z-\rangle\,, \tag{17}$$

where $|n\pm\rangle$ is the eigenstate of $\hat{\sigma}_n$ with eigenvalue ± 1. Using the pseudoinverse method, reconstruct the density matrices for $\vec{p}$ given in files `p1.csv` and `p2.csv`. If the density matrix originates from a pure state, give the state.

2. Redo the same analysis, but this time only with the first 4 projection operators. Does it give the same density matrices? Compute the singular values of the measurement matrix and comment.

Part C: QST with experimental constraints

Experimentally, it can happen that the measurement cannot be performed along an arbitrary direction in spin space, but rather only along a given axis. This axis can be specified by two angles θ and ϕ, yielding

$$|\psi(\theta,\phi)\rangle := \begin{pmatrix} \cos(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) \end{pmatrix} \tag{18}$$

and the projection operator

$$\hat{E} = |\psi(\theta,\phi)\rangle \langle\psi(\theta,\phi)| . \tag{19}$$

From what we saw in the previous section, it is not enough to retrieve the density matrix. However, due to the external magnetic field, measuring at different times is equivalent to rotating the axis, because

$$e^{i\hat{H}t/\hbar}|\psi(\theta,\psi)\rangle = |\psi(\theta,\psi-\Omega t)\rangle . \tag{20}$$

This equality holds only up to a global phase, which is not important because it cannot be measured. The rotation allows to gain a lot more information about the system, but it is not guaranteed to be sufficient to fully reconstruct the density matrix.

1. Consider the following set of projection operators: $|\psi(\theta,\phi_m)\rangle\langle\psi(\theta,\phi_m)|$, where $\phi_m = 0, 2\pi/M, 2\cdot 2\pi/M, \ldots, (M-1)\cdot 2\pi/M$. As seen above, this is equivalent to a measurement along the $(\theta, \phi = 0)$ axis, for M different times, uniformly distributed between $t = 0$ and $t = 2\pi/\Omega$, the period of the two-level system. Look at the SVD decomposition of the measurement matrix for the following values of θ: $\theta = 0$, $\theta = \pi/2$ and $\theta = \pi/3$. In which case can you reconstruct the density matrix?

2. A collection of $M = 100$ measurements with $\theta = 5\pi/7$ was conducted, and the probabilities $\vec{p}$ can be found in file `p3.csv`. Reconstruct the density matrix.

3. Given the probabilities $\vec{p}$ are measured experimentally, there are uncertainties $\Delta\vec{p}$ associated with them. These uncertainties will propagate to yield an uncertainty on the reconstructed density matrix. To assess the robustness of our tomography scheme, we define the equally weighted variance (EWV)

$$EWV = \sum_{n=1}^{3}\sum_{m=1}^{M}(M^{+}_{nm})^2(\Delta p_m)^2, \tag{21}$$

where M^+ is the pseudoinverse of M. In the experiment of the previous question, we estimate $\Delta p_m = 0.1 + 0.001(m-1)$ (the uncertainty is larger at later times). Plot the EWV as a function of angle $\theta \in [0,\pi]$ to find the measurement axis that minimizes the uncertainty.

Submit: your report as a PDF file as well as your scripts. The points are distributed in the following way:

- Part A: [2 pts] for each question;
- Parts B and C: [4 pts] for each question.