

COMPUTATIONAL METHODS IN RESEARCH

ASSIGNMENT 4

Exercise 1: Integrals

Check the codes written by the groups in class to solve integrals via the trapezoidal and the Simpson's rule. They can be found on

Canvas → Pages → Please, check!!

Are they correct? If you find a mistake, copy the code, comment out the wrong lines, and write your own lines.

Exercise 2: Jacobian

Solve the double integrals. **Solve on a piece of paper** and use a computer to verify your answers.

2.1) Use the new variables $x = u$ and $y = u + v$ to solve

$$\int_1^3 dx \int_{x+2}^{x+3} \frac{dy}{\sqrt{xy - x^2}}$$

When changing the limits of the integral in y , use

$$y = x + 2 \Rightarrow u + v = u + 2$$

2.2) Use the new variables $x = u^2$ and $y = v$ to solve

$$\int_1^3 dx \int_0^{\sqrt{x}} ye^{\sqrt{x}} dy$$

2.3) Use polar coordinates to solve

$$\int_{-1}^1 dx \int_{-\sqrt{1-x^2}}^0 \cos(x^2 + y^2) dy$$

Notice that the lower limit for y is $-\sqrt{1-x^2}$, which looks like the bottom of the circle of radius 1 centered at the origin. This implies that after the change of variables, we will have

$$0 \leq r \leq 1$$

and

$$\pi \leq \theta \leq 2\pi$$

Exercise 3: Taylor expansion

Solve on a piece of paper.

3.1) Using Taylor expansion, explain why the use of the *central difference* improves over the *forward difference* when solving the derivative of a function.

Solve 3.2 on a piece of paper and check with a computer.

3.2) Taylor expansion up to x^3 of

a) e^x around $x = 0$.

b) $\frac{1}{1-x}$ around $x = 0$.

c) $\ln(1+x)$ around $x = 1$.

3.3) Solve in the computer the Taylor expansion of $\exp(\sin(x))$

a) Up to x

b) Up to x^2

c) Up to x^4

d) Up to x^7

e) Show the given function and the 4 approximations obtained in (a), (b), (c) and (d) in a figure with a legend and $-3 \leq x \leq 3$.

Exercise 4 (6.2 from book)

Consider the following four simultaneous equations

$$0 + x + 4y + z = -4$$

$$3w + 4x - y - z = 3$$

$$w - 4x + y + 5z = 9$$

$$2w - 2x + y + 3z = 7,$$

which can be written in the matrix form $\mathbf{Ax} = \mathbf{v}$.

1. Show analytically (**on a piece of paper**) the steps involved in the Gaussian elimination and pivoting of the system of equations above. Show all the steps up to the point where you get the upper triangular matrix.
2. Solve the equations above using "solve" from `numpy.linalg`.
3. Solve the equations above using the inverse of a matrix from `numpy.linalg`.
4. Write a program to solve the four equations using Gaussian elimination and pivoting.

Exercise 5 (part of 6.3 from book)

LU decomposition

Consider the following four simultaneous equations

$$2w + x + 4y + z = -4$$

$$3w + 4x - y - z = 3$$

$$w - 4x + y + 5z = 9$$

$$2w - 2x + y + 3z = 7,$$

which can be written in the matrix form $\mathbf{Ax} = \mathbf{v}$.

This exercise invites you to write your own program to solve simultaneous equations using the method of LU decomposition.

1. Write a Python function that calculates the LU decomposition of the matrix \mathbf{A} above. The calculation is same as that for Gaussian elimination, except that at each step of the calculation you need to extract the appropriate elements of the matrix and assemble them to form the lower diagonal matrix \mathbf{L} . Test your function by calculating the LU decomposition of the matrix \mathbf{A} , then multiplying the \mathbf{L} and \mathbf{U} you get and verifying that you recover the original matrix once more.
2. Build on your LU decomposition function to create a complete program to solve the simultaneous equations above by performing a double backsubstitution.

Exercise 6

1. Find the eigenvalues and the normalized eigenvectors analytically (on a piece of paper) of the matrix

$$\begin{bmatrix} 3 & 1 & 0 \\ 1 & 3 & 1 \\ 0 & 1 & 3 \end{bmatrix}$$

2. Compare with the solution from `numpy.linalg`.

Exercise 7

The QR algorithm

In this exercise you'll write a program to calculate the eigenvalues and eigenvectors of a real symmetric matrix using the QR algorithm. The first challenge is to write a program that finds the QR decomposition of a matrix. Then we'll use that decomposition to find the eigenvalues.

1. Write a Python function that takes as its argument the real square matrix \mathbf{A} below and returns the two matrices \mathbf{Q} and \mathbf{R} that form its QR decomposition.

$$\mathbf{A} = \begin{pmatrix} 1 & 4 & 8 & 4 \\ 4 & 2 & 3 & 7 \\ 8 & 3 & 6 & 9 \\ 4 & 7 & 9 & 2 \end{pmatrix}.$$

Check the results by multiplying \mathbf{Q} and \mathbf{R} together to recover the original matrix \mathbf{A} again.

- Using your function, write a complete program to calculate the eigenvalues and eigenvectors of a real symmetric matrix using the QR algorithm. Continue the calculation until the magnitude of every off-diagonal element of the matrix is smaller than 10^{-6} . You should find that the eigenvalues are 1, 21, -3 , and -8 .
- Compare the results using “solve” from `numpy.linalg`.

Exercise 8

On Canvas, in the “Lectures” folder of “Pages”, you will find some files about the Google Matrix. Our class last week followed closely the file ‘LA03.pdf’. At the end of this file, you will find Problems 3 and 4.

(a) Find the PageRank in Problem 3 for $p = 0$ and $p = 0.15$ using the Power Method (that is, iteration of an initial vector, where all entries are equal, up to convergence).

(b) Find the PageRank in Problem 3 for $p = 0$ and $p = 0.15$ via diagonalization. Careful with the issue of normalization.

Exercise 9

Read the article ‘The World Wide Web and High-Energy Physics’ that was distributed in class (if you did not come to class, you can find it on Canvas) and summarize it with at least 250 words (it can be longer, but not shorter). It should be a pedagogical summary accessible to other science and math Stern students. You can do this in group, if you want. You have two options:

*) Write your text down.

or

*) Record it (just voice or an entire video, as you prefer).

Exercise 10

Solve analytically **on a piece of paper** the Gaussian integrals below. Use a computer to double check your answers.

$$10.1) \int_{-\infty}^{\infty} \exp(-ax^2) dx$$

[If you do not remember what we did in class, you can watch a YouTube video available in the “Lectures” on Canvas.

$$10.2) \int_{-\infty}^{\infty} x \exp(-ax^2) dx$$

[You do not need to solve this integral. You can justify its solution with one simple comment.]

$$10.3) \int_{-\infty}^{\infty} x^2 \exp(-ax^2) dx$$

[You may be able to find how to solve this integral online.]