



MATH2019 Introduction to Scientific Computation

— Coursework 2 (10%) —

Submission deadline: **3pm, Tuesday, 6 December 2022**

Note: This is currently **version 3-3** of the PDF document. (26th November, 2022)

Further questions will be added to this PDF in the upcoming weeks.

This coursework contributes **10%** towards the overall grade for the module.

Rules:

- Each student is to submit their own coursework.
- You are allowed to work together and discuss in small groups (2 to 3 people), but *you must write your own coursework and program all code by yourself*.
- Please be informed of the [UoN Academic Misconduct Policy](#) (incl. plagiarism, false authorship, and collusion).

Coursework Aim and Coding Environment:

- In this coursework you will develop Python code related to algorithms that solve linear systems, and you will study some of the algorithms' behaviour.
- As discussed in the lecture, you should **write (and submit) plain Python code** (.py), and you are strongly encouraged to **use the Spyder IDE** (integrated development environment). Hence you should **not write IPython Notebooks** (.ipynb), and you should **not use Jupyter**.

How and Where to run Spyder:

- Spyder comes as part of the Anaconda package (recall that Jupyter is also part of Anaconda). Here are three options on how to run Spyder:
 - (1) You can choose to install [Anaconda](#) on your personal device (if not done already).
 - (2) You can open Anaconda on any University of Nottingham computer.
 - (3) You can open a [UoN Virtual Desktop](#) on your own personal device, which is virtually the same as logging onto a University of Nottingham computer, but through the virtual desktop. The simply open Anaconda. Here is [further info on the UoN Virtual Desktop](#).
- The A18 Computer Room in the Mathematical Sciences building has a number of computers available, as well as desks with dual monitors that you can plug into your own laptop.

Time-tabled Support Sessions (Mondays 12-1pm, Fridays 11-12noon, ESLC C13 Computer Room):

- You can work on the coursework whenever you prefer.
- We especially encourage you to work on it during the (optional) time-tabled drop-in sessions.

Piazza (<https://piazza.com/class/l7z5sbys7m74fq>):

- You are allowed and certainly encouraged(!) to also ask questions using Piazza to obtain clarification of the coursework questions, as well as general Python queries.
- However, **when using Piazza, please ensure that you are not revealing any answers to others**. Also, **please ensure that you are not directly revealing any code that you wrote**. Doing so is considered Academic Misconduct.
- **When in doubt, please simply attend a drop-in session to meet with a PGR Teaching Assistant or the Lecturer.**

Helpful resources:

- [Python 3 Online Documentation](#) – [Spyder IDE \(integrated development editor\)](#) – [NumPy User Guide](#) – [Matplotlib Quick Start Guide](#) – [Moodle: Core Programming 2021-2022](#) – [Moodle: Core Programming 2020-2021](#)
- You are expected to have basic familiarity with Python, in particular: logic and loops, functions, NumPy and matplotlib.pyplot. **Note that it will always be assumed that the package numpy is imported as np, and matplotlib.pyplot as plt.**

Some Further Advice:

- Write your code as neatly and read-able as possible so that it is easy to follow. Add some comments to your code that indicate what a piece of code does. Frequently run your code to check for (and immediately resolve) mistakes and bugs.
- Coursework Questions with a “*” are more tedious, but can be safely skipped, as they don’t affect follow-up questions.

Submission Procedure:

- Submission will open **after 28 November 2022**.
- To submit, simply upload the requested .py-files on [Moodle](#). (Your submission will be checked for plagiarism using *turnitin*.)
- Your work will be marked (mostly) automatically: This is done by running your functions and comparing their output against the true results.

Getting Started:

- Download the contents of the “**Coursework 2 Pack**” folder from [Moodle](#) into a single folder. (More files may be added in later weeks.)

► Gaussian elimination without pivoting

(This is a warm up exercise. No marks will be awarded for it. Its solution is available on Moodle as file warmup_solution.py. Further clarification of what you need to do to obtain marks is given in Question 2 below.)

Let $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$. Suppose that A is such that there exists a unique solution $x \in \mathbb{R}^n$ to $Ax = b$ and that forward elimination can be performed without any row interchanges to arrive at an augmented matrix to which backward substitution can be applied to find x .

- 1 Open the file `warmup.py`. Note that this file already contains an unfinished function with the following first line:

```
def no_pivoting(A,b,n,c)
```

This function returns the output M which is of type `numpy.ndarray` and has shape $(n, n + 1)$. The input A is of type `numpy.ndarray` and has shape (n, n) and represents the square matrix A . The input b is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the column vector b . The input n is an integer such that $n \geq 2$. The input c is an integer such that $1 \leq c \leq n - 1$, and it is used to (prematurely) stop the forward elimination algorithm; see details below.

- A pseudocode algorithm for performing forward elimination without row interchanges on the matrix $M \in \mathbb{R}^{n \times n+1}$ is the following:

```

For  $i = 1$  to  $n - 1$  do
    For  $j = i + 1$  to  $n$  do
        Set  $g = m_{j,i}/m_{i,i}$ 
        Set  $m_{j,i} = 0$ 
        For  $k = i + 1$  to  $n + 1$  do
            Set  $m_{j,k} = m_{j,k} - gm_{i,k}$ 
        End do
    End do
End do

```

In the above pseudocode algorithm, the entries of the matrix M are $m_{i,j}$ for $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, n + 1$. However, the elements in M (a `numpy.ndarray` with shape $(n, n + 1)$) are $M[i, j]$ for $i = 0, 1, \dots, n - 1$ and $j = 0, 1, \dots, n$.

- Complete the `no_pivoting` function so that the output M is an array representing the augmented matrix arrived at by starting from the augmented matrix $[A \ b]$ and performing forward elimination without row interchanges until all of the entries below the main diagonal in the first c columns are 0.
- The `warmup.py` file contains an unfinished function with the following first line:

```
def backward_substitution(M, n)
```

The input M is of type `numpy.ndarray` and has shape $(n, n + 1)$ and represents an augmented matrix of the form $[U \ v]$ where $U \in \mathbb{R}^{n \times n}$ is an upper triangular matrix with all entries on its main diagonal being nonzero and $v \in \mathbb{R}^n$. The input n is an integer such that $n \geq 2$.

- Complete the `backward_substitution` function so that the output x is of type `numpy.ndarray` and has shape $(n, 1)$, and represents the solution x to $Ux = v$.
- Hint:** See Lecture 4 Slides, Algorithm 6.1, Steps 8–9 for a pseudocode of backward substitution.

- The `warmup.py` file contains the following finished function:

```
def no_pivoting_solve(A, b, n)
```

The input A is of type `numpy.ndarray` and has shape (n, n) and represents the matrix A . The input b is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the vector b . The input n is an integer such that $n \geq 2$. The output x is of type `numpy.ndarray` and has shape $(n, 1)$, and represents the solution x to $Ax = b$ computed using Gaussian elimination without pivoting. One may note that the `no_pivoting_solve` function calls the `no_pivoting` and

backward_substitution functions in order to do this.

- Test your no_pivoting and backward_substitution, and the no_pivoting_solve functions by running the main_warmup.py file. For the A, b and n in the main_warmup.py file, with c=1, the output from the no_pivoting function should be:

```
[[ 1.  -5.   1.   7.]  
 [ 0.  50.  10. -64.]  
 [ 0.  35.  -6. -31.]]
```

For the A, b and n in the main_warmup.py file, with c=2, the output from the no_pivoting function should be:

```
[[ 1.  -5.   1.   7. ]  
 [ 0.  50.  10. -64. ]  
 [ 0.   0. -13.  13.8]]
```

The output from the backward_substitution function and the no_pivoting_solve function obtained by running the main_warmup.py file should be:

```
[[ 2.72307692]  
 [-1.06769231]  
 [-1.06153846]]
```

► **Gaussian elimination with scaled partial pivoting**

Let $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$. Suppose that A is such that there exists a unique solution $x \in \mathbb{R}^n$ to $Ax = b$ and that forward elimination with scaled partial pivoting can be performed to arrive at an augmented matrix to which backward substitution can be applied to find x .

2 A pseudocode algorithm for finding the smallest positive integer p such that

$$|v_p| = \max_{j \in \{1, 2, \dots, n\}} |v_j|$$

is the following:

Set $m = 0$

Set $p = 0$

For $j = 1$ to n do

 If $|v_j| > m$

 Set $m = |v_j|$

 Set $p = j$

 End If

End do

- Open the file `systemsolvers.py`. The `systemsolvers.py` file contains an unfinished function with the following first line:

```
def find_max(M,s,n,i)
```

The input M is of type `numpy.ndarray` and has shape $(n, n + 1)$. The input s is of type `numpy.ndarray` and has shape $(n,)$ and is such that all of its elements are positive. The input n is an integer such that $n \geq 2$. The input i is a nonnegative integer such that $i \leq n - 2$.

- Complete the `find_max` function so that the output p is of type `int` and is the smallest integer such that $p \geq i$ and

$$\frac{|M[p, i]|}{s[p]} = \max_{j \in \{i, i+1, \dots, n-1\}} \frac{|M[j, i]|}{s[j]}.$$

Hint: To calculate the absolute value, one can use the command `abs`, `np.abs` or `np.absolute`; see numpy.org/doc.

- Test your `find_max` ~~scaled partial pivoting and app solve functions~~ by running the `main.py` file. The output from the `find_max` function obtained by running the `main.py` file should be $p = 1$ (because $\frac{|M[j, 0]|}{s[j]}$ is 0.2, 0.5 and 0.5, for $j = 0, 1, 2$, respectively).

Sentence
corrected on
18 Oct, 11am
←

► Assessment

When submitting your coursework, you will only be asked to upload your `systemsolvers.py` file.

Marks can be obtained for your `find_max` function definition for generating the required output, for certain set(s) of inputs for $\{M, s, n, i\}$. The correctness of the following will be checked:

[8 / 40]

- The type of output p
- The value of output p .

- 3 • The `systemsolvers.py` file contains an unfinished function with the following first line:

```
def scaled_partial_pivoting(A,b,n,c)
```

The input A is of type `numpy.ndarray` and has shape (n, n) and represents the square matrix A . The input b is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the column vector b . The input n is an integer such that $n \geq 2$. The input c is an integer such that $1 \leq c \leq n - 1$, and it is used to (prematurely) stop the forward elimination with scaled partial pivoting algorithm; see details below.

- Complete the `scaled_partial_pivoting` function so that the output M is of type `numpy.ndarray` and has shape $(n, n + 1)$, and represents the augmented matrix arrived at by starting from the augmented matrix $[A \ b]$ and performing forward elimination with scaled partial pivoting (as described in the Linear Systems: Direct Methods II slides) until all of the entries below the main diagonal in the first c columns are 0. The `scaled_partial_pivoting` function should call the `find_max` function in order to do this.

Hint: Note that $M[[i,p], :] = M[:, [p,i], :]$ can be used to interchange the row $M[i, :]$ and the row $M[p, :]$. Also note that $s[[i,p]] = s[[p,i]]$ can be used to interchange $s[i]$ and $s[p]$.

- The `systemsolvers.py` file contains an unfinished function with the following first line:

```
def spp_solve(A,b,n)
```

The input A is of type `numpy.ndarray` and has shape (n, n) and represents the matrix A . The input b is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the vector b . The input n is an integer such that $n \geq 2$.

- Complete the `spp_solve` function so that the output x is of type `numpy.ndarray` and has shape $(n, 1)$, and represents the solution x to $Ax = b$ computed using Gaussian elimination with scaled partial pivoting. In order to do this, the `spp_solve` function should call the `scaled_partial_pivoting` function and the `backward_substitution` function. Note that a completed version of the

backward_substitution function is in the warmup_solution module that is imported in systemsolvers.py.

- Test your scaled_partial_pivoting and spp_solve functions by running the main.py file. The output from the scaled_partial_pivoting function obtained by running the main.py file should be:

```
[[ 10.    0.   20.    6. ]
 [  0.   -5.   -1.   6.4]
 [  0.   10.  -11.    1. ]]
```

The output from the spp_solve function obtained by running the main.py file should be:

```
[[ 2.72307692]
 [-1.06769231]
 [-1.06153846]]
```

► Assessment

When submitting your coursework, you will only be asked to upload your systemsolvers.py file.

Marks can be obtained for your scaled_partial_pivoting function definition for generating the required output, for certain set(s) of inputs for $\{A, b, n, c\}$. The correctness of the following will be checked:

[10 / 40]

- The type of output M
- The np.shape of output M
- The values of output M.

Marks can be obtained for your spp_solve function definition for generating the required output, for certain set(s) of inputs for $\{A, b, n\}$. The correctness of the following will be checked:

- The type of output x
- The np.shape of output x
- The values of output x.

Note that in marking your work, different input(s) may be used.

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► **PLU factorisation**

Given an appropriate matrix $A \in \mathbb{R}^{n \times n}$, a pseudocode algorithm for obtaining a permutation matrix P , a lower triangular matrix L and an upper triangular matrix U such that $A = PLU$ is the following:

Set $P = I$, the $n \times n$ identity matrix

Set L to be the $n \times n$ zero matrix

Set $U = A$

For $i = 1$ to $n - 1$ do

Find the smallest integer s such that $i \leq s \leq n$ and $|u_{s,i}| > 10^{-15}$

If $s \neq i$

Interchange row i and row s of P

Interchange row i and row s of L

Interchange row i and row s of U

End if

For $j = i + 1$ to n do

Set $l_{j,i} = u_{j,i}/u_{i,i}$

Set $u_{j,i} = 0$

For $k = i + 1$ to n do

Set $u_{j,k} = u_{j,k} - l_{j,i}u_{i,k}$

End do

End do

End do

Set $P = P^T$

Set $L = L + I$

Note: As a first attempt to Question 4, you can ignore the blue parts related to the row interchanges (for P , L and U). Indeed, without the blue parts the algorithm then simply implements the LU factorisation. There is a dedicated test that should work without the blue parts (see below).

- 4 • The `systemsolvers.py` file has been updated to include an unfinished function with the following first line:

```
def PLU(A, n)
```

The input A is of type `numpy.ndarray` and has shape (n, n) and represents an $n \times n$ matrix A which is assumed to be such that the above pseudocode algorithm can be used to obtain a PLU factorisation of A . The input n is an integer such that $n \geq 2$.

- Complete the `PLU` function so that it implements the above pseudocode algorithm for obtaining matrices P , L and U such that $A = PLU$. The output P is of type `numpy.ndarray` and has shape (n, n) and is an array representing the permutation matrix P , the output L is of type `numpy.ndarray` and has shape

(n, n) and is an array representing the lower triangular matrix L , and the output U is of type `numpy.ndarray` and has shape (n, n) and is an array representing the upper triangular matrix U .

- In the pseudocode algorithm, the entries of the matrices P , L and U are, respectively, $p_{i,j}$, $l_{i,j}$ and $u_{i,j}$ for $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, n$. However, the elements in P , L and U are, respectively, $P[i, j]$, $L[i, j]$ and $U[i, j]$ for $i = 0, 1, \dots, n - 1$ and $j = 0, 1, \dots, n - 1$.

Hint: Note that `np.transpose(P)` returns the transpose of P .

Hint: Recall from Question 3, the hint on how to interchange rows in a matrix.

- Test your PLU function by running the updated `main.py` file. There are two test matrices A_1 and A_2 : For A_1 , the PLU function should do a factorisation without doing row exchanges, hence the output should be (for P , L , U , respectively):

```
[[1.  0.  0.]
 [0.  1.  0.]
 [0.  0.  1.]]
[[ 1.  0.  0.]
 [ 1.  1.  0.]
 [ 2. -2.  1.]]
[[ 1. -1.  2.]
 [ 0. -1. -3.]
 [ 0.  0. -8.]]
```

For A_2 , the PLU function should do a factorisation involving row exchanges, and the output should be:

```
[[1.  0.  0.]
 [0.  0.  1.]
 [0.  1.  0.]]
[[1.  0.  0.]
 [2.  1.  0.]
 [1.  0.  1.]]
[[ 1. -1.  2.]
 [ 0.  2. -2.]
 [ 0.  0. -3.]]
```

► Assessment

When submitting your coursework, you will only be asked to upload your `systemsolvers.py` file.

Marks can be obtained for your **PLU** function definition for generating the required output, for certain set(s) of inputs for $\{A, n\}$. The correctness of the following will be checked:

- The values of outputs P , L , and U .

Note that in marking your work, different input(s) may be used.

[12 / 40]

(turn page)

► Jacobi method

Suppose $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$, and $x \in \mathbb{R}^n$ is the unique solution to $Ax = b$. Let $x^{(k)}$ be the approximation to x obtained after performing k iterations of the Jacobi method, starting from the initial approximation $x^{(0)}$.

- 5 The `systemsolvers.py` file has been updated to include an unfinished function with the following first line:

```
def Jacobi(A,b,n,x0,N):
```

- The input A is of type `numpy.ndarray` and has shape (n, n) and represents the square matrix A . The input b is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the column vector b . The input n is an integer such that $n \geq 2$. The input $x0$ is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the initial approximation $x^{(0)}$. The input N is a positive integer that is the number of iterations to be performed.

- Complete the `Jacobi` function so that the output `x_approx` is of type `numpy.ndarray` and has shape $(n, N+1)$ and is such that, for $j = 0, 1, \dots, n-1$, `x_approx[j,0] = $x_{j+1}^{(0)}$` and `x_approx[j,k] = $x_{j+1}^{(k)}$` for $k = 1, 2, \dots, N$.

Hint: You can choose to implement directly the element-based form of the ~~Jacobi method~~ ~~Gauss-Seidel method~~ (see Lecture 7 Slides and Notes), or you can choose to implement a vector-based form of the ~~Jacobi method~~ ~~Gauss-Seidel method~~ (see also Lecture 7). The following functions could be useful: `np.dot`, `np.tril`, `np.triu`, `np.diag`, `np.linalg.inv`, `np.matmul` or the '@' operator for matrix multiplication.

- Test your `Jacobi` function by running the updated `main.py` file. The output from the `Jacobi` function obtained by running the `main.py` file should be:

```
[[ 0.    12.    12.375]
 [ 0.     1.5     3.75 ]
 [ 0.     6.     6.375]]
```

Sentence
corrected on
25 Oct, 12noon

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←

► Assessment

When submitting your coursework, you will only be asked to upload your `systemsolvers.py` file.

Marks can be obtained for your `Jacobi` function definition for generating the required output, for certain set(s) of inputs for $\{A, b, n, x0, N\}$. The correctness of the following will be checked:

[6 / 40]

- The type of output `x_approx`
- The `np.shape` of output `x_approx`
- The values of output `x_approx`.

(turn page)

- 6 The `systemsolvers.py` file contains an unfinished function with the following first line:

```
def Jacobi_plot(A,b,n,x0,N):
```

- The input `A` is of type `numpy.ndarray` and has shape (n, n) and represents the square matrix A . The input `b` is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the column vector b . The input `n` is an integer such that $n \geq 2$. The input `x0` is of type `numpy.ndarray` and has shape $(n, 1)$ and represents the initial approximation $x^{(0)}$. The input `N` is a positive integer that is the number of iterations to be performed.

- Complete the `Jacobi_plot` function so that it plots (in the same figure using the same axes) $\|x - x^{(k)}\|_\infty$ for $k = 0, 1, \dots, N$ and $\|x - x^{(k)}\|_2$ and ~~$\|x - x^{(k)}\|_\infty$~~ for $k = 0, 1, \dots, N$. The approximations $x^{(k)}$ to x should be computed by calling the `Jacobi` function. The solution x to $Ax = b$ should be computed by calling the `no_pivoting_solve` function. Note that a completed version of the `no_pivoting_solve` function is in the `warmup_solution` module that is imported in `systemsolvers.py`.

Hint: To calculate the l_∞ norm of a one-dimensional array v , one can use the command `np.linalg.norm(v, np.inf)`; see numpy.org/doc.

Hint: To calculate the l_2 norm of a one-dimensional array v , one can use the command `np.linalg.norm(v, 2)`; see numpy.org/doc.

Hint: If `w` is of type `numpy.ndarray` and has shape (n, m) and `p` is a nonnegative integer less than `m` then `w[0:n-1, p]` is of type `numpy.ndarray` and has shape $(n,)$ not $(n, 1)$.

- Test your `Jacobi_plot` function by running the updated `main.py` file.

► Assessment

When submitting your coursework, you will only be asked to upload your `systemsolvers.py` file.

Marks can be obtained for your `Jacobi_plot` function definition for generating the required output, for certain set(s) of inputs for $\{A, b, n, x0, N\}$. The correctness of the following will be checked:

- The points plotted.

Note that in marking your work, different input(s) may be used.

Sentence
corrected on
26 Oct, 4:30pm
←

[4 / 40]

► Finished!