

project3_demo1

December 3, 2024

1 Finite Difference method for solving discrete Laplace Equation

1.0.1 Exercise 1: solve the 4x4 linear equation $A \cdot x = b$

$$4u[i,j] - u[i-1,j] - u[i+1,j] - u[i,j-1] - u[i,j+1] = 0$$

Derive and solve the linear system $A \cdot x = b$

REF: <https://docs.scipy.org/doc/scipy/reference/generated/scipy.linalg.solve.html#scipy.linalg.solve>

```
[1]: import numpy as np
      from scipy import linalg
      from scipy.linalg import solve
```

```
[59]: A = np.array([
        [4, -1, -1, 0],
        [-1, 4, 0, -1],
        [-1, 0, 4, -1],
        [0, -1, -1, 4]
    ])

    b = np.array([0, 0, 1, 1])

    x = solve(A, b)

    print(x)
```

```
[0.125 0.125 0.375 0.375]
```

1.0.2 Exercise 2: arbitrary size of the matrix.

If we want our solve could solve an arbitrary size of the system $N \times N$ in 2D.

First, we need to generate the left-hand matrix.

The left-hand matrix contains two components: One is an diagonal matrix with only three banded values.

The other component contains negative identity matrix.

we could use the `dia_matrix` in `scipy.sparse` and `np.identity()` for these components.

REF: <https://docs.scipy.org/doc/scipy/reference/sparse.html>

```
[2]: import numpy as np
from scipy.sparse import dia_array # if dia_array is not able, use dia_matrix
from scipy.sparse import dia_matrix
from numba import jit, njit, prange
```

Part 1:

Write a function to generate the matrix A with arbitrary size N.

The shape of the matrix A is (N^2, N^2) .

Hints: depending on your implementation, you might want to use `numba` to speed it up.

We could decompose the matrix into several (N, N) submatrix and initialize the diagonal matrices and the offset terms separately.

```
[3]: def generate_the_laplace_matrix_with_size(N=4):
    """
    assume sqrt(N) is an integer.

    """
    nsq = N*N
    A = np.zeros((nsq, nsq))

    # TODO
    for i in range(N):
        for j in range(N):
            index = i * N + j
            A[index, index] = 4
            if j > 0:
                A[index, index - 1] = -1
            if j < N - 1:
                A[index, index + 1] = -1
            if i > 0:
                A[index, index - N] = -1
            if i < N - 1:
                A[index, index + N] = -1

    return A
```

```
[4]: N = 4
A = generate_the_laplace_matrix_with_size(N)
print(A)
```

```
[ [ 4. -1.  0.  0. -1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
  [-1.  4. -1.  0.  0. -1.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
  [ 0. -1.  4. -1.  0.  0. -1.  0.  0.  0.  0.  0.  0.  0.  0.  0.]
  [ 0.  0. -1.  4.  0.  0.  0. -1.  0.  0.  0.  0.  0.  0.  0.  0.]
  [-1.  0.  0.  0.  4. -1.  0.  0. -1.  0.  0.  0.  0.  0.  0.  0.]
  [ 0. -1.  0.  0. -1.  4. -1.  0.  0. -1.  0.  0.  0.  0.  0.  0.]
  [ 0.  0. -1.  0.  0. -1.  4. -1.  0.  0. -1.  0.  0.  0.  0.  0.]
```

```
[ 0.  0.  0. -1.  0.  0. -1.  4.  0.  0.  0. -1.  0.  0.  0.  0.]
[ 0.  0.  0.  0. -1.  0.  0.  0.  4. -1.  0.  0. -1.  0.  0.  0.]
[ 0.  0.  0.  0.  0. -1.  0.  0. -1.  4. -1.  0.  0. -1.  0.  0.]
[ 0.  0.  0.  0.  0.  0. -1.  0.  0. -1.  4. -1.  0.  0. -1.  0.]
[ 0.  0.  0.  0.  0.  0.  0. -1.  0.  0. -1.  4.  0.  0.  0. -1.]
[ 0.  0.  0.  0.  0.  0.  0.  0. -1.  0.  0.  0.  4. -1.  0.  0.]
[ 0.  0.  0.  0.  0.  0.  0.  0.  0. -1.  0.  0. -1.  4. -1.  0.]
[ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0. -1.  0.  0. -1.  4. -1.]
[ 0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. -1.  0.  0. -1.  4.]]
```

Part2:

The right hand side of the linear equation is a vector.
generate a vector is simple with `np.array()`

```
[4]: def generate_the_rhs_vector_with_size(N=4):
      b = np.zeros(N*N)
      #TODO
      b[-N:] = 1    # Setting the boundary conditions for the first few points
      return b
```

```
[6]: b = generate_the_rhs_vector_with_size(N=N)
      print(b)
```

```
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 1. 1. 1. 1.]
```

Part 3:

Once we have the linear problem $A x = b$, we could solve the system with `scipy.linalg.solve`

REF: <https://docs.scipy.org/doc/scipy/reference/generated/scipy.linalg.solve.html#scipy.linalg.solve>

```
[5]: from scipy import linalg
```

```
[8]: x = linalg.solve(A, b)
```

Part 4:

Once we have the solution, we should convert the solution vector to the finite difference grids `u[i,j]`.

```
[6]: def convert_solution(x):
      usize = np.sqrt(len(x))
      u = x.reshape(int(usize),int(usize)).transpose()
      return u
```

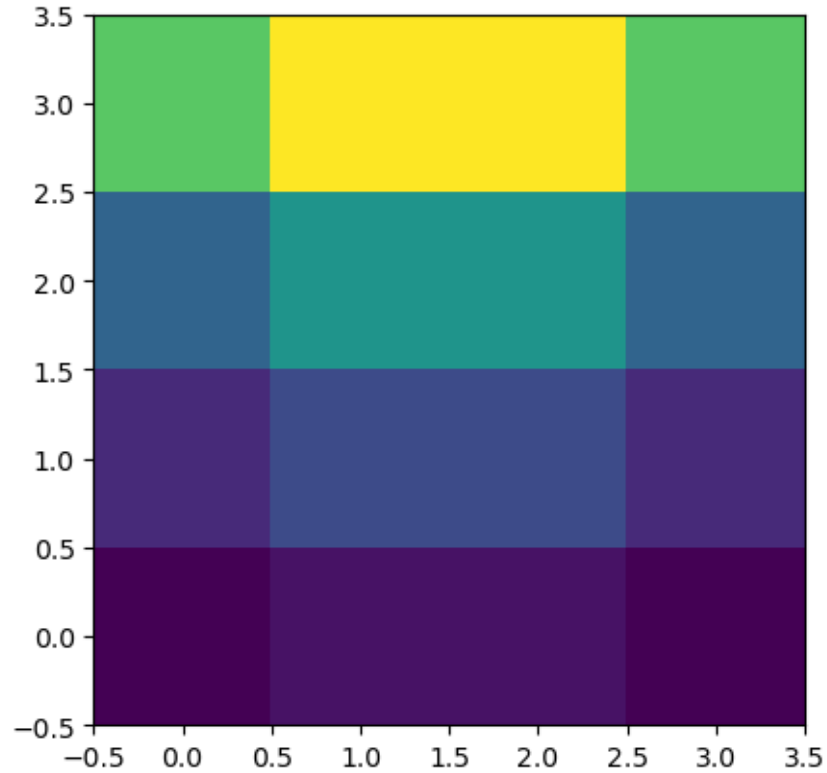
Part 5:

Now, let's visualize the solution with `matplotlib`

```
[7]: import matplotlib.pyplot as plt
```

```
[11]: u = convert_solution(x)
plt.imshow(u.T,origin="lower")
```

```
[11]: <matplotlib.image.AxesImage at 0x21b672181d0>
```



Part 6:

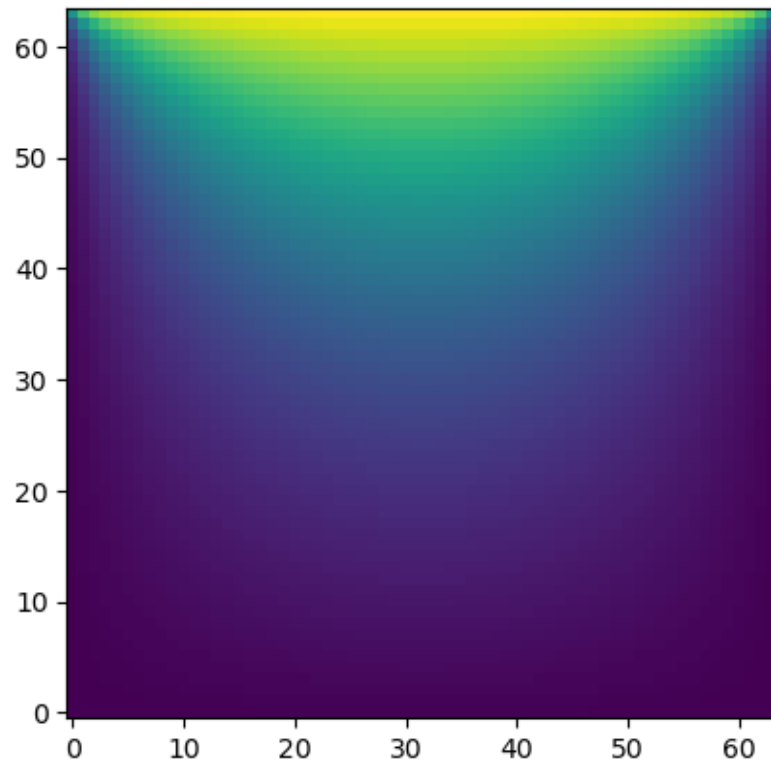
Now we have tested our code, we could write a “solver” function to wrap all necessary codes. This solver function could be either in the notebook or in a separate python file.

```
[8]: def solve_laplace(N=16):
      A = generate_the_laplace_matrix_with_size(N=N)
      b = generate_the_rhs_vector_with_size(N=N)
      x = linalg.solve(A,b)
      u = convert_solution(x)
      return u
```

```
[13]: u = solve_laplace(N=64)
```

```
[14]: plt.imshow(u.T,origin="lower")
```

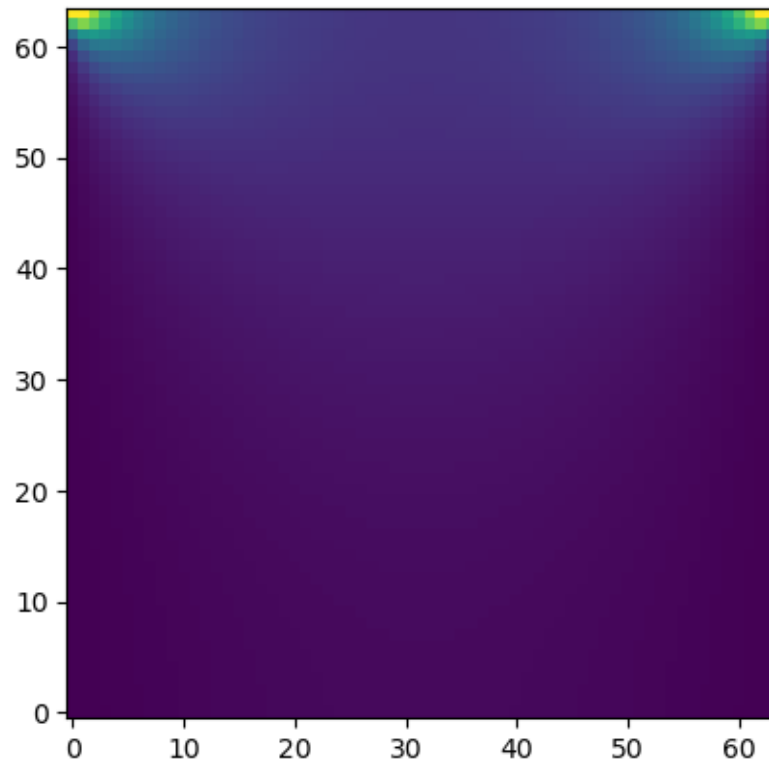
```
[14]: <matplotlib.image.AxesImage at 0x21b07186e90>
```



```
[15]: field = np.gradient(u)
```

```
[16]: plt.imshow(field[1].T,origin="lower")
```

```
[16]: <matplotlib.image.AxesImage at 0x21b672083d0>
```



Part 7:

The bottleneck of this solver is in the `linalg.solve()`.

Let's measure the performance of `linalg.solve()` with different resolutions.

```
[9]: import time

[13]: resolutions = np.array([8,16,32,64,128])
      times      = np.zeros(len(resolutions))

      for i, N in enumerate(resolutions):
          print("Measuring resolution N = ", N)
          A = generate_the_laplace_matrix_with_size(N)
          b = generate_the_rhs_vector_with_size(N)
          t1 = time.time()
          x = linalg.solve(A,b)
          t2 = time.time()
          times[i] = (t2-t1)
```

```
Measuring resolution N = 8
Measuring resolution N = 16
Measuring resolution N = 32
Measuring resolution N = 64
```

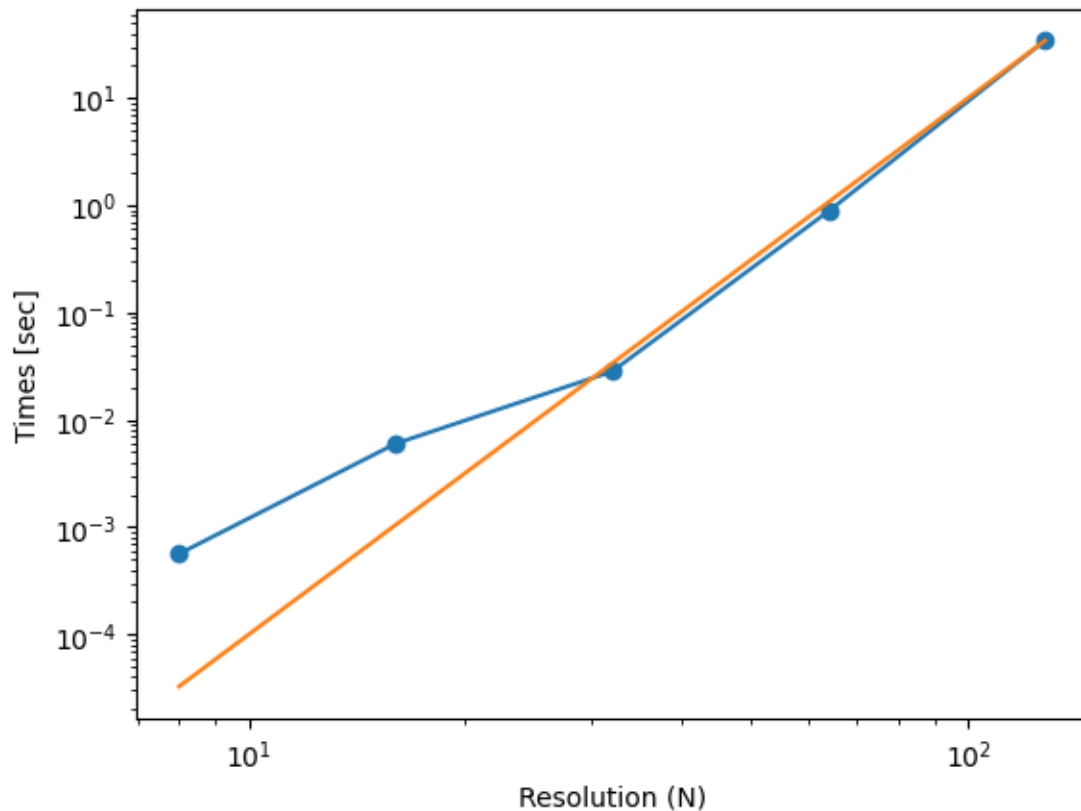
Measuring resolution $N = 128$

Part 8:

Plot Computing time vs N in log-log scale.

```
[12]: plt.figure(1)
plt.plot(resolutions,times,'-o')
plt.plot(resolutions,times[-1]*resolutions**5/resolutions[-1]**5)
plt.xscale('log')
plt.yscale('log')
plt.xlabel("Resolution (N)")
plt.ylabel("Times [sec]")
```

```
[12]: Text(0, 0.5, 'Times [sec]')
```



You could see that the performance is proportional to N^5 !

This is because the size of the matrix A is proportional to N^2 and the calculation time of `linalg.solve(M,b)` is proportional to the cubic of the size of M , N^3 , giving N^5 at the end.

The `scipy.linalg.solve` is robust, but since the matrix A is a sparse matrix, we could use special method to solve it.

REF: <https://docs.scipy.org/doc/scipy/reference/generated/scipy.sparse.linalg.spsolve.html>

```
[10]: from scipy.sparse import csc_matrix
import scipy.sparse.linalg as splinalg
```

```
[14]: N = 16
A = generate_the_laplace_matrix_with_size(N)
A = csc_matrix(A)
b = generate_the_rhs_vector_with_size(N)
x = splinalg.spsolve(A,b)
```

Let's measure the performance again with `spsolve()`

```
[16]: resolutions = np.array([8,16,32,64,128,256])
times_sp = np.zeros(len(resolutions))

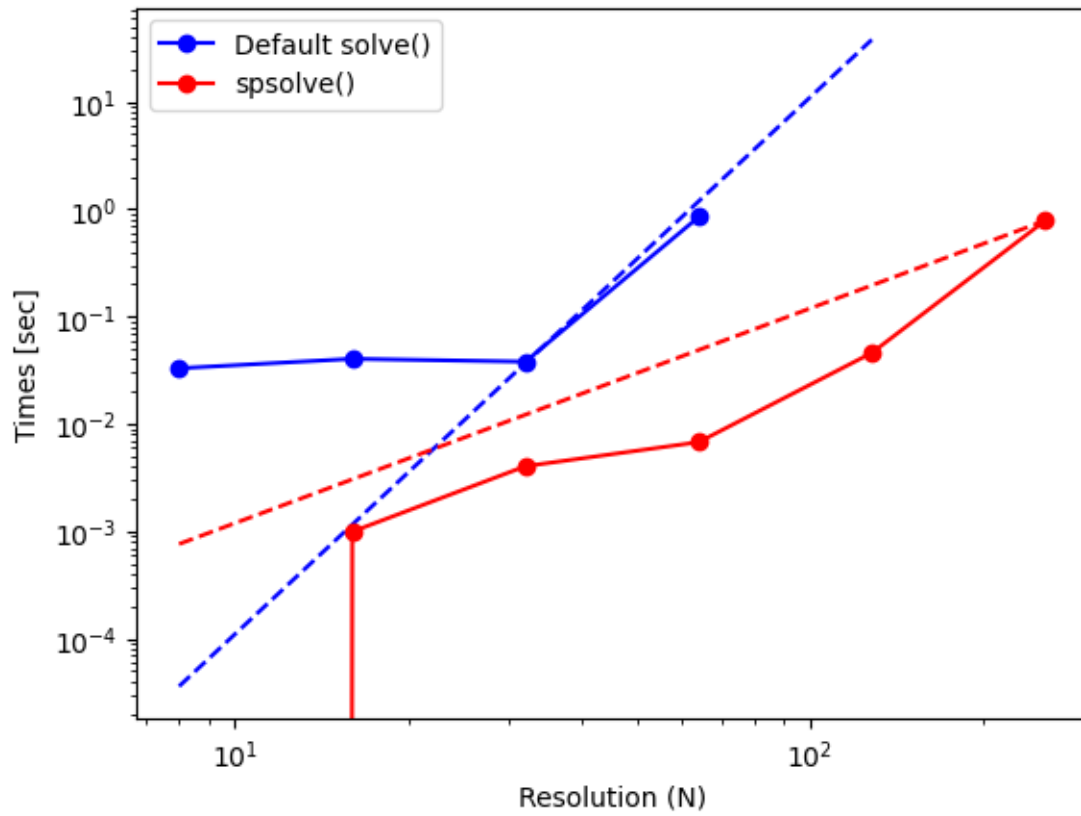
for i, N in enumerate(resolutions):
    print("Measuring resolution N = ", N)
    A = generate_the_laplace_matrix_with_size(N)
    A = csc_matrix(A)
    b = generate_the_rhs_vector_with_size(N)
    t1 = time.time()
    x = splinalg.spsolve(A,b)
    t2 = time.time()
    times_sp[i] = (t2-t1)
```

```
Measuring resolution N = 8
Measuring resolution N = 16
Measuring resolution N = 32
Measuring resolution N = 64
Measuring resolution N = 128
Measuring resolution N = 256
```

```
[17]: resolutions1 = np.array([8,16,32,64,128])

plt.figure(1)
plt.plot(resolutions1[:-1],times[:-1], 'b-o',label="Default solve()")
plt.plot(resolutions1,times[-1]*resolutions1**5/resolutions1[-1]**5, 'b--')
plt.plot(resolutions,times_sp, 'r-o', label="spsolve()")
plt.plot(resolutions,times_sp[-1]*resolutions**2/resolutions[-1]**2, 'r--')
plt.xscale('log')
plt.yscale('log')
plt.legend(loc='upper left')
plt.xlabel("Resolution (N)")
plt.ylabel("Times [sec]")
```

```
[17]: Text(0, 0.5, 'Times [sec]')
```

You got several orders of speedup if you know the matrix is a sparse matrix.