

PHYS-E0412 Computational Physics -Homework 7

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a) Dimension 1. Implement a solver for the one-dimensional problem

```
In [198]: import numpy as np
import matplotlib.pyplot as plt
```

Function for calculating the solution for one dimensional problem.

```
In [207]: def oned_solve(N):
    h = 1 / (N - 1)

    a = np.diag(np.ones(N))
    b = np.diag(np.ones(N-1), k = 1)
    c = np.diag(np.ones(N-1), k = -1)

    #constructing the stencil from the diagonal matrices
    s = (- b + 2 * a - c)

    #boundary conditions
    s[0,0] = 1
    s[0, 1] = 0
    s[-1,-1] = 1
    s[-1, -2] = 0

    #scaling
    s *= 1 / h**2

    #sampling the u''(x)
    x = np.linspace(0, 1, N)
    b = (x - 0.5)**3 - 2*(x - 0.5)

    #boundary conditions
    b[0] = 0
    b[-1] = 0

    #solve and return the linear system
    return np.linalg.solve(s, b)
```

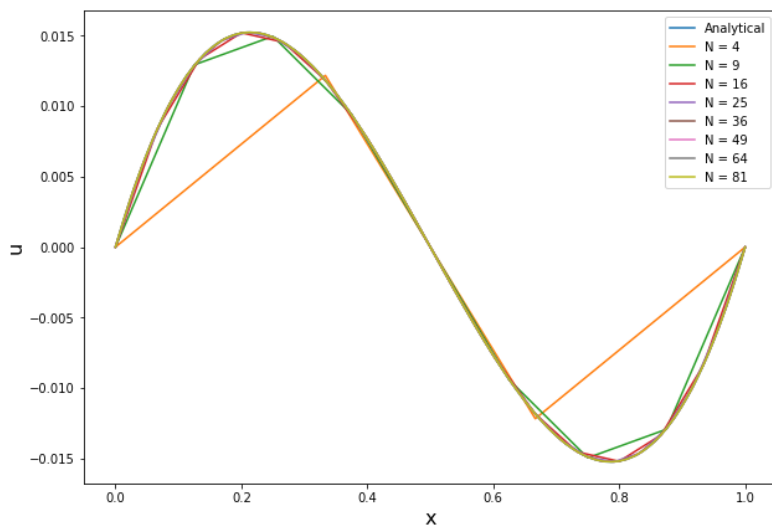
Analytical solution for the function u calculated symbolically.

```
In [200]: def analytical(N):
    x = np.linspace(0, 1, N)
    return -1./20 * (x-0.5) ** 5 + x**3 / 3. - x**2 / 2. +163 * x / 960. - 1./640
```

Plotting u with multiple grid spacings and comparing them to the analytical solution. We see that the solution converges to the analytical solution rather quickly.

```
In [201]: x = np.linspace(0,1,100)
plt.figure(1, (10, 7))
plt.plot(x, analytical(100), label = "Analytical")
for i in range(2, 10):
    N = i ** 2
    x = np.linspace(0, 1, N)
    plt.plot(x, oned_solve(N), label = "N = " + str(i ** 2))

plt.xlabel("x", size = 16)
plt.ylabel("u", size = 16)
plt.legend()
plt.show()
```

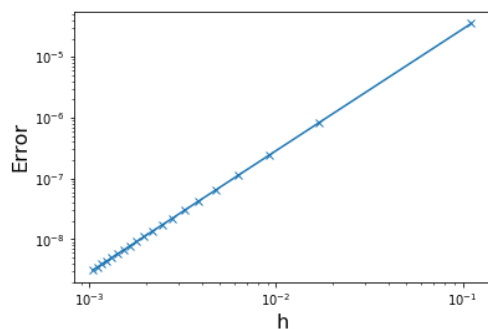


The error can be calculated using formula $\sqrt{h} \|u_{\text{analytical}} - u\|$.

```
In [204]: def error(N):
    h = 1 / (N - 1)
    return np.sqrt(h) * np.linalg.norm(analytical(N) - oned_solve(N))

In [208]: N = np.array(list(range(10, 1000, 50)))

#calculating the error with different values of N and plotting them.
errors = [error(i) for i in N]
plt.loglog(1 / (N-1), errors, marker = "x")
plt.xlabel("h", size = 16)
plt.ylabel("Error", size = 16)
plt.show()
```



From the loglog plot we can see that the error converges with some power law as a function of the grid spacing.

```
In [209]: #fitting a linear model
np.polyfit(np.log(1 / (N-1)), np.log(errors), 1)

Out[209]: array([ 1.9997664 , -5.85304734])
```

If we fit a line to the logarithm we can see that the speed of convergence is about h^2 .

b) Change the boundary conditions to $u(0) = 0$, $u'(1) = 0$

Let's make a new function that implements the new boundary conditions using backwards scheme for first order finite difference.

```
In [210]: def neumann_oned_solve(N):
h = 1 / (N - 1)

a = np.diag(np.ones(N))
b = np.diag(np.ones(N-1), k = 1)
c = np.diag(np.ones(N-1), k = -1)

s = (- b + 2 * a - c)

#new boundary conditions, this time with backwards finite difference scheme for u'(1)
s[0,0] = 1
s[0, 1] = 0
s[-1,-1] = 1
s[-1, -2] = -1

s *= 1 / h**2

x = np.linspace(0, 1, N)
b = (x - 0.5)**3 - 2*(x - 0.5)

b[0] = 0
b[-1] = 0

return np.linalg.solve(s, b)
```

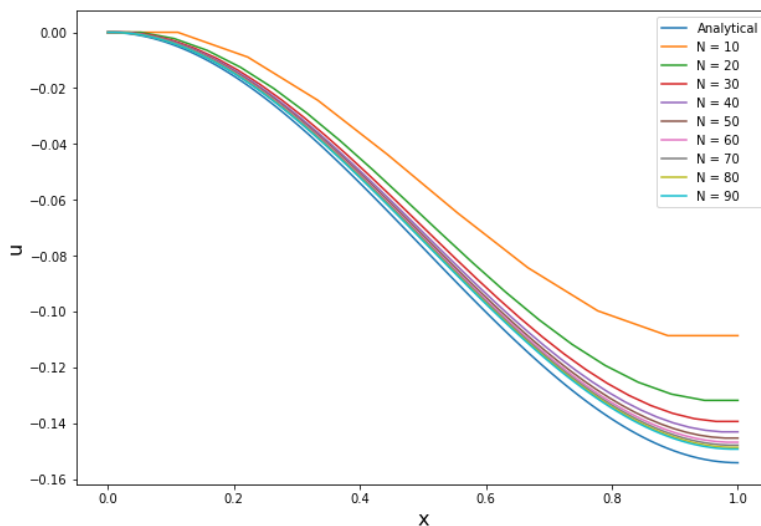
Again the analytical solutions is obtained symbolically.

```
In [9]: def neumann_analytic(N):
x = np.linspace(0, 1, N)
return -(1 / 20 * x**5 - 1/8* x**4 - 5/24* x**3 + 7/16* x **2)
```

If we again calculate values for u with different grid spacings we see that the solution converges to the analytical at some rate.

```
In [34]: x = np.linspace(0,1,100)
plt.figure(1, (10,7))
plt.plot(x, neumann_analytic(100), label = "Analytical")
for i in range(1, 10):
    N = i * 10
    x = np.linspace(0, 1, N)
    plt.plot(x, neumann_oned_solve(N), label = "N = " + str(i * 10))

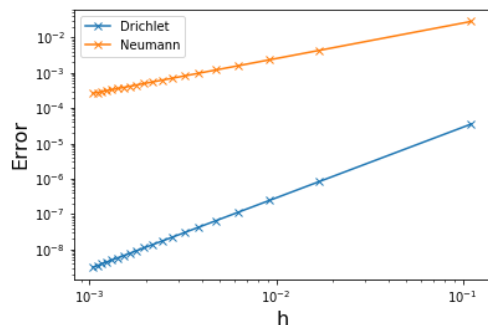
plt.xlabel("x", size = 16)
plt.ylabel("u", size = 16)
plt.legend()
plt.show()
```



```
In [11]: def neumann_error(N):
h = 1 / (N - 1)
return np.sqrt(h) * np.linalg.norm(neumann_analytic(N) - neumann_oned_solve(N))
```

```
In [206]: N = np.array(list(range(10, 1000, 50)))

neumann_errors = [neumann_error(i) for i in N]
errors = [error(i) for i in N]
plt.loglog(1/(N-1), errors, marker = "x", label = "Dirichlet")
plt.loglog(1/(N-1), neumann_errors, marker = "x", label = "Neumann")
plt.xlabel("h", size = 16)
plt.ylabel("Error", size = 16)
plt.legend()
plt.show()
```



```
In [13]: np.polyfit(np.log(1 / (N-1)), np.log(neumann_errors), 1)
```

```
Out[13]: array([ 1.00224725, -1.36165818])
```

Again if we fit a line to the loglog plot we see that the convergence follows a power law, but at this time it is just linearly. The rate is thus lower than with the dirichlet boundary conditions.

If we put Neumann boundary conditions on both edges we get a singular solution.

c) Dimension 2. Implement a solver for the two-dimensional problem

```
In [176]: def d2(N):
    #constructing the D matrix for 5 point stencil
    D = 4 * np.diag(np.ones(N)) - np.diag(np.ones(N-1), k = -1) - np.diag(np.ones(N-1), k = 1)

    #boundary conditions
    D[0] = D[-1] = 0
    D[0,0] = D[-1,-1] =

    #identity matrix for off diagonals
    I = np.diag(np.ones(N))
    IO = np.copy(I)

    #boundary conditions
    IO[0] = IO[-1] = 0

    s = np.diag(np.zeros(N**2))

    #filling the stencil with block matrices
    for i in range(0, N):
        if i == 0:
            #first row
            s[:,0:N] = I
        elif i == N - 1:
            #last row
            s[i*N:,N*i:] = I
        else:
            #other rows
            s[i*N:(i+1)*N,N*(i-1):N*(i+2)] = np.hstack((-IO,D,-IO))

    #scaling
    s *= 1 / (1 / (N-1)**2)

    #the b matrix
    b = np.zeros((N,N))
    x = y = np.linspace(0,1,N)

    #calculating the values
    for i in range(N):
        for j in range(N):
            b[i, j] = np.exp(-((x[i] - 0.5)**2 + (y[j]-0.5)**2) / 18)

    #boundary conditions
    b[0,:] = 0
    b[:,0] = 0
    b[-1,:] = 0
    b[:,-1] = 0

    #flatten the matrix for 1-d array
    b = b.flatten()

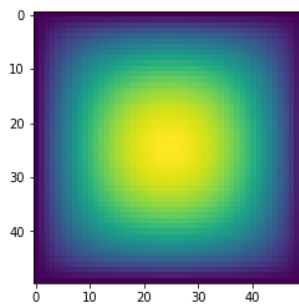
    #solve the system
    z = np.linalg.solve(s, b).reshape((N,N))

    return x,y,z
```

Plotting a heatmap of the solution

```
In [194]: plt.imshow(d2(50)[-1])
```

```
Out[194]: <matplotlib.image.AxesImage at 0x7efe55e3f940>
```



Same in 3D

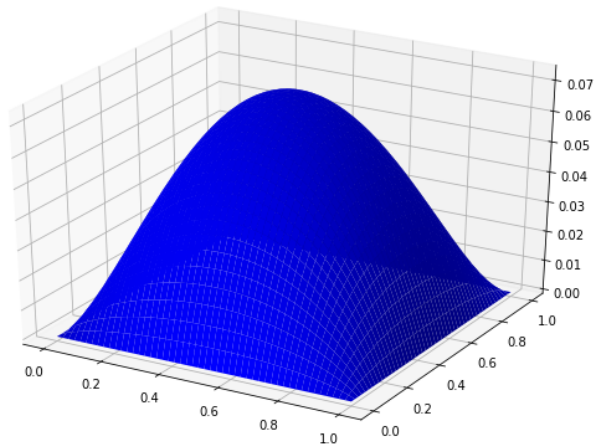
```
In [197]: from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
import numpy as np

fig = plt.figure(1, (10, 7))
ax = fig.add_subplot(111, projection='3d')

sol = d2(50)

X, Y = np.meshgrid(sol[0], sol[1])
# Plot the surface
ax.plot_surface(X, Y, sol[2], color='b')

plt.show()
```



We seem to get a solution with this solver.

Since this problem does not have an analytical solution we can investigate the error by calculating the solution with a dense grid and see how the solution converges to that.

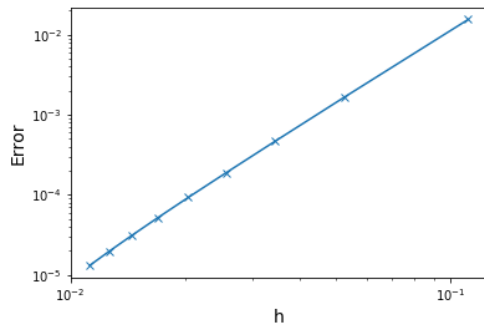
```
In [212]: from scipy.interpolate import interp2d
```

```
In [213]: analytical = d2(100)
```

```
In [217]: errors = []
hs = []
for i in range(10, 100, 10):
    hs.append(1 / (i - 1))
    print(i)
    s = d2(i)
    #interpolate the sparser solution unto a tighter "analytical solution" grid
    interp = interp2d(s[0], s[1], s[2])
    polated = interp(analytical[0], analytical[1])
    #calculate the error as the Frobenius norm of the solution matrices
    errors.append(np.linalg.norm(analytical[2] - polated)* 1 / (i - 1))

10
20
30
40
50
60
70
80
90
```

```
In [218]: plt.loglog(hs, errors, marker = "x")
plt.xlabel("h", size = 14)
plt.ylabel("Error", size = 14)
plt.show()
```



```
In [219]: np.polyfit(np.log(hs), np.log(errors), 1)
```

```
Out[219]: array([3.0820963 , 2.66533682])
```

Again if we fit a line we see that the convergence rate is about h^3

d) I used 8 hours for this exercise