Numerical solution for 1-D Poisson(Laplace) equation

Assignment #3

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For the students who are studying the quantum mechanics, the 1-D infinite potential problem is very basic problem to understand the wave property.

In this assignment, we use numerical method for solving the Laplace and Poisson equation. Basically those two equations have same structure. In the electrodynamics, the Poisson's equation and Laplace equation give us the electric field properties correspond to the given boundary condition and the source distribution.

The Poisson equation is as follows:

$$\nabla^2 \Phi(\mathbf{r}) = s(\mathbf{r})$$

If the source function is zero then we call those equation as Laplace equation.

Problem 1.

Solve the Laplace equation with boundary condition $\Phi(\mathrm{a}) = -1, \Phi(0) = 1$.

Analytical solution

$$\nabla^2 \Phi(x) = 0$$

$$\nabla \Phi(x) = \mathrm{C}_1$$

$$\Phi(x) = \mathrm{C}_1 x + \mathrm{C}_2$$

By applying boundary condition, we can get exact solution.

$$\Phi(x) = -\frac{2}{a}x + 1$$

For convenience of the calculation. I assume the constant <u>'a' as 1.</u>

Numerical solution

Likewise, the potential well problem, we should treat second derivative numerically. Which is:

$$\frac{d^2}{dx^2}\Psi(x_n) \approx \frac{\Psi(x_{n-1}) - 2\Psi(x_n) + \Psi(x_{n+1})}{\Delta x^2} = 0$$

In case of N=5, we can build the equation as follows

Ax=b, where A is the N×N matrix and x and b is N×1 vectors.

$$
A\Phi = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 & 0 & 0 \\ 0 & 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 & 0 \\ 0 & 0 & 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 \\ 0 & 0 & 0 & 0 & 1/(\Delta x)^2 \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -1 \end{bmatrix} = b
$$

The number ‘1’ and ‘-1’ is the boundary condition in this problem.

```
prompt = 'What is the number N?';
N= input(prompt);

A=[];
A(1,1)=1;
A(N,N)=1;

for i=2:(N-1);
    A(i,i-1)=1/(1/(N-1))^2;
    A(i,i)=-2/(1/(N-1))^2;
    A(i,i+1)=1/(1/(N-1))^2;

end

b=zeros(N,1);
b(N,1)=-1;
b(1,1)=1;

x=A₩b;
y=0:1/(N-1):1;

plot(y,x(:,1))
xlabel('x');
ylabel('₩Phi');
```

The figure 1 shows N = 5 and figure 2 shows N= 500 cases.

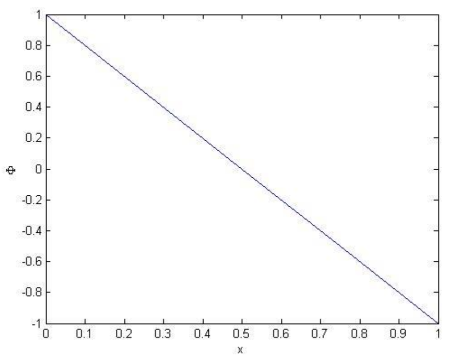


Figure 1 N= 5 case

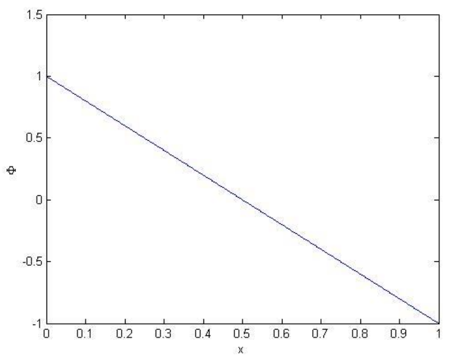


Figure 2 N= 500 case

Problem 2.

Solve the Poisson equation with boundary condition $\Phi(\mathrm{a}) = 0, \Phi(0) = 0$. For convenience of the calculation, we assume a=1.

Analytical solution

$$\frac{d^2}{dx^2}\phi = \delta(x - \tfrac{1}{2}), \quad \phi(0) = \phi(1) = 0.$$

i) $x > \frac{1}{2}$

$$\frac{d^2}{dx^2}\phi = 0.$$

$$\Rightarrow \phi(x) = cx + d.$$

$$\phi(1) = c + d = 0$$

$$\therefore c = -d$$

ii) $x < \frac{1}{2}$

$$\phi(x) = c'x + d'$$

$$\phi(0) = d' = 0$$

iii) Continuity of $\phi(x)$ at $x = \frac{1}{2}$.

$$\therefore \phi(\tfrac{1}{2}) = \frac{1}{2}c + d = -\frac{1}{2}c = \frac{1}{2}c'$$

$$\therefore c = -c'$$

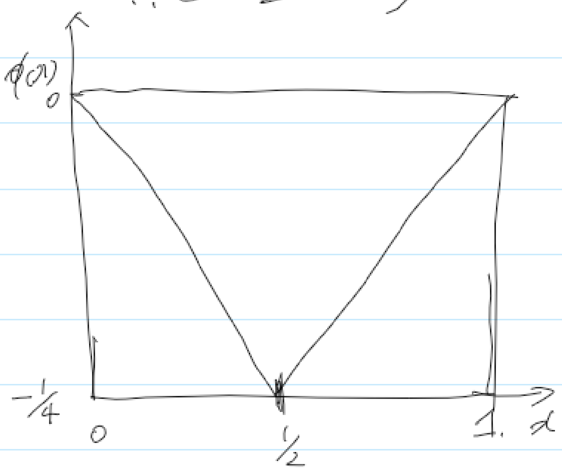
$\therefore c = -c$

iv) near $x = \frac{1}{2}$.

$$\int_{\frac{1}{2}-\epsilon}^{\frac{1}{2}+\epsilon} \phi''(x)\,dx = \int_{\frac{1}{2}-\epsilon}^{\frac{1}{2}+\epsilon} \delta(x-\tfrac{1}{2}) = 1.$$

$$\left.\frac{d\phi}{dx}\right|_{\frac{1}{2}+\epsilon} - \left.\frac{d\phi}{dx}\right|_{\frac{1}{2}-\epsilon} = c - c' = 2c = 1.$$

$\therefore c = \frac{1}{2}$. so, $d = -\frac{1}{2}$, $c' = -\frac{1}{2}$



Numerical solution

This Poisson equation is almost same with P1 in this assignment. However, treat the delta function is only one problem. I use their property for making the numerical version of delta function. That is integration of delta function give us value 1.

Here is delta function code.

```
b=zeros(N,1);

if mod(N,2)==1

    b(((N+1)/2),1)=(N-1);
else

    b((N/2),1)=(N-1)/2;
    b((N/2+1),1)=(N-1)/2;
end
```

And next figure N=5 and N=6 case of delta function graph.

For N = 5(odd number) case, we can choose exact mid-point so, we can set 3rd ((N+1)/2-th)component height as 4 (N-1). However, for the N = 6(even number) there are no component in the mid-point so, we choose two points(3rd and 4th) have 5/2. You can also check their area is nothing but 1.

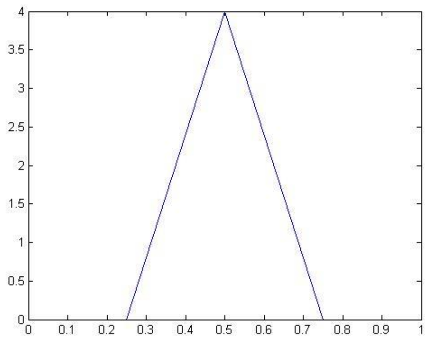


Figure 3 The delta function for N=5

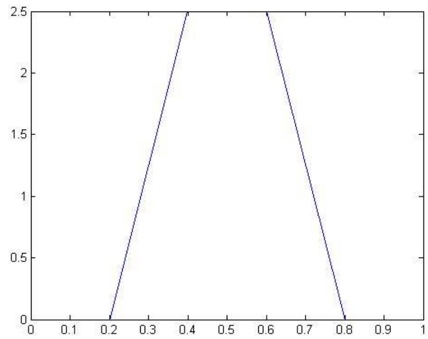
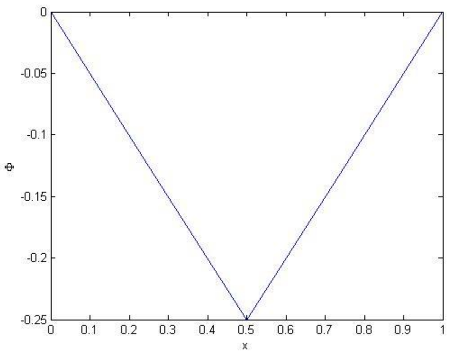
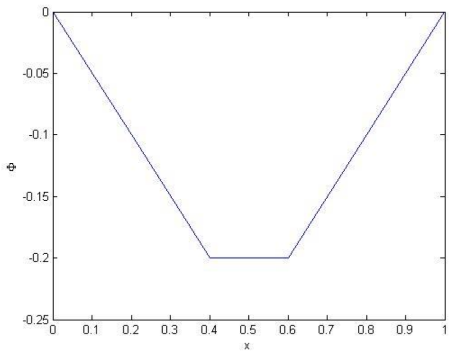
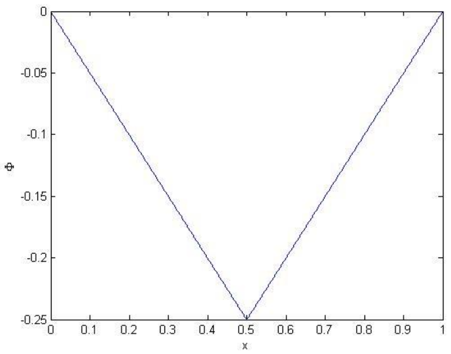
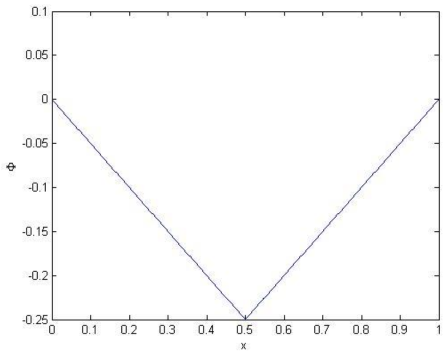


Figure 4 The delta function for N =6

$$A\Phi = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 & 0 & 0 \\ 0 & 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 & 0 \\ 0 & 0 & 1/(\Delta x)^2 & -2/(\Delta x)^2 & 1/(\Delta x)^2 \\ 0 & 0 & 0 & 0 & 1/(\Delta x)^2 \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 4 \\ 0 \\ 0 \end{bmatrix} = b$$

Here are the results for N= 5, 6, 499, 500.

N = odd	N = even
	
N= 5	N = 6
	
N = 499	N = 500

In my choice of delta function, for the odd number, it is exact same even N is small number. However, N = even case, because the delta function has width through mid-point, N = 6 case shows quite similar but near the mid-point is not same as analytical solution. But N = 500 case, because the segment is very small, it is almost same with analytical solution.