

Implementing direct methods for boundary value problems

$$\frac{d^2y}{dx^2} = f(x) \tag{1}$$

Given $y(0) = \alpha$ and $y(1) = \beta$... find $y(x)$.

HERE: $f(x) = x^2 - \frac{1}{2} \sin(6x)$

$y(0) = 4$ and $y(1) = 5$


```
% Plot the result
figure; set(gca,'FontSize',18)
subplot(211)
set(gca,'FontSize',18)
plot(x,y,'o'), title('y(x)')

%Check our answer -- interior points
for j=2:m+1
    yd(j)=(y(j+1)-2*y(j)+y(j-1))/(dx^2);
end

subplot(212)
set(gca,'FontSize',18)
plot(xint,yd(2:m+1),'o'); hold on
plot(xint,f(xint))
title('second deriv of y(x)')
```

A direct approach to energy level (eigenvalue) problem of Schrödinger equation from quantum mechanics:

$$\frac{d^2\psi}{dx^2} + [n_0 - \beta]\psi = 0 \quad (5)$$

Boundary conditions $\psi(\pm 1) = 0$.

QUESTION: what values of β satisfy this?

Discretize:

$$\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\Delta x^2} + (n_0 - \beta)\psi_n = 0 \quad n = 1, 2, 3, \dots, N - 1. \quad (6)$$

Multiplying through by Δx^2 , rearranging:

$$\psi_{n+1} + (-2 + \Delta x^2 n_0)\psi_n + \psi_{n-1} = \Delta x^2 \beta \psi_n \quad n = 1, 2, 3, \dots, N - 1. \quad (7)$$

Strategy: put UNKNOWN β on right hand side. Define $\lambda = \Delta x^2 \beta$:

$$\psi_{n+1} + (-2 + \Delta x^2 n_0)\psi_n + \psi_{n-1} = \lambda \psi_n \quad n = 1, 2, 3, \dots, N - 1. \quad (8)$$

!!! This gives eigenvalue problem:

$$\mathbf{A}\vec{\psi} = \lambda\vec{\psi} \quad (9)$$

where

$$\mathbf{A} = \begin{bmatrix} -2 + \Delta x^2 n_0 & 1 & 0 & \dots & 0 \\ 1 & -2 + \Delta x^2 n_0 & 1 & 0 & \dots \\ 0 & \ddots & \ddots & \ddots & \\ \vdots & & & & \vdots \\ \vdots & & & \ddots & \ddots \\ 0 & \dots & 0 & 1 & -2 + \Delta x^2 n_0 \end{bmatrix} \quad (10)$$

and

$$\vec{\psi} = \begin{bmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_{N-2}) \\ \psi(x_{N-1}) \end{bmatrix}. \quad (11)$$

- **Eigenvalues** $\lambda = \Delta x^2 \beta \rightarrow \beta = \lambda / \Delta x^2$
- **Eigenvector with eigenvalue λ is solution to b.v.p. with this β**

CODE: direct_boundary_solve_schrodinger.m

```
for i=1:m % Main Diagonal
    A1(i,i) = (-2+dx^2*n0);
end
for i=1:m-1 % Off diagonals
```

```
A1(i,i+1) = 1;
```

```
A1(i+1,i) = 1;
```

```
end
```

```
% Solve the eigen value problem
```

```
[V,D] = eig(A1);
```

```
%largest values of lambda
```

```
lambda_list=diag(D);
```

```
beta_list=lambda_list/(dx^2);
```

```
largest_lambda_list=lambda_list(end-4:end)
```

```
largest_beta_list=largest_lambda_list/(dx^2)
```

Comparing results from shooting vs. direct methods for boundary value problems

n=1500 for direct (slower)

```
>> schrodinger_shoot
```

```
beta =  
    97.532714843750000
```

```
beta =  
    90.129980468750006
```

```
beta =  
    77.799511718750011
```

```
beta =  
    60.527636718750017
```

```
beta =  
    38.326074218750016
```

```
>> direct_boundary_value_solve_schrodinger
```

```
largest_beta_list =
```

```
38.315536953535783
```

```
60.521813598809025
```

```
77.793463251968603
```

```
90.130410049325704
```

```
97.532599803055106
```