Finite Differences

1. Linear Boundary Value Problems
   - Dirichlet and Neumann conditions
   - finite differences applied to Dirichlet conditions
   - finite differences applied to Neumann conditions
2. Characteristic Value Problems
   - a boundary value problem with a parameter
   - reduction to an eigenvalue problem
3. Nonlinear Boundary Value Problems
   - derivation of a nonlinear system
   - Newton's method in several variables

MCS 471 Lecture 34
Numerical Analysis
Jan Verschelde, 10 November 2021

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Dirichlet and Neumann conditions

Consider the second order differential equation:

$$\frac{d^2y}{dx^2} = f\left(x, y, \frac{dy}{dx}\right), \quad x \in [a, b].$$

We distinguish between two "pure" types of boundary conditions:

1. Dirichlet imposes conditions on values at end points.

$$y(a) = A \quad \text{and} \quad y(b) = B.$$

2. Neumann imposes conditions on derivatives at the end points.

$$y'(a) = A \quad \text{and} \quad y'(b) = B.$$

Previously, we reduced the Boundary Value Problem (BVP)
to an initial value problem by shooting.

Now, we will reduce the BVP to a system of linear equations.

a linear boundary value problem

Consider the linear boundary value problem:

$$\frac{d^2y}{dx^2} = 4y, \quad x \in [0,1], \quad y(0) = 1, \quad y(1) = 3.$$

Observe that for $y(x) = e^{2x}$, $y'(x) = 2e^{2x}$, and $y''(x) = 4e^{2x}$.

So e^{2x} is one solution. Another solution is e^{-2x}.

Because the problem is linear, the solution is $y(x) = c_1 e^{2x} + c_2 e^{-2x}$.

Using the boundary conditions to determine c_1 and c_2:

$$\begin{array}{rcl} y(0) = c_1 \quad + c_2 & = & 1 \\ y(1) = c_1 e^2 + c_2 e^{-2} & = & 3 \end{array}$$

gives $y(t) = \dfrac{3 - e^{-2}}{e^2 - e^{-2}} e^{2t} + \dfrac{e^2 - 3}{e^2 - e^{-2}} e^{-2t}$.

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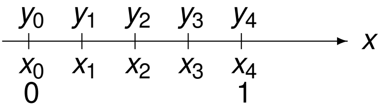
finite differences

Consider

$$\frac{d^2y}{dx^2} = 4y, \quad x \in [0,1], \quad y(0) = 1, \quad y(1) = 3.$$

We will discretize the interval $[0,1]$:



Let $h = 1/4$, then $x_i = 1 + i\,h = 1 + i/2$, $i = 0,1,2,3,4$.

As $y(0) = 1$: $y_0 = 1$, and $y_4 = 3$, as $y(1) = 3$.

We have three unknowns left: y_1, y_2, and y_3.

forward and backward differences

Forward differences:

$$\Delta y_i = \frac{1}{h}\left(y(x+h) - y(x) \right) = \frac{1}{h}\left(y_{i+1} - y_i \right).$$

Backward differences:

$$\nabla y_i = \frac{1}{h}\left(y(x) - y(x-h) \right) = \frac{1}{h}\left(y_i - y_{i-1} \right).$$

Then the second derivative is

$$y_i'' = \frac{1}{h}\left(\Delta y_i - \nabla y_i \right) = \frac{1}{h^2}\left(y_{i+1} - 2y_i + y_{i-1} \right).$$

The equation $y'' = 4y$ is then discretized by

$$\frac{1}{h^2}\left(y_{i+1} - 2y_i + y_{i-1} \right) = 4y_i, \quad i = 1, 2, 3.$$

a system of linear equations

$$\frac{1}{h^2}\left(y_{i+1} - 2y_i + y_{i-1}\right) = 4y_i, \quad i = 1, 2, 3,$$

is equivalent to

$$\begin{array}{rcl} y_0 + (-4h^2 - 2)y_1 + y_2 & = & 0 \\ y_1 + (-4h^2 - 2)y_2 + y_3 & = & 0 \\ y_2 + (-4h^2 - 2)y_3 + y_4 & = & 0. \end{array}$$

In matrix form:

$$\left[\begin{array}{ccc} -4h^2 - 2 & 1 & 0 \\ 1 & -4h^2 - 2 & 1 \\ 0 & 1 & -4h^2 - 2 \end{array}\right]\left[\begin{array}{c} y_1 \\ y_2 \\ y_3 \end{array}\right] = \left[\begin{array}{c} -y_0 \\ 0 \\ -y_4 \end{array}\right],$$

$h = 1/4$, $y_0 = 1$, $y_4 = 3$.

defining the linear system in Julia

```
"""
    A, b = setup(dim::Int)

returns the linear system to solve a BVP
with finite differences over the interval [a,b]
with dim points, with a step size h of (b-a)/(dim+1).
"""
function setup(dim::Int, a::Float64, b::Float64)
    h = (b - a)/(dim+1)
    d = (-4*h^2 - 2)*ones(dim)
    e = ones(dim-1)
    f = ones(dim-1)
    A = diagm(d) + diagm(+1 => e) + diagm(-1 => f)
    b = zeros(dim)
    b[1] = -1
    b[dim] = -3
    return A, b
end
```

for ten points

```
 approximation  :  exact value   :  error
9.78554113e-01 : 9.78153999e-01 : 4.00e-04
9.89457123e-01 : 9.88732845e-01 : 7.24e-04
1.03306946e+00 : 1.03208722e+00 : 9.82e-04
1.11083285e+00 : 1.10965427e+00 : 1.18e-03
1.22531799e+00 : 1.22400527e+00 : 1.31e-03
1.38030951e+00 : 1.37893085e+00 : 1.38e-03
1.58093110e+00 : 1.57956663e+00 : 1.36e-03
1.83381487e+00 : 1.83256350e+00 : 1.25e-03
2.14732062e+00 : 2.14630805e+00 : 1.01e-03
2.53181217e+00 : 2.53120062e+00 : 6.12e-04
```

For 10 points, $h = 1/11$, and $h^2 =$ `9.09e-02`.

We expect the error to be $O(h^2)$.

Dirichlet conditions

Dirichlet conditions give values for $y(a)$ and $y(b)$.
For $n+1$ points, or n intervals, $y_0 = y(a)$ and $y_n = y(b)$,
and thus the linear system has dimension $n-1$.

Exercise 1:
Consider the boundary value problem over $[0,1]$:

$$\frac{d^2y}{dx^2} = 6x, \quad y(0) = 0 \quad \text{and} \quad y(1) = 1.$$

1. Divide $[0,1]$ into 5 intervals of equal size and apply the method of finite differences to set up the linear system to find approximations of $y(x)$ over $[0,1]$.
2. Solve the system for 5, 20, 100, 200.
   How good is the computed approximation?

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finite differences applied to Neumann conditions

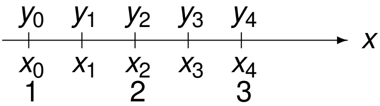
Consider

$$\frac{d^2y}{dx^2} = y, \quad x \in [1,3]$$

with conditions on the boundaries

$$y'(1) = 1.17520 \quad \text{and} \quad y'(3) = 10.0179.$$

We will discretize the interval $[1,3]$:



Let $h = 1/2$, then $x_i = 1 + i\,h = 1 + i/2$, $i = 0,1,2,3,4$.

a tridiagonal linear system

With $y'' = (y_{i+1} - 2y_i + y_{i-1})/h^2$, we discretize $y'' = y$ into

$$\frac{1}{h^2}\left(y_{i+1} - 2y_i + y_{i-1}\right) = y_i, \quad i = 0, 1, 2, 3, 4,$$

and rewritten into $y_{i+1} - 2y_i + y_{i-1} = h^2 y_i$, and

$$y_{i+1} - (2 + h^2)y_i + y_{i-1} = 0, \quad i = 0, 1, 2, 3, 4.$$

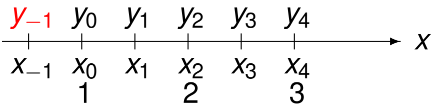
We have 5 equations in 7 unknowns:

$$\begin{array}{lrcl}
i = 0 & y_1 - (2 + h^2)y_0 + y_{-1} & = & 0 \\
i = 1 & y_2 - (2 + h^2)y_1 + y_0 & = & 0 \\
i = 2 & y_3 - (2 + h^2)y_2 + y_1 & = & 0 \\
i = 3 & y_4 - (2 + h^2)y_3 + y_2 & = & 0 \\
i = 4 & y_5 - (2 + h^2)y_4 + y_3 & = & 0
\end{array}$$

What is y_{-1}? What is y_5?

determine y_{-1} by boundary conditions

We work on the interval $[1, 3]$:



What is y_{-1}? Consider central differences on $y'(1)$:

$$y'(1) = \frac{y(1+h) - y(1-h)}{2h} = \frac{y_1 - y_{-1}}{2h}.$$

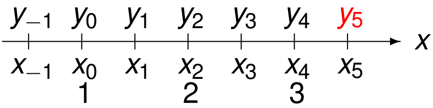
This leads to

$$2hy'(1) = y_1 - y_{-1} \quad \Rightarrow \quad y_{-1} = y_1 - 2hy'(1).$$

Given is $y'(1) = 1.17520$.

determine y_5 by boundary conditions

We work on the interval $[1, 3]$:



What is y_5? Consider central differences on $y'(3)$:

$$y'(3) = \frac{y(3+h) - y(3-h)}{2h} = \frac{y_5 - y_3}{2h}.$$

This leads to

$$2hy'(3) = y_5 - y_3 \quad \Rightarrow \quad y_5 = y_3 + 2hy'(3).$$

Given is $y'(3) = 10.0179$.

a tridiagonal linear system

$$A = \begin{bmatrix} -(2+h^2) & 2 & 0 & 0 & 0 \\ 1 & -(2+h^2) & 1 & 0 & 0 \\ 0 & 1 & -(2+h^2) & 1 & 0 \\ 0 & 0 & 1 & -(2+h^2) & 1 \\ 0 & 0 & 0 & 2 & -(2+h^2) \end{bmatrix}$$

The two 2 in A are coming from y_{-1} and y_5.

This leads to the linear system

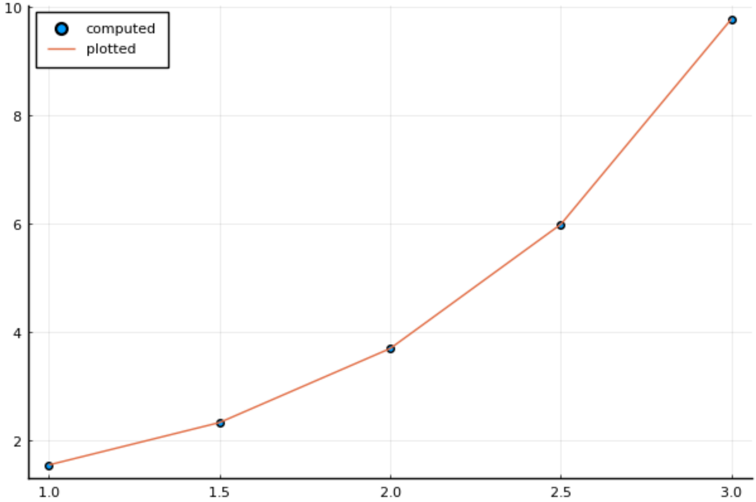
$$A \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 2hy'(1) \\ 0 \\ 0 \\ 0 \\ -2hy'(3) \end{bmatrix}.$$

the setup of the linear system

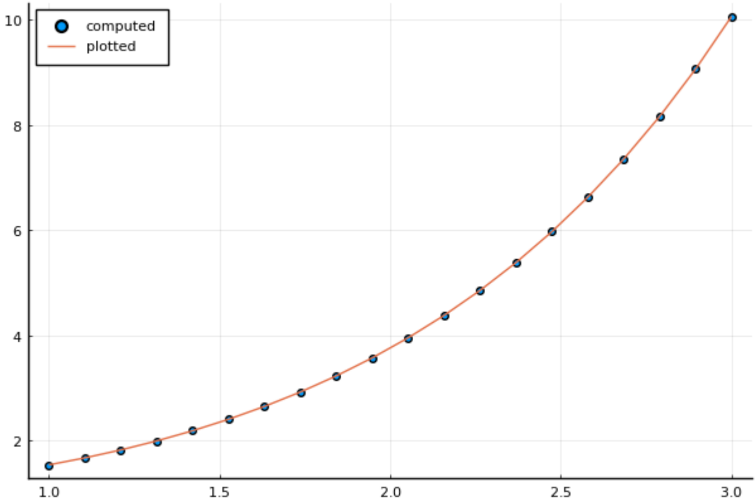
```
"""
    A, b = setup(dim::Int)

returns the linear system to solve a BVP
with finite differences over the interval [a,b]
with dim points, with a step size h of (b-a)/(dim-1).
"""
function setup(dim::Int, a::Float64, b::Float64)
    h = (b - a)/(dim-1)
    d = -(2 + h^2)*ones(dim)
    e = ones(dim-1); e[1] = 2
    f = ones(dim-1); f[dim-1] = 2
    A = diagm(d) + diagm(+1 => e) + diagm(-1 => f)
    b = zeros(dim)
    yprime1 = 1.17520
    yprime3 = 10.0179
    b[1] = 2*h*yprime1
    b[dim] = -2*h*yprime3
    return A, b
end
```

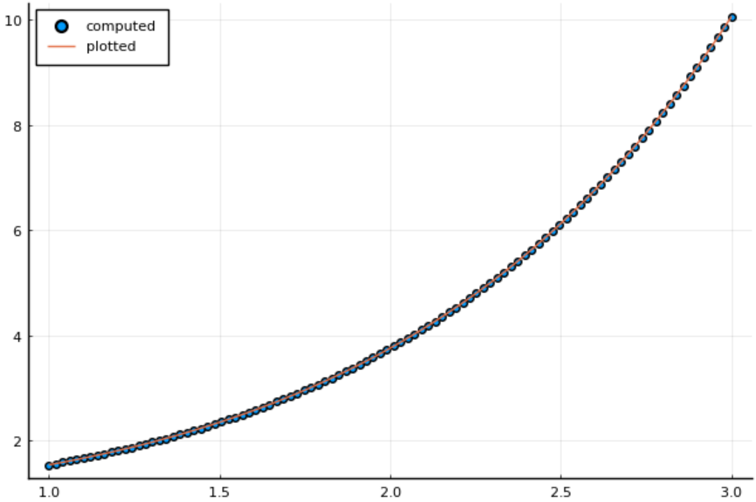
for 5 points



for 20 points



for 100 points



How good is the approximation?

The given slopes are $y'(1) = 1.17520$ and $y'(3) = 10.0179$.

With the numerical solution, we can approximate the slopes:

$$y'(1) \approx \frac{y_2 - y_1}{h} \quad \text{and} \quad y'(3) \approx \frac{y_n - y_{n-1}}{h}.$$

```
dim =   5 left slope : 1.563e+00, right slope : 7.574e+00
dim =  20 left slope : 1.256e+00, right slope : 9.489e+00
dim = 100 left slope : 1.191e+00, right slope : 9.916e+00
dim = 800 left slope : 1.177e+00, right slope : 1.001e+01
```

For 800 points, the errors are `1.800e-03` and `7.900e-03`.

Neumann conditions

Neumann conditions give values for $y'(a)$ and $y'(b)$.
For $n+1$ points, or n intervals, the linear system has dimension $n+1$.

Exercise 2:
Consider the boundary value problem over $[0,1]$:

$$\frac{d^2y}{dx^2} = 6x, \quad y'(0) = 0 \quad \text{and} \quad y'(1) = 1.$$

1. Divide $[0,1]$ into 5 intervals of equal size and apply the method of finite differences to set up the linear system to find approximations of $y(x)$ over $[0,1]$.
2. Solve the system for 5, 20, 100, 200.
   How good is the computed approximation?

Finite Differences

characteristic value problems

Consider for example

$$\frac{d^2y}{dx^2} + k^2 y = 0, \quad x \in [0,1], \quad y(0) = 0, \quad y(1) = 0.$$

The general solution has the form

$$y(x) = a \sin(kx) + b \cos(kx),$$

but this solution exists only for specific values of k,
the so-called *characteristic values*.

imposing the boundary conditions

The boundary conditions are $y(0) = 0$ and $y(1) = 0$.

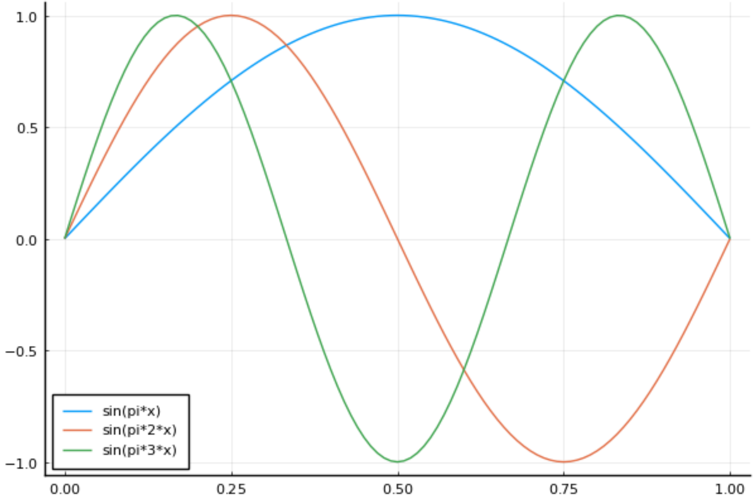
The general solution is $y(x) = a\sin(kx) + b\cos(kx)$.

We determine the constants a and b by the boundary conditions:

$$\begin{array}{rcl} y(0) = 0 & : & a\sin(0) + b\cos(0) = b = 0 \\ y(1) = 0 & : & a\sin(k1) = 0 \quad \Rightarrow \quad k = n\pi, n \in \mathbb{Z}. \end{array}$$

The symbolic solution is $\displaystyle\sum_{n=-\infty}^{\infty} a_n \sin(n\pi x)$.

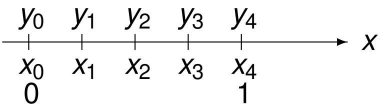
sine waves



Finite Differences

finite differences

Let $h = 1/4$, $x_i = i/4$, $i = 0, 1, 2, 3, 4$:



Note that $y_0 = 0$ and $y_4 = 0$, so we are left with 3 unknowns.

On the grid we have

$$y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}.$$

deriving an eigenvalue problem

Applied to $y'' + k^2 y = 0$, the equations are

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + k^2 y_i = 0, \quad i = 1, 2, 3.$$

Multiply by h^2:

$$\begin{array}{c} y_{i+1} - 2y_i + y_{i-1} + h^2 k^2 y_i = 0 \\ y_{i+1} + (h^2 k^2 - 2) y_i + y_{i-1} = 0. \end{array}$$

The three equations are then:

$$\begin{array}{lcl} i = 1 & : & y_2 + (h^2 k^2 - 2) y_1 + y_0 = 0 \\ i = 2 & : & y_3 + (h^2 k^2 - 2) y_2 + y_1 = 0 \\ i = 3 & : & y_4 + (h^2 k^2 - 2) y_3 + y_2 = 0 \end{array}$$

and we have that $y_0 = 0$ and $y_4 = 0$.

an eigenvalue problem

$$\begin{bmatrix} h^2k^2-2 & 1 & 0 \\ 1 & h^2k^2-2 & 1 \\ 0 & 1 & h^2k^2-2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

The linear system with parameter k is then

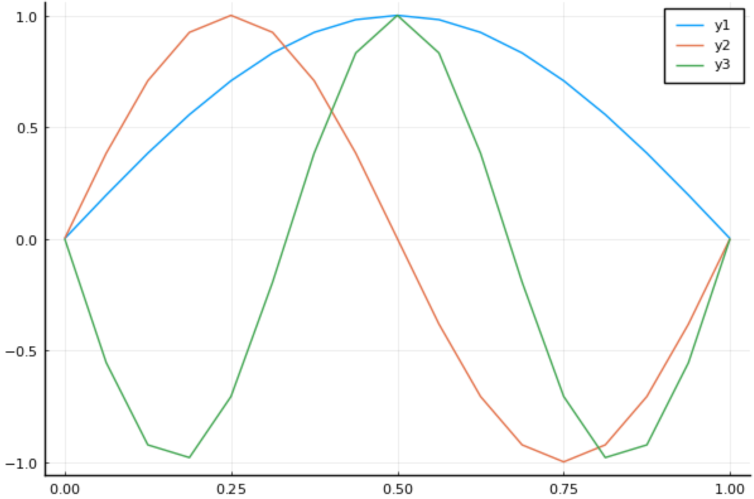
$$\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = h^2k^2 \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix},$$

which is an eigenvalue problem $A\mathbf{v} = \lambda\mathbf{v}$.

For every eigenvalue λ, we have $\lambda = h^2k^2$, or $k^2 = \lambda/h^2$.

The eigenvectors $\mathbf{v}$ hold the values for y on the grid.

the first 3 eigenvectors with 15 interior points



another characteristic value problem

Exercise 3:

Consider the characteristic-value problem (for some parameter k):

$$y'' - k^2 xy = 0, \quad y(0) = 1, \quad y(1) = 2.$$

1. Use finite differences with $h = 1/4$ to set up the corresponding eigenvalue problem.
2. Solve the eigenvalue problem.
   What is the accuracy of the solutions for $h = 1/4$?

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a nonlinear BVP

Consider

$$y'' = y - y^2, \quad y(0) = 1, \quad y(1) = 4.$$

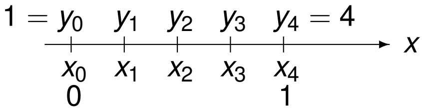
We apply finite differences $y_i \approx y(x_i)$, $x_i = ih$, $h > 0$.

For $i = 0, 1, \ldots, n$:

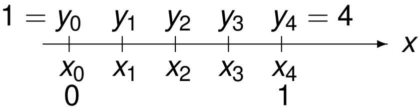
$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} - y_i + y_i^2 = 0.$$

Or equivalently: $h^2 y_i^2 + y_{i-1} - (2 + h^2)y_i + y_{i+1} = 0$.

For $n = 4$, $h = 1/4$:



a nonlinear system



$$h^2 y_i^2 + y_{i-1} - (2 + h^2) y_i + y_{i+1} = 0$$

$$\begin{array}{rcl} i = 1 & : & h^2 y_1^2 + y_0 - (2 + h^2) y_1 + y_2 = 0 \\ i = 2 & : & h^2 y_2^2 + y_1 - (2 + h^2) y_2 + y_3 = 0 \\ i = 3 & : & h^2 y_3^2 + y_2 - (2 + h^2) y_3 + y_4 = 0 \end{array}$$

Using $y_0 = 1$ and $y_4 = 4$:

$$f(y_1, y_2, y_3) = \left\{ \begin{array}{rcl} h^2 y_1^2 + 1 - (2 + h^2) y_1 + y_2 & = & 0 \\ h^2 y_2^2 + y_1 - (2 + h^2) y_2 + y_3 & = & 0 \\ h^2 y_3^2 + y_2 - (2 + h^2) y_3 + 4 & = & 0 \end{array} \right.$$

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Newton's method in several variables

$$f(y_1, y_2, y_3) = \begin{cases} h^2 y_1^2 + 1 - (2 + h^2) y_1 + y_2 & = & 0 \\ h^2 y_2^2 + y_1 - (2 + h^2) y_2 + y_3 & = & 0 \\ h^2 y_3^2 + y_2 - (2 + h^2) y_3 + 4 & = & 0 \end{cases}$$

The Jacobian matrix J_f is

$$\begin{bmatrix} 2h^2 y_1 - (2 + h^2) & 1 & 0 \\ 1 & 2h^2 y_2 - (2 + h^2) & 1 \\ 0 & 1 & 2h^2 y_3 - (2 + h^2) \end{bmatrix}.$$

Let $\mathbf{y} = (y_1, y_2, y_3)$. In a Newton step, we solve a linear system:

$$J_f(\mathbf{y}^{(k)})\Delta\mathbf{y} = -f(\mathbf{y}^{(k)}),$$

and then $\mathbf{y}^{(k+1)} := \mathbf{y}^{(k)} + \Delta\mathbf{y}$, for $k = 0, 1, \ldots$

What is $\mathbf{y}^{(0)}$?

where to start?

$$f(y_1, y_2, y_3) = \begin{cases} h^2 y_1^2 + 1 - (2 + h^2) y_1 + y_2 & = & 0 \\ h^2 y_2^2 + y_1 - (2 + h^2) y_2 + y_3 & = & 0 \\ h^2 y_3^2 + y_2 - (2 + h^2) y_3 + 4 & = & 0 \end{cases}$$

Observe that the nonlinear terms appear with a coefficient h^2.

Consider the system for $h = 0$:

$$\begin{cases} 1 - 2y_1 + y_2 & = & 0 \\ y_1 - 2y_2 + y_3 & = & 0 \\ y_2 - 2y_3 + 4 & = & 0 \end{cases}$$

and observe that this system is linear.

Take $\mathbf{y}^{(0)}$ as the solution to the system for $h = 0$.

five steps with Newton's method suffice

The output of running five Newton steps:

```
||f(y)|| : 2.12e-02  ||dy|| : 4.27e+00
||f(y)|| : 2.07e-03  ||dy|| : 7.97e-01
||f(y)|| : 7.30e-05  ||dy|| : 3.04e-02
||f(y)|| : 1.06e-07  ||dy|| : 4.45e-05
||f(y)|| : 2.28e-13  ||dy|| : 9.54e-11
```

Observe the quadratic convergence in `||dy||`.

another nonlinear BVP

Exercise 4: Consider

$$y'' = 10y(1-y), \quad y(0) = 0, \quad y(1) = 1.$$

1. Apply finite differences to define the nonlinear system to compute the approximations $y_i \approx y(x_i)$, $x_i = ih$, $i = 0, 1, \ldots, n$.
2. Run Newton's method on the system for $n = 10, 20, 40$.