## ME 310

## Numerical Methods

# Ordinary Differential Equations 

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## Differential Equations

Differential Equation: Contains an unknown function and its derivatives.
They are important because physics of many engineering problems involve rate of changes (derivatives). And it is easier to understand the relationships in terms of derivatives.

PDE: involves more than one independent variable $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}+\frac{\partial \mathbf{f}}{\partial \mathbf{y}}=\mathbf{f}(\mathbf{x}, \mathbf{y})$
ODE: involves only one independent variable. $\quad \mathbf{A} \frac{\mathbf{d}^{2} \mathbf{f}}{\mathbf{d} \mathbf{x}^{2}}+\mathbf{B} \frac{\mathbf{d f}}{\mathbf{d x}}=\mathbf{C f}(\mathbf{x})$
Order: depends on the highest derivative. $\quad-\frac{\mathbf{d}^{2} \mathbf{f}}{\mathbf{d} \mathbf{x}^{2}}+\mathbf{2} \frac{\mathbf{d} \mathbf{f}}{\mathbf{d} \mathbf{x}}=\mathbf{0} \quad$ is a $2^{\text {nd }}$ order ODE.
Nonlinearity: Due the terms like $f^{2},\left(\frac{d f}{d x}\right)^{2}, f \frac{d f}{d x}, e^{x}, \cos (x)$, etc
Coupled system of ODEs: $\left.\quad \mathbf{2} \frac{\mathbf{d} \mathbf{y}}{\mathbf{d} \mathbf{x}}+\mathbf{3} \frac{\mathbf{d z}}{\mathbf{d} \mathbf{x}}=\mathbf{4}\right\} \quad y(x)=$ ?

$$
\frac{\mathbf{d}^{2} \mathbf{y}}{\mathbf{d} \mathbf{x}^{2}}-\frac{\mathbf{d z}}{\mathbf{d x}}=0 \quad \int \quad \mathrm{z}(\mathrm{x})=?
$$

## Examples of ODEs

Newton's $2^{\text {nd }}$ Law of Motion: $\quad \frac{\mathbf{d} \mathbf{v}}{\mathbf{d} \mathbf{t}}=\frac{\mathbf{F}}{\mathbf{m}}$

Fourier's Heat Law: $\quad \mathbf{q}=-\mathbf{k} \frac{\mathbf{d} \mathbf{T}}{\mathbf{d} \mathbf{x}}$


Swing of a Pendulum: $\quad \frac{\mathbf{d}^{2} \theta}{\mathbf{d} \mathbf{t}^{\mathbf{2}}}+\frac{\mathbf{g}}{\mathbf{L}} \boldsymbol{\operatorname { s i n }}(\theta)=\mathbf{0}$


Mass-Spring-Damper System: $\quad \mathbf{m} \frac{\mathbf{d}^{2} \mathbf{y}}{\mathbf{d t}^{2}}+\mathbf{c} \frac{\mathbf{d} \mathbf{y}}{\mathbf{d} \mathbf{t}}+\mathbf{k y}=\mathbf{0}$

Solar Heater Collector: $\quad \mathbf{x}\left(\frac{\mathbf{d} \mathbf{y}}{\mathbf{d} \mathbf{x}}\right)^{\mathbf{2}}-\mathbf{2 y} \frac{\mathbf{d} \mathbf{y}}{\mathbf{d x}}=\mathbf{0}$


## Mathematical Background

- Consider the function $y=x^{3}-x^{2}-4 x+4$

- An ODE can be formed by taking $\mathrm{dy} / \mathrm{dx}$ $d y / d x=3 x^{2}-2 x-4$

- They both describe the same behavior. One directly shows the dependent variable. The other shows the rate of change of it.
- Solving an ODE is actually going back from dy/dx to $y(x)$. This can be done by integration.

$$
y(x)=x^{3}-x^{2}-4 x+C
$$

- C is the integration constant. For different integration constants different equations will be obtained (If the ODE was $2^{\text {nd }}$ order than we would integrate twice and got two constants).
- Only C=4 corresponds to the original function.
- C can be determined if $y(x)$ is known at one point. This value is known as the INITIAL VALUE.
- For example if the INITIAL CONDITION $y(0)=4$ is known, than $C$ can be determined.
- A typical numerical solution of an ODE starts from the initial value and discretely constructs $y(x)$ using the differential equation.


## Euler's Method

- General form of the ODEs that we will study is

$$
\frac{d y}{d x}=f(x, y)
$$

- $f(x, y)$ is known and $y(x)$ is to be determined.


$$
\mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+\left.\frac{\mathbf{d y}}{d x_{i}}\right|_{i} \rightarrow \quad \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{h}
$$

- Start from the initial condition $\mathrm{x}_{\mathbf{0}}$. Choose a step size h and apply Euler's method successively.




## Example 40:

- Solve the following initial value problem over the interval $[0,2]$ using
(a) $h=0.5$, (b) $h=0.25$. Note that the analytical solution is $y(x)=e^{x^{\mathbf{3} / 3-1.2 x}}$

$$
\frac{d y}{d x}=y x^{2}-1.2 y \quad y(0)=1
$$

(a) $h=0.5 . \quad y_{i+1}=y_{i}+f\left(x_{i}, y_{i}\right) h \quad$ where $f(x)=y x^{2}-1.2 y$
$\mathrm{i}=0 \quad \mathrm{y}_{1}=\mathrm{y}_{\mathbf{0}}+\mathrm{f}\left(\mathrm{x}_{\mathbf{0}}, \mathrm{y}_{\mathbf{0}}\right) \mathrm{h} \quad \rightarrow \quad \mathrm{y}_{1}=\mathrm{y}(0.5)=1+\left(1^{*} 0^{2}-1.2^{*} 1\right) 0.5=0.4$
$\mathrm{i}=1 \quad \mathrm{y}_{2}=\mathrm{y}_{1}+\mathrm{f}\left(\mathrm{x}_{1}, \mathrm{y}_{1}\right) \mathrm{h} \quad \rightarrow \quad \mathrm{y}_{2}=\mathrm{y}(1.0)=0.4+\left(0.4^{*} 0.5^{2}-1.2^{*} 0.4\right) 0.5=0.21$
$\mathrm{i}=2 \quad \mathrm{y}_{3}=\mathrm{y}_{2}+\mathrm{f}\left(\mathrm{x}_{2}, \mathrm{y}_{2}\right) \mathrm{h} \quad \rightarrow \quad \mathrm{y}_{3}=\mathrm{y}(1.5)=0.21+\left(0.21^{*} 1^{2}-1.2 * 0.21\right) 0.5=0.189$
$i=3 \quad y_{4}=y_{3}+f\left(x_{3}, y_{3}\right) h \quad \rightarrow \quad y_{4}=y(2.0)=0.189+\left(0.189 * 1.5^{2}-1.2 * 0.189\right) 0.5=0.28823$

- Analytical solution is shown with blue.
- Solution for $h=0.5$ is shown with red.

Exercise 45: Solve the above example for $\mathrm{h}=0.25$ to obtain the solution shown in the middle (with black).


## Error Analysis of Euler's Method

- Truncation Error (TE) for the Euler's Method is composed of two parts.
- Local TE: Error due to the application of the method over a single step.
- Propagated TE: Error due to the approximations produced in the previous steps.
- Global TE: The sum of these two.
- For error analysis Euler's Method can be derived from Taylor Series Exapnsion.

$$
\begin{aligned}
& y_{i+1}=y_{i}+y_{i}^{\prime} h+\frac{y_{i}^{\prime \prime}}{2!} h^{2}+\ldots .+\frac{y_{i}^{(n)}}{n!} h^{n}+R_{n}
\end{aligned}
$$

$$
\begin{aligned}
& E_{a}=\frac{f^{\prime}\left(x_{i}, y_{i}\right)}{2!} h^{2}=\mathbf{O}\left(h^{2}\right) \\
& \text { Et: TRUNCATON ERROR FOR EULER'S METHOD }
\end{aligned}
$$

- Local error of Euler's Method is of order O(h²).
- But actually Euler's Method is first order and its global error is of order $O(h)$. It can give exact predictions only if $y(x)$ is linear.
- Exercise 46: For the previous example, calculate the true local and global errors at each step. To calculate local errors you need to use the exact value at the beginning of each step. Also estimate the local errors with the above formula and compare the true and estimated values.


## Higher Order Methods

- Higher order methods can be derived by using more terms in the TSE.
- For example the second order method will be

$$
y_{i+1}=y_{i}+f\left(x_{i}, y_{i}\right) h+\frac{f^{\prime}\left(x_{i}, y_{i}\right)}{2!} h^{2}+E_{t}
$$

- This requires the $1^{\text {st }}$ derivative of the given function $f(x, y)$. It can be obtained using the chain rule.

$$
f^{\prime}\left(x_{i}, y_{i}\right)=\frac{\partial \mathbf{f}}{\partial \mathbf{x}}+\frac{\partial \mathbf{f}}{\partial \mathbf{y}} \frac{\mathbf{d y}}{\frac{\mathbf{f}_{(x, y)}}{\mathbf{d x}}}
$$

- Formuas for higher derivatives is even more complicated.
- These methods are not preferred. We will learn other accurate methods that uses only the given function $f(x, y)$ but not its derivatives. These methods are
- Heun's Method
- Midpoint Method
- Runge-Kutta Methods


## Heun's Method

- Euler's Method: $y_{i+1}=y_{i}+f\left(x_{i}, y_{i}\right) h$.
- Can we use a better estimate for the derivative instead of $f\left(x_{i} y_{i}\right)$.



## Predictor step:

- Use Euler's Method to find a first estimate for $y_{i+1}$.

$$
\mathbf{y}_{i+1}^{0}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{h}
$$

- Using $\mathrm{y}^{\mathbf{0}}{ }_{\mathrm{i}+\mathbf{1}}$ calculate the slope at $\mathrm{x}_{\mathbf{i + 1}}$.



## Corrector step:

- Take the average of slopes at $x_{i}$ and $x_{i+1}$.
- Use it to calculate a new estimate for $y_{i+1}$.

$$
y_{i+1}=y_{i}+\frac{f\left(x_{i}, y_{i}\right)+f\left(x_{i+1}, y_{i+1}^{0}\right)}{2} h
$$

## Heun's Method (cont'd)

- Heun's Method is a predictor-corrector method.
- Corrector step can be used more than once to get better estimates for $\mathrm{y}_{\mathrm{i}+\mathbf{1}}$.

Predictor: $\quad y_{i+1}^{\mathbf{0}}=y_{i}+f\left(x_{i}, y_{i}\right) h$
Corrector: $\quad y^{\mathbf{1}}{ }_{\mathbf{i}+\mathbf{1}}=y_{i}+\left[f\left(x_{i}, y_{i}\right)+f\left(x_{i+1}, y^{\mathbf{0}}{ }_{i+1}\right)\right] / 2 * h$
Corrector: $\quad y^{\mathbf{2}}{ }_{i+1}=y_{i}+\left[f\left(x_{i}, y_{i}\right)+f\left(x_{i+1}, y^{\mathbf{1}}{ }_{i+1}\right)\right] / 2 * h$
... continue until the error falls below the tolerance

- If $f=f(x)$ only, than the predictor step is not required. Corrector step becomes

$$
\mathbf{y}_{i+1}=\mathbf{y}_{i}+\frac{f\left(\mathbf{x}_{i}\right)+f\left(\mathbf{x}_{i+1}\right)}{2} h
$$

Note the similarity between the above formula and the trapezoidal Rule.

- Heun's Method is $2^{\text {nd }}$ order accurate. It can obtain exact results when the solution $y(x)$ is quadratic.
- It has a global error of $\mathrm{O}\left(\mathrm{h}^{2}\right)$ and local error of $\mathrm{O}\left(\mathrm{h}^{\mathbf{3}}\right)$.


## Midpoint Method

- Similar to Heun's Method this also tries to improve the Euler's Method by using a better slope.

- Use Euler's Method to find an estimate for $\mathrm{y}_{\mathrm{i+1/2}}$.

$$
\mathbf{y}_{i+1 / 2}=\mathbf{y}_{\mathrm{i}}+\mathbf{f}\left(\mathbf{x}_{i}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{h} / \mathbf{2}
$$

- Using $y_{i+1 / 2}$ calculate the slope at $x_{i+1 / 2}$.

- Use the slope at $x_{i+1 / 2}$ to calculate an estimate for $y_{i+1}$.

$$
y_{i+1}=y_{i}+f\left(x_{i+1 / 2}, y_{i+1 / 2}\right) h
$$

- Unlike Heun's Method, second step can NOT be applied more than once.
- If $\mathrm{f}=\mathrm{f}(\mathrm{x})$ only, than there is no need to perform the first step.
- Midpoint Method is $2^{\text {nd }}$ order accurate. Its global error is $\mathrm{O}\left(\mathrm{h}^{\mathbf{2}}\right)$.


## Example 41:

Solve $\mathbf{d y} / \mathbf{d x}=\mathbf{y x} \mathbf{- 1 . 2 y}$ with the initial condition $\mathbf{y}(\mathbf{0})=\mathbf{1}$ over the interval $[0,2]$ using Heun's method. Use $h=0.5$. Iterate the corrector to $\varepsilon_{s}=1 \%$. Analytical solution is $y(x)=e^{x^{3} / 3-1.2 x}$
$h=0.5, f(x)=y x^{\mathbf{2}}-1.2 y, \quad y^{\mathbf{0}}{ }_{\mathbf{i + 1}}=y_{i}+f\left(x_{i}, y_{i}\right) h, y_{i+1}^{k}=y_{i}+\left[f\left(x_{i}, y_{i}\right)+f\left(x_{i+1}, y^{\mathbf{k}-1} \mathbf{1}_{\mathbf{i}+\mathbf{1}}\right)\right] / 2 * h$
$\mathrm{i}=0 \quad$ Predictor: $\quad \mathrm{y}^{\mathbf{0}}{ }_{\mathbf{1}}=1+\left(1^{*} 0^{\mathbf{2}}-1.2^{*} 1\right) 0.5=0.4$
Corrector:

$$
\begin{array}{lll}
\mathrm{k}=1 & \mathrm{y}^{\mathbf{1}}=1+\left[\left(1^{*} 0^{2}-1.2^{*} 1\right)+\left(0.4^{*} 0.5^{2}-1.2^{*} 0.4\right)\right] / 2 * 0.5=0.605 & \varepsilon_{\mathrm{a}}=33.9 \% \\
\mathrm{k}=2 & \mathrm{y}^{\mathbf{2}}=1+\left[\left(1^{*} 0^{2}-1.2^{*} 1\right)+\left(0.605^{*} 0.5^{2}-1.2^{*} 0.605\right)\right] / 2 * 0.5=0.5563125 & \varepsilon_{\mathrm{a}}=8.75 \% \\
\mathrm{k}=3 & \mathrm{y}^{\mathbf{3}}=1+\left[\left(1^{*} 0^{2}-1.2^{*} 1\right)+\left(0.5563 * 0.5^{2}-1.2^{*} 0.5563\right)\right] / 2 * 0.5=0.5678757 & \varepsilon_{\mathrm{a}}=2.04 \% \\
\mathrm{k}=4 & \mathrm{y}^{4}{ }_{\mathbf{a}}=1+\left[\left(1^{*} 0^{2}-1.2^{*} 1\right)+\left(0.5679 * 0.5^{2}-1.2^{*} 0.5679\right)\right] / 2 * 0.5=0.5651295 & \varepsilon_{\mathrm{a}}=0.49 \% \\
\mathrm{y}_{\mathbf{1}}=\mathrm{y}(0.5)=0.5651295 &
\end{array}
$$

$\mathrm{i}=1$ Predictor: $\quad \mathrm{y}_{\mathbf{2}}^{\mathbf{2}}=0.5651295+\left(0.5651295 * 0.5^{\mathbf{2}}-1.2 * 0.5651295\right) 0.5=0.2966930$
Corrector:
$\mathrm{k}=1 \quad \mathrm{y}^{\mathbf{1}}{ }_{\mathbf{2}}=0.5651295+\left[\left(05651295 * 0.5^{\mathbf{2}}-1.2^{*} 05651295\right)+\left(0.296693 * 1^{2}-1.2 * 0.296693\right)\right] / 2^{*} 0.5$ $=0.4160766 \quad \varepsilon_{a}=28.7 \%$

Continue like this to find

$$
y(1)=0.4104059, \quad y(1.5)=0.5279021, \quad y(2)=2.181574
$$

## Example 42:

Solve the previous problem using the Midpoint Method with (a) $h=0.5$, (b) $h=0.25$.
$f(x)=y x^{2}-1.2 y, \quad y_{i+1 / 2}=y_{i}+f\left(x_{i}, y_{i}\right) h / 2, y_{i+1}=y_{i}+f\left(x_{i+1 / 2}, y_{i+1 / 2}\right) h$
(a) $\mathrm{h}=0.5$
$\mathrm{i}=0 \quad$ Predictor: $\quad \mathrm{y}_{0+1 / 2}=1+\left(1^{*} 0^{2}-1.2^{*} 1\right) 0.25=0.7$
Corrector: $\mathrm{y}_{\mathbf{1}}=\mathrm{y}(0.5)=1+\left(0.7 * 0.25^{2}-1.2 * 0.7\right) 0.5=\mathbf{0 . 6 0 1 8 7 5}$
$\mathrm{i}=1 \quad$ Predictor: $\quad \mathrm{y}_{\mathbf{1 + 1 / 2}}=0.601875+\left(0.601875 * 0.5^{2}-1.2 * 0.601875\right) 0.25=0.4589297$
Corrector: $y_{2}=y(1)=0.601875+\left(0.4589297 * 0.75^{2}-1.2 * 0.4589297\right) 0.5=\mathbf{0 . 4 5 5 5 9 1 1}$
$\mathrm{i}=2$ Predictor: $\quad \mathrm{y}_{2+1 / 2}=0.4555911+\left(0.4555911^{*} 1^{2}-1.2 * 0.4555911\right) 0.25=0.4328116$
Corrector: $\mathrm{y}_{\mathbf{3}}=\mathrm{y}(1.5)=0.4555911+\left(0.4328116 * 1.25^{2}-1.2 * 0.4328116\right) 0.5=\mathbf{0 . 5 3 4 0 3 8 3}$
$\mathrm{i}=3$ Predictor: $\quad \mathrm{y}_{3+1 / 2}=0.5340383+\left(0.5340383 * 1.5^{2}-1.2^{*} 0.5350383\right) 0.25=0.6742233$
Corrector: $y_{4}=y(2)=0.5340383+\left(0.6742233 * 1.75^{2}-1.2 * 0.6742233\right) 0.5=\mathbf{1 . 1 6 1 9 0 8 7}$

Exercise 47: Solve part (b) of the above example

## Generalized Runge-Kutta Methods

- Euler's Method: $\quad \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{y}_{\mathbf{i}}\right) \mathbf{h}$
- Heun's Method: $\quad \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+\frac{f\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right)+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}+1}, \mathbf{y}_{i+1}^{0}\right)}{\mathbf{2}} \mathbf{h} \quad \mathbf{y}_{i+1}^{0}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{h}$
- Midpoint Method: $\quad \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathbf{i + 1 / 2}}, \mathbf{y}_{\mathbf{i + 1 / 2}}\right) \mathbf{h} \quad \mathbf{y}_{\mathbf{i + 1 / 2}}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{y}_{\mathbf{i}}\right) \mathbf{h} / \mathbf{2}$
- These methods can be generalized as Runge Kutta (RK) Methods:

$$
\begin{aligned}
& \mathbf{y}_{i+1}=\mathbf{y}_{i}+\phi\left(x_{i}, y_{i}, h\right) h \\
& \phi=a_{1} k_{1}+a_{2} k_{2}+\ldots \ldots+a_{n} k_{n} \\
& k_{1}=f\left(x_{i}, y_{i}\right) \\
& k_{2}=f\left(x_{i}+p_{1} h, y_{i}+q_{11} k_{1} h\right) \\
& k_{3}=f\left(x_{i}+p_{2} h, y_{i}+q_{21} k_{1} h+q_{22} k_{2} h\right) \\
& \ldots \ldots \\
& k_{n}=f\left(x_{i}+p_{n-1} h, y_{i}+q_{(n-1) 1} k_{1} h+q_{(n-2) 2} k_{2} h+\ldots+q_{(n-2)(n-1)} k_{n-1} h\right)
\end{aligned}
$$

- RK Methods are a generalization of ODE solvers that only use the known function $f(x, y)$ but not its derivatives. Therefore their applications are very simple.
- $1^{\text {st }}$ order ( $\mathrm{n}=1$ ) RK Method is actually the Euler's Method.


## $\underline{\text { nd }^{\text {nd }} \text { order Runge Kutta }}$

$$
\begin{align*}
& y_{i+1}=y_{i}+\left(a_{1} k_{1}+a_{2} k_{2}\right)  \tag{Eq.1}\\
& k_{1}=f\left(x_{i}, y_{i}\right) \\
& k_{2}=f\left(x_{i}+p_{1} h, y_{i}+q_{11} k_{1} h\right)
\end{align*}
$$

A Taylor Series analysis can be used to determine the constants $a_{1}, a_{2}, p_{1}, q_{11}$.
$y_{i+1}=y_{i}+f\left(x_{i}, y_{i}\right) h+\frac{f^{\prime}\left(x_{i}, y_{i}\right)}{2} h^{\mathbf{2}}+\mathbf{O}\left(h^{3}\right)$
where $\quad f^{\prime}\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right)=\frac{\partial \mathbf{f}(\mathbf{x}, \mathbf{y})}{\partial \mathbf{x}}+\frac{\partial \mathbf{f}(\mathbf{x}, \mathbf{y})}{\partial \mathbf{y}} \underbrace{\frac{\mathbf{d y}}{\mathbf{d x}}}_{\mathrm{f}}$
therefore $\quad \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{h}+\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}+\frac{\partial \mathbf{f}}{\partial \mathbf{y}} \mathbf{f}\right) \frac{\mathbf{h}^{\mathbf{2}}}{\mathbf{2}}+\mathbf{O}\left(\mathbf{h}^{\mathbf{3}}\right)$

Now write a TSE of $\mathrm{k}_{\mathbf{2}}$ around $\left(\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}\right)$
$f\left(x_{i}+p_{1} h, y_{i}+q_{11} k_{1} h\right)=f\left(x_{i}, y_{i}\right)+p_{1} h \frac{\partial f}{\partial x}+\mathbf{q}_{11} k_{1} h \frac{\partial f}{\partial \mathbf{y}}+\mathbf{O}\left(h^{2}\right)$
Using this in (Eq. 1) we get
$y_{i+1}=y_{i}+\left[a_{1} f\left(x_{i}, y_{i}\right)+a_{2} f\left(x_{i}, y_{i}\right)\right] h+\left[a_{2} p_{1} \frac{\partial f}{\partial x}+a_{2} q_{11} f\left(x_{i}, y_{i}\right) \frac{\partial f}{\partial \mathbf{y}}\right] h^{2}+O\left(h^{3}\right)$

## $\underline{2}^{\text {nd }}$ order Runge Kutta (cont'd)

- Compare equal order terms in (Eq. 2) and (Eq. 3)
$a_{1}+a_{2}=1 \quad$ There are 4 unknowns and 3 equations.
$a_{2} p_{1}=1 / 2$
$a_{2} q_{11}=1 / 2 \quad$ This means there are many different $2^{\text {nd }}$ order Runge Kutta Methods.
- Select $a_{2}=1 / 2 \rightarrow a_{1}=1 / 2, p_{1}=1, q_{11}=1$. This is Heun's Method

$$
y_{i+1}=y_{i}+\left(1 / 2 k_{1}+1 / 2 k_{2}\right) h, \quad k_{1}=f\left(x_{i}, y_{i}\right), \quad k_{2}=f\left(x_{i}+h, y_{i}+h k_{1}\right)
$$

- Select $a_{2}=1 \rightarrow a_{1}=0, p_{1}=1 / 2, q_{11}=1 / 2$. This is the Midpoint Method

$$
y_{i+1}=y_{i}+k_{2} h, \quad k_{1}=f\left(x_{i}, y_{i}\right), \quad k_{2}=f\left(x_{i}+h / 2, y_{i}+h / 2 k_{1}\right)
$$

- Select $a_{2}=2 / 3 \rightarrow a_{1}=1 / 3, p_{1}=3 / 4, q_{11}=3 / 4$. This is Ralston's Method

$$
y_{i+1}=y_{i}+\left(1 / 3 k_{1}+2 / 3 k_{2}\right) h \quad, \quad k_{1}=f\left(x_{i}, y_{i}\right) \quad, \quad k_{2}=f\left(x_{i}+3 / 4 h, y_{i}+3 / 4 k_{1}\right)
$$

- Although these are all $2^{\text {nd }}$ order methods, error of the Ralston's Method is somewhat smaller than the other two and it is the preferred $2^{\text {nd }}$ order RK Method.


## Graphical Depiction of the Ralston's Method



- Use Euler's Method to find an estimate for $\mathrm{y}_{\mathrm{i}+\mathbf{3 / 4}}$.

$$
\mathbf{y}_{i+3 / 4}=\mathbf{y}_{i}+f\left(\mathbf{x}_{i}, y_{i}\right) \mathbf{3 h / 4}
$$

- Using $y_{i+3 / 4}$ calculate the slope at $x_{i+3 / 4}$ as $f\left(x_{i+3 / 4}, y_{i+3 / 4}\right)$
- Calculate a weighted slope using the slope at $x_{i}$ and $x_{i+3 / 4}$ as

$$
\frac{f\left(x_{i}, y_{i}\right)+2 f\left(x_{i+3 / 4}, y_{i+3 / 4}\right)}{3}
$$

- Use this slope and estimate $y_{i+1}$.

$$
y_{i+1}=y_{i}+\left[\frac{1}{3} f\left(x_{i}, y_{i}\right)+\frac{2}{3} f\left(x_{i+3 / 4}, y_{i+3 / 4}\right)\right] h
$$

## 3rd order RK Method

- Again, many different $3^{\text {rd }}$ order RK Methods can be written. The preferred one is

$$
\begin{aligned}
& y_{i+1}=y_{i}+h\left(k_{1}+4 k_{2}+k_{3}\right) / 6 \\
& k_{1}=f\left(x_{i}, y_{i}\right) \\
& k_{2}=f\left(x_{i}+h / 2, y_{i}+k_{1} h / 2\right) \\
& k_{3}=f\left(x_{i}+h, y_{i}-k_{1} h+2 k_{2} h\right)
\end{aligned}
$$

## $4^{\text {th }}$ order RK Method

- The preferred $4^{\text {th }}$ order RK Method is

$$
\begin{aligned}
& y_{i+1}=y_{i}+h\left(k_{1}+2 k_{2}+2 k_{3}+k_{4}\right) / 6 \\
& k_{1}=f\left(x_{i}, y_{i}\right) \\
& k_{2}=f\left(x_{i}+h / 2, y_{i}+k_{1} h / 2\right) \\
& k_{3}=f\left(x_{i}+h / 2, y_{i}+k_{2} h / 2\right) \\
& k_{4}=f\left(x_{i}+h, y_{i}+k_{3} h\right)
\end{aligned}
$$

- This method is $4^{\text {th }}$ order accurate and used very often for solving ODEs.

Exercise 48: What happens to the Runge Kutta Methods in the simplified case of $f=f(x)$ only?

## Example 43:

- Solve $\mathbf{d y} / \mathbf{d x}=\mathbf{y x} \mathbf{- 1 . 2 y}$ with the initial condition $\mathbf{y}(\mathbf{0})=\mathbf{1}$ over the interval $[0,2]$ using RK4 method. Use $h=0.5$.

$$
\begin{aligned}
& y_{i+1}=y_{i}+h\left(k_{1}+2 k_{2}+2 k_{3}+k_{4}\right) / 6 \\
& k_{1}=f\left(x_{i}, y_{i}\right) \quad k_{2}=f\left(x_{i}+h / 2, y_{i}+k_{1} h / 2\right) \quad k_{3}=f\left(x_{i}+h / 2, y_{i}+k_{2} h / 2\right) \quad k_{4}=f\left(x_{i}+h, y_{i}+k_{3} h\right) \\
& i=0, k_{1}=f(0,1)=-1.2, k_{2}=f(0.25,0.7)=-0.79625 \\
& k_{3}=f(0.25,0.800938)=-0.91107, \quad k_{4}=f(0.5,0.544467)=-0.51724 \\
& y_{1}=y(0.5)=0.572344 \quad \varepsilon_{\mathrm{t}}=\mathbf{0 . 0 3 2} \% \\
& i=1, k_{1}=f(0.5,0.572344)=-0.54373, k_{2}=f(0.75,0.436412)=-0.27821 \\
& k_{3}=f(0.75,0.50279)=-0.32053, k_{4}=f(1,0.412079)=-0.08242 \\
& y_{2}=y(1)=0.420375 \quad \varepsilon_{\mathrm{t}}=\mathbf{0 . 0 0 6} \% \\
& \mathrm{i}=2, \mathrm{k}_{1}=\mathrm{f}(1,0.420375)=-0.08407, \mathrm{k}_{2}=\mathrm{f}(1.25,0.399356)=0.144767 \\
& \mathrm{k}_{3}=\mathrm{f}(1.25,0.456567)=0.165505, \mathrm{k}_{4}=\mathrm{f}(1.5,0.503128)=0.528284 \\
& y_{3}=y(1.5)=0.509104 \quad \varepsilon_{t}=\mathbf{0 . 0 1} \% \\
& i=3, k_{1}=f(1.5,0.509104)=0.534559, k_{2}=f(1.75,0.642744)=1.197111 \\
& k_{3}=f(1.75,0.808382)=0.505611, k_{4}=f(2,1.26191)=3.533348 \\
& y_{4}=y(2)=1.29855 \quad \varepsilon_{t}=0.54 \%
\end{aligned}
$$

## Solving System of ODEs

- We can use any of the methods that we learned to solve a system of ODEs.
- An example of this is obtained when we reduce a second order ODE to first order by change of variables.


## Example 44:

Solve the following ODE in the range $[0,5]$ using $\mathrm{h}=0.1$ with Euler's Method.

$$
\frac{d^{2} y}{d t^{2}}-t+y=0, \quad y(0)=2, \quad \frac{d y}{d t}(0)=0
$$

Separate this $2^{\text {nd }}$ order ODE into two $1^{\text {st }}$ order ODEs by defining a new variable $z=d y / d t$

$$
\begin{aligned}
& \frac{d y}{d t}=f_{1}=z, \quad y(0)=2 \\
& \frac{d z}{d t}=f_{2}=t-y, \quad z(0)=0
\end{aligned}
$$

$i=0, \quad t_{0}=0, \quad y_{0}=2, \quad z_{0}=0$.
$y_{1}=y_{0}+f_{1}\left(z_{0}\right) h=2+(0)(0.1)=2$
$z_{1}=z_{0}+f_{2}\left(t_{0}, y_{0}\right) h=0+(0-2)(0.1)=-0.2$
$\mathrm{i}=2, \quad \mathrm{t}_{1}=0.1, \quad \mathrm{y}_{1}=2, \quad \mathrm{z}_{1}=-0.2$.
$y_{2}=y_{1}+f_{1}\left(z_{1}\right) h=2+(-0.2)(0.1)=1.98$
$\mathrm{z}_{\mathbf{2}}=\mathrm{z}_{1}+\mathrm{f}_{\mathbf{2}}\left(\mathrm{t}_{1}, \mathrm{y}_{\mathbf{1}}\right) \mathrm{h}=-0.2+(0.1-2)(0.1)=-0.39 \quad$ Continue like this until $\mathrm{i}=50$.

## Stability of Numerical Solutions of ODEs

- Consider the following ODE

$$
\frac{d y}{d t}=-a y, \quad y(0)=y_{0} \quad y_{\text {exact }}=y_{0} e^{-a t}
$$

- If we solve this with the Euler's Method

$$
\mathbf{y}_{i+1}=\mathbf{y}_{i}+\left.\frac{d y}{d t}\right|_{i} h=y_{i}-a y_{i} h=y_{i}(\mathbf{1}-a h)
$$

- Consider positive "a" values, which means that the solution asymptotically approaches to zero. Our numerical solution will behave like this if $y_{i+1}$ is smaller than $y_{i}$ at all steps. This requires

$$
1-a h<1 \rightarrow h<\frac{2}{a}
$$

- This is the stability condition of the Euler's Method for this problem. The step size we can use has an upper limit. For larger step sizes, $\mathrm{y} \rightarrow \infty$ as $\mathrm{i} \rightarrow \infty$, which means that the solution is unstable.
- Euler's Method is explicit. That is in Euler's equation the unknown $y_{i+1}$, appears only at the left hand side and it can be solved explicitly using the known quantities at the right hand side.
- Explicit methods need to satisfy a stability condition.
- We can derive implicit methods that have better stability characteristics or even unconditionally stable. A simple one is the Backward Euler's (Implicit Euler) Method.


## Implicit Euler (unconditional stability)

- In Euler's Method use the slope at point $x_{i+1}$ instead of $x_{i}$.
- This new method is called Implicit Euler. Use it to solve the previous problem.

$$
\mathbf{y}_{i+1}=\mathbf{y}_{i}+\left.\frac{\mathbf{d y}}{d t}\right|_{i+1} \mathbf{h}=\mathbf{y}_{\mathbf{i}}-\mathbf{a} \mathbf{y}_{i+1} \mathbf{h} \quad \rightarrow \quad \mathbf{y}_{i+1}=\frac{\mathbf{y}_{\mathbf{i}}}{(\mathbf{1}+\mathbf{a h})}
$$

- For positive "a" values, $y_{i+1}$ is always smaller than $y_{i}$
- y $\rightarrow 0$ as $\mathrm{i} \rightarrow \infty$, regardless of the step size $h$. Therefore this method is unconditionally stable. We can select large step sizes and the solution will still be stable.
- However very large step sizes might not capture the details of the solution properly.
- The disadvantage of implicit methods is that their solution requires more work compared to explicit methods. This can be seen better when an implicit method is applied to solve a set of ODEs. This requires the solution of a system of equations at each step (see page 729 for details).

Exercise 49: Solve $\frac{\mathbf{d y}}{\mathbf{d t}}=\mathbf{- 2 0 y}, \quad \mathbf{y}(\mathbf{0})=\mathbf{0}$ using
(a) Explicit Euler with $\mathrm{h}=0.1, \mathrm{~h}=0.2$, $\mathrm{h}=0.5$
(b) Implicit Euler with $\mathrm{h}=0.1, \mathrm{~h}=10$

Calculate 5 steps for each case and check the true error at each step. Do you observe any instability?

## Multistep Methods

- The methods discussed up to here are all one-step methods.
- They use the information at a single point $x_{i}$ to predict the value $y_{i+1}$.
- Multistep methods use the available information at point $\mathrm{x}_{\mathrm{i}-1}, \mathrm{x}_{\mathrm{i}-2}$, etc.
- Note that they can not be used at the first few steps of the computation.


## Non-Self-Starting Heun's Method

- The original Heun's method is

$$
\begin{array}{lll}
\text { Predictor: } & \mathbf{y}_{i+1}^{0}=\mathbf{y}_{\mathbf{i}}+\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{y}_{\mathbf{i}}\right) \mathbf{h} & \text { Local Error is } \mathrm{O}\left(\mathrm{~h}^{2}\right) \\
\text { Corrector: } & \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\frac{\mathbf{f}\left(\mathbf{x}_{\mathbf{i}}, \mathbf{y}_{\mathbf{i}}\right)+\mathbf{f}\left(\mathbf{x}_{\mathbf{i}+1}, \mathbf{y}_{\mathbf{i + 1}}^{0}\right)}{\mathbf{2}} \mathbf{h} & \text { Local Error is } \mathrm{O}\left(\mathrm{~h}^{3}\right)
\end{array}
$$

- The overall efficiency of the method can be improved by using a better predictor.
- We can use the Midpoint Method for the predictor instead of Euler's Method.



$$
\begin{aligned}
& \mathbf{y}_{i+1}^{0}=\mathbf{y}_{i-1}+\mathbf{f}\left(\mathbf{x}_{i}, \mathbf{y}_{\mathrm{i}}\right) \mathbf{2 h} \\
& \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+\frac{\mathbf{f}\left(\mathbf{x}_{i}, \mathbf{y}_{\mathrm{i}}\right)+\mathbf{f}\left(\mathbf{x}_{\mathrm{i}+1}, \mathbf{y}_{i+1}^{0}\right)}{\mathbf{2}} \mathbf{h}
\end{aligned}
$$

## Error Analysis for the N-S-S Heun's Method

- Local errors of the predictor and corrector steps of the Non-Self-Starting Heun's Method can be derived using TSE analyses

$$
\text { Predictor : } \mathbf{E}_{\mathbf{p}}=\frac{\mathbf{1}}{\mathbf{3}} \mathbf{h}^{\mathbf{3}} \mathbf{f}^{\prime \prime}\left(\xi_{\mathrm{p}}\right) \quad \text { Corrector: } \quad \mathbf{E}_{\mathbf{c}}=-\frac{\mathbf{1}}{\mathbf{1 2}} \mathbf{h}^{\mathbf{3}} \mathbf{f}^{\prime \prime}\left(\xi_{\mathrm{c}}\right)
$$

- Using these in the definition of true error we get

$$
\text { T.V }=y_{i+1}^{0}+\frac{1}{3} h^{3} f^{\prime \prime}\left(\xi_{\mathrm{p}}\right) \quad T . V=y_{i+1}-\frac{1}{12} h^{3} f^{\prime \prime}\left(\xi_{c}\right)
$$

- Subtract the first one from the second

$$
0=y_{i+1}-y_{i+1}^{0}-\frac{5}{12} h^{3} f^{\prime \prime}(\xi) \quad \rightarrow \quad \frac{y_{i+1}^{0}-y_{i+1}}{5}=-\frac{1}{12} h^{3} f^{\prime \prime}(\xi)
$$

- Note that the right-hand-side is equal to the error of the corrector $\left(\mathrm{E}_{\mathrm{c}}\right)$ except the second derivative of the function is evaluated at a different point. Assuming that f " does not vary much in the region of interest

$$
E_{c}=\frac{\mathbf{y}_{i+1}^{0}-\mathbf{y}_{i+1}}{5}
$$

- This formula can be used to estimate the error at each step of the Non-Self-Starting-Heun's Method. It uses the predicted and corrected values of $y_{i+1}$.


## Modifiers for the N-S-S Heun's Method

- Previously derived $\mathrm{E}_{\mathrm{c}}$ can be added to $\mathrm{y}_{\mathrm{i}+\mathbf{1}}$ to get even a better result. It is therefore called the corrector modifier.

$$
\mathbf{y}_{i+1} \leftarrow \mathbf{y}_{i+1}+\frac{\mathbf{y}_{i+1}-\mathbf{y}_{i+1}^{0}}{5}
$$

- Similarly a modifier for the predictor step can be derived (see page 737 for details).

$$
y_{i+1}^{0} \leftarrow y_{i+1}^{0}+\frac{4}{5}\left(y_{i}-y_{i}^{0}\right)
$$

- These modifiers can be applied after each predictor and corrector step to increase the accuracy of the method. If we use multiple correctors than the modifier can also be applied multiple times.

Example 45: Solve $\mathbf{d y} / \mathbf{d x}=\mathbf{y x} \mathbf{} \mathbf{- 1 . 2 y}$ with the initial condition $\mathbf{y ( 0 ) = 1}$ over the interval $[0,2]$ using the $\mathrm{N}-\mathrm{S}-\mathrm{S}$ Heun's Method with modifiers. Use $\mathrm{h}=0.5$. Note that the exact solution is $y(x)=e^{x^{3} / 3-1.2 x}$.
predictor: $\mathrm{y}^{\mathbf{0}}{ }_{\mathbf{i}+\mathbf{1}}=\mathrm{y}_{\mathbf{i} \mathbf{- 1}}+\mathrm{f}\left(\mathrm{x}_{\mathbf{i}}, \mathrm{y}_{\mathbf{i}}\right) 2 \mathrm{~h} \quad$ modifier: $\quad \mathrm{y}^{\mathbf{0}}{ }_{\mathbf{i}+\mathbf{1}} \leftarrow \mathrm{y}^{\mathbf{0}} \mathbf{i}_{\mathbf{+ 1}}+4 / 5\left(\mathrm{y}_{\mathbf{i}}-\mathrm{y}_{\mathbf{i}}^{\mathbf{0}}\right)$
corrector: $y_{i+1}=y_{\mathbf{i}}+0.5\left[f\left(x_{\mathbf{i}}, y_{i}\right)+f\left(x_{\mathbf{i}+\mathbf{1}}, y_{i+1}^{\mathbf{0}}\right)\right] h \quad$ modifier: $\quad y_{i+1} \leftarrow y_{i+1}+\left(y_{i+1}-y_{i+1}^{0}\right) / 5$
$x_{0}=0, y_{0}=1$ are given.
$\mathrm{i}=0$. The predictor needs $\mathrm{x}_{-1}$, which is not given. It can be obtained using the known exact solution. Or this step can be done with a different method, for example the Midpoint Method.

## Example 45 (cont'd):

$x_{0}=0, y_{0}=1$ are given.
$\mathrm{i}=0$. Use the Midpoint Method
Predictor: $\quad y_{0+1 / 2}=1+\left(1^{*} 0^{2}-1.2^{*} 1\right) 0.25=0.7$
Corrector: $y_{1}=y(0.5)=1+\left(0.7^{*} 0.25^{2}-1.2 * 0.7\right) 0.5=0.601875 \quad \varepsilon_{t}=5.19 \%$
$\mathrm{i}=1$. Predictor: $\mathrm{y}^{\mathbf{0}}{ }_{\mathbf{2}}=1+\left(0.601875^{*} 0.5^{\mathbf{2}}-1.2^{*} 0.601875\right)\left(2^{*} 0.5\right)=0.428219$
Predictor modifier: Can not be applied because we do not have $\mathrm{y}^{\mathbf{0}}{ }_{\mathbf{1}}$.
Corrector: $\mathrm{y}_{\mathbf{2}}=0.601875+0.5\left[\left(0.601875 * 0.5^{2}-1.2^{*} 0.601875\right)+\right.$ $\left.\left(0.428219 * 1^{2}-1.2 * 0.428219\right)\right]^{*} 0.5=0.437519$
Corrector modifier: $\mathrm{y}_{\mathbf{2}}=0.437519+(0.437519-0.428219) / 5=0.439379 \quad \varepsilon_{\mathrm{t}}=4.08 \%$
$\mathrm{i}=2$ \& $\mathrm{i}=3$ are exercises for you.

- Note that N-S-S Heun's method is not a popular multi-step method. Adams formulas that we will study next are generally preferred.


## Adam's Basforth Formulas

- They can be derived using appropriate derivative estimates in the TSE for $y_{i+1}$.
- They are explicit formulas.
- Their general formula is

$$
y_{i+1}=y_{i}+h \sum_{k=0}^{n-1}\left(\beta_{k} f_{i-k}\right)+\mathbf{O}\left(h^{n+1}\right)
$$

where the constants $\beta_{\mathbf{k}}$ are given at Table 26.1

- $1^{\text {st }}$ order: $\quad \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{h} \mathbf{f}_{\mathbf{i}}+\frac{\mathbf{1}}{\mathbf{2}} \mathbf{h}^{\mathbf{2} \mathbf{f}^{\prime}(\xi)}$
- $2^{\text {nd }}$ order: $\quad \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{h}\left(\frac{\mathbf{3}}{\mathbf{2}} \mathbf{f}_{\mathbf{i}}-\frac{\mathbf{1}}{\mathbf{2}} \mathbf{f}_{\mathbf{i - 1}}\right)+\frac{\mathbf{5}}{\mathbf{1 2}} \mathbf{h}^{\mathbf{3}} \mathbf{f}^{\prime \prime}(\xi)$
- $3^{\text {rd }}$ order: $\quad \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+h\left(\frac{\mathbf{2 3}}{12} f_{i}-\frac{16}{12} f_{i-1}+\frac{\mathbf{5}}{12} f_{i-2}\right)+\frac{9}{\mathbf{2 4}} h^{4} f^{(3)}(\xi)$


## Derivation of the 3rd order Adam's Basforth Formula

- Write TSE for $\mathrm{y}_{\mathrm{i}+1}$

$$
\mathbf{y}_{i+1}=\mathbf{y}_{i}+\mathbf{f}_{i} h+\frac{\mathbf{f}_{i}^{\prime}}{\mathbf{2}} \mathbf{h}^{2}+\frac{\mathbf{f}_{i}^{\prime \prime}}{\mathbf{6}} \mathbf{h}^{3}+\mathbf{O}\left(h^{4}\right)+\ldots \ldots
$$

- Use backward estimates for $\mathrm{f}^{\prime}$ and $\mathrm{f}^{\prime \prime}$ (They are given in Figure 23.2).

$$
\begin{aligned}
& f_{i}^{\prime}=\frac{3 f_{i}-4 f_{i-1}+f_{i-2}}{2 h}+\mathbf{O}\left(h^{2}\right) \\
& \mathbf{f}_{i}^{\prime \prime}=\frac{f_{i}-2 f_{i-1}+f_{i-2}}{h^{2}}+\mathbf{O}(\mathbf{h})
\end{aligned}
$$

- Substitute these into the $1^{\text {st }}$ equation

$$
y_{i+1}=y_{i}+f_{i} h+\left(\frac{3 f_{i}-4 f_{i-1}+f_{i-2}}{2 h}+O\left(h^{2}\right)\right) \frac{h^{2}}{2}+\left(\frac{f_{i}-2 f_{i-1}+f_{i-2}}{h^{2}}+O(h)\right) \frac{h^{3}}{6}+O\left(h^{4}\right)+\ldots \ldots
$$

- Arrange the terms to get

$$
y_{i+1}=y_{i}+h\left(\frac{23}{12} f_{i}-\frac{16}{12} f_{i-1}+\frac{5}{12} f_{i-2}\right)+O\left(h^{4}\right)
$$

Exercise 50: To get the exact error term we need to use the exact errors in the derivative estmates. Figure 23.2 does not provide them. You need to derive them.

## Adam's Moulton Formulas

- Their general formula is

$$
\mathbf{y}_{i+1}=\mathbf{y}_{i}+h \sum_{k=0}^{n-1}\left(\beta_{k} f_{i+1-k}\right)+\mathbf{O}\left(h^{n+1}\right)
$$

where the constants $\beta_{\mathbf{k}}$ are given at Table 26.2

- $2^{\text {nd }}$ order: $\quad \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+\mathbf{h}\left(\frac{\mathbf{1}}{\mathbf{2}} \mathbf{f}_{\mathbf{i + 1}}+\frac{\mathbf{1}}{\mathbf{2}} \mathbf{f}_{\mathbf{i}}\right)-\frac{\mathbf{1}}{\mathbf{1 2}} \mathbf{h}^{\mathbf{3} \mathbf{f}^{\prime \prime}(\xi)}$
-3rd order: $\quad \mathbf{y}_{i+1}=\mathbf{y}_{\mathbf{i}}+h\left(\frac{\mathbf{5}}{12} f_{i+1}+\frac{\mathbf{8}}{12} f_{i}-\frac{\mathbf{1}}{12} f_{i-1}\right)-\frac{\mathbf{1}}{\mathbf{2 4}} h^{4} f^{(3)}(\xi)$
- These are implicit formulas because the unknown $\mathrm{y}_{\mathrm{i}+1}$ appears on both sides of the equation.

Exercise 51: Derive the 3rd order formula and the corresponding error term using a proper derivative estimates in the TSE for $\mathrm{y}_{\mathrm{i}+\mathbf{1}}$.

- Other higher order formulas can be derived. Two popular ones are the fourth-order Adams Method and the Milne's Method. (see page 746-747 for details).


## Example 46:

- Solve the following initial value problem in the range $[0,2.5]$ using 4 th order Adams Method with multiple correctors. If necessary start the solution with the RK4 Method. Use $h=0.5$

$$
\frac{d y}{d x}=\frac{-y}{1+x}, \quad y(0)=2
$$

- Fourth-order Adams Method is a predictor corrector method.

$$
\begin{array}{ll}
\text { Predictor : } & \mathbf{y}_{\mathbf{i + 1}}^{0}=\mathbf{y}_{\mathbf{i}}+\mathbf{h}\left(\frac{\mathbf{5 5}}{\mathbf{2 4}} \mathbf{f}_{\mathbf{i}}-\frac{\mathbf{5 9}}{\mathbf{2 4}} \mathbf{f}_{\mathbf{i}-1}+\frac{\mathbf{3 7}}{\mathbf{2 4}} \mathbf{f}_{\mathrm{i}-2}-\frac{\mathbf{9}}{\mathbf{2 4}} \mathbf{f}_{\mathrm{i}-3}\right) \\
\text { Corrector: } & \mathbf{y}_{\mathbf{i + 1}}=\mathbf{y}_{\mathbf{i}}+\mathbf{h}\left(\frac{\mathbf{9}}{\mathbf{2 4}} \mathbf{f}_{\mathbf{i}+1}+\frac{\mathbf{1 9}}{\mathbf{2 4}} \mathbf{f}_{\mathbf{i}}-\frac{\mathbf{5}}{\mathbf{2 4}} \mathbf{f}_{\mathrm{i}-1}+\frac{\mathbf{1}}{\mathbf{2 4}} \mathbf{f}_{\mathbf{i}-2}\right)
\end{array}
$$

- To find $y_{i+1}$, Adams Method needs $f_{i-3}$, which needs $y_{i-3}$. Therefore we can not use the Adams Method until we get $y_{1}, y_{2}$ and $y_{3}$ using the fourth-order Runge-Kutta Method.

$$
\begin{array}{lll}
i=0 & i=1 & i=2 \\
k_{1}=f\left(x_{0}, y_{0}\right)=-2 & k_{1}=-0.888889 & k_{1}=-0.5 \\
k_{2}=f\left(x_{0}+h / 2, y_{0}+k_{1} h / 2\right)=-1.2 & k_{\mathbf{2}}=-0.634921 & k_{\mathbf{2}}=-0.388889 \\
k_{\mathbf{3}}=f\left(x_{0}+h / 2, y_{0}+k_{2} h / 2\right)=-1.36 & k_{\mathbf{3}}=-0.671202 & k_{\mathbf{3}}=-0.401235 \\
k_{\mathbf{4}}=f\left(x_{0}+h, y_{0}+k_{\mathbf{3}} h\right)=-0.88 & k_{4}=-0.498866 & k_{\mathbf{4}}=-0.319753 \\
y_{\mathbf{1}}=y_{0}+h\left(k_{\mathbf{1}}+2 k_{\mathbf{2}}+2 k_{\mathbf{3}}+k_{4}\right) / 6=1.333333 & y_{\mathbf{2}}=1.000000 & y_{\mathbf{3}}=0.8
\end{array}
$$

## Example 46 (cont'd):

- Now that we have $\mathrm{y}_{\mathbf{0}}=2, \mathrm{y}_{\mathbf{1}}=1.333333, \mathrm{y}_{\mathbf{2}}=1$ and $\mathrm{y}_{3}=0.8$ we can start using the Adams Method.
$i=3$. Predictor: $y^{\mathbf{0}}{ }_{4}=y_{3}+0.5\left(55 f_{3}-59 f_{2}+37 f_{1}-9 f_{0}\right) / 24=0.737731$
Corrector: $\mathrm{y}^{\mathbf{1}}{ }_{4}=\mathrm{y}_{\mathbf{3}}+0.5\left(9 \mathrm{f}_{\mathbf{4}}+19 \mathrm{f}_{\mathbf{3}}-5 \mathrm{f}_{\mathbf{2}}+\mathrm{f}_{\mathbf{1}}\right) / 24=0.660790$
Corrector: $\mathrm{y}^{\mathbf{2}}{ }_{4}=0.665599$
Corrector: $\mathrm{y}^{\mathbf{3}}{ }_{4}=0.665298$
Corrector: $\mathrm{y}_{4}^{\mathbf{4}}=0.665317$
$\mathrm{i}=4$. Predictor: $\mathrm{y}_{\mathbf{0}}^{\mathbf{0}}=\mathrm{y}_{\mathbf{4}}+0.5\left(55 \mathrm{f}_{\mathbf{4}}-59 \mathrm{f}_{\mathbf{3}}+37 \mathrm{f}_{\mathbf{2}}-9 \mathrm{f}_{\mathbf{1}}\right) / 24=0.585786$
Corrector: $\mathrm{y}^{\mathbf{1}}{ }_{5}=\mathrm{y}_{4}+0.5\left(9 \mathrm{f}_{5}+19 \mathrm{f}_{4}-5 \mathrm{f}_{\mathbf{3}}+\mathrm{f}_{2}\right) / 24=0.569067$
Corrector: $\mathrm{y}^{\mathbf{2}}{ }_{5}=0.569963$
Corrector: $\mathrm{y}^{\mathbf{3}} \mathbf{5}=0.569915$


## Boundary Value Problems (BVP)

- For a system of ODEs or for an ODE of order 2 or more, we need to specify multiple initial/boundary conditions.
- If all these conditions are provided at the same point, the problem is said to be an Initial Value Problem (IVP).

$$
\begin{array}{ll}
\frac{d y_{1}}{d t}=f_{1}\left(t, y_{1}, y_{2}\right), & y_{1}(0)=y_{1,0} \\
\frac{d y_{2}}{d t}=f_{2}\left(t, y_{1}, y_{2}\right), & \mathbf{y}_{2}(0)=y_{2,0}
\end{array}
$$



- If these conditions are not provided at the same point, the problem is said to be a Boundary Value problem (BVP).



## The Shooting Method

- Consider the following boundary value problem

$$
\begin{array}{ll}
\frac{d^{2} T}{d x^{2}}=f\left(x, T, T^{\prime}\right) & T(0)=T_{0} \\
T(L)=T_{L}
\end{array}
$$



- Define a new variable $z=d T / d x$ and separate the above ODE into two $1^{\text {st }}$ order ODEs.

$$
\begin{aligned}
& \frac{d T}{d x}=z \quad T(0)=T_{0} \\
& \frac{d z}{d x}=f\left(x, T, T^{\prime}\right) \quad z(0)=?
\end{aligned}
$$

- This is not an initial value problem and $z(0)$ is not known.
- Shooting method assumes a $z(0)$ value and solves the problem as if it was an initial value problem.
- This is a trial-error method.
- Assume a $z(0)$ value, solve the problem. Check the calculated $T(10)$ with the given condition.
- Based on the above comparison assume another z(0). Repeat the solution and the comparison.
- Continue like this. For a linear problem exact $\mathrm{T}(10)$ can be found after 3 solutions. A nonlinear problem is more difficult to solve with the shooting method.


## Example 47:

- Solve the following boundary value problem

$$
\begin{aligned}
& \frac{d^{2} T}{d(0)}=40 \\
& d x^{2}=0.01 T-0.2 \\
& T(10)=200
\end{aligned}
$$



- Separate the problem into two $1^{\text {st }}$ order ODEs.

$$
\begin{aligned}
& \frac{d T}{d x}=z \quad T(0)=40 \\
& \frac{d z}{d x}=0.01 T-0.2 \quad z(0)=?
\end{aligned}
$$

- Assume a value for $z(0)$, the slope at $x=0$. For example $z(0)=15$.
- Select a method and a step size and solve this initial value problem. For example use the Euler's Method with $\mathrm{h}=2$. The results are shown below.

$$
\begin{array}{ll}
\mathrm{T}_{0}=40 \quad \mathrm{z}_{0}=15 & \\
\mathrm{~T}_{1}=\mathrm{T}_{0}+\mathrm{z}_{0}(2)=70 & \mathrm{z}_{1}=\mathrm{z}_{0}+\left(0.01 \mathrm{~T}_{0}-0.2\right)(2)=15.4 \\
\mathrm{~T}_{2}=\mathrm{T}_{1}+\mathrm{z}_{1}(2)=100.8 & \mathrm{z}_{2}=\mathrm{z}_{1}+\left(0.01 \mathrm{~T}_{1}-0.2\right)(2)=16.4 \\
\mathrm{~T}_{3}=\mathrm{T}_{2}+\mathrm{z}_{2}(2)=133.6 & \mathrm{z}_{3}=\mathrm{z}_{2}+\left(0.01 \mathrm{~T}_{2}-0.2\right)(2)=18.016 \\
\mathrm{~T}_{4}=\mathrm{T}_{\mathbf{3}}+\mathrm{Z}_{3}(2)=169.632 & \mathrm{z}_{4}=\mathrm{z}_{3}+\left(0.01 \mathrm{~T}_{3}-0.2\right)(2)=20.288 \\
\mathrm{~T}_{5}=\mathrm{T}_{4}+\mathrm{z}_{4}(2)=210.208 & \mathrm{z}_{5}=\mathrm{z}_{4}+\left(0.01 \mathrm{~T}_{4}-0.2\right)(2)=23.28064
\end{array}
$$



## Example 47 (cont'd):

- The guess $\mathrm{z}(0)=15$ resulted in $\mathrm{T}(10)=210.208$. This time assume a lower value, like $\mathrm{z}(0)=10$.
- The solution with Euler's Method and $\mathrm{h}=2$ is given below
$T_{0}=40 \quad z_{0}=10$
$\mathrm{T}_{1}=\mathrm{T}_{0}+\mathrm{z}_{0}(2)=60 \quad \mathrm{z}_{1}=\mathrm{z}_{0}+\left(0.01 \mathrm{~T}_{0}-0.2\right)(2)=10.4$
$\mathrm{T}_{\mathbf{2}}=\mathrm{T}_{1}+\mathrm{z}_{1}(2)=80.8 \quad \mathrm{z}_{\mathbf{2}}=\mathrm{z}_{\mathbf{1}}+\left(0.01 \mathrm{~T}_{1}-0.2\right)(2)=11.2$
$\mathrm{T}_{3}=\mathrm{T}_{\mathbf{2}}+\mathrm{z}_{\mathbf{2}}(2)=103.2 \quad \mathrm{z}_{3}=\mathrm{z}_{\mathbf{2}}+\left(0.01 \mathrm{~T}_{\mathbf{2}}-0.2\right)(2)=12.416$
$\mathrm{T}_{4}=\mathrm{T}_{3}+\mathrm{z}_{3}(2)=128.032 \quad \mathrm{z}_{4}=\mathrm{z}_{3}+\left(0.01 \mathrm{~T}_{3}-0.2\right)(2)=14.08$

$\mathrm{T}_{5}=\mathrm{T}_{4}+\mathrm{z}_{4}(2)=156.192 \quad \mathrm{z}_{5}=\mathrm{z}_{4}+\left(0.01 \mathrm{~T}_{4}-0.2\right)(2)=16.24064$
- The first guess of $z(0)=15$ resulted in $T(10)=210.208$.

Second guess of $z(0)=10$ resulted in $T(10)=156.192$.

- Third guess can be obtained by performing a linear interpolation with the first two guesses.


$$
\begin{aligned}
& z(0)=10+\frac{15-10}{210.208-156.192}(200-156.192) \\
& z(0)=14.055095
\end{aligned}
$$

## Example 47 (cont'd):

- Perform another solution with the third guess, $z(0)=14.055095$.

$$
\begin{array}{ll}
T_{0}=40 & z_{0}=14.055095 \\
T_{1}=T_{0}+z_{0}(2)=68.1102 & z_{1}=z_{0}+\left(0.01 T_{0}-0.2\right)(2)=14.4551 \\
T_{2}=T_{1}+z_{1}(2)=97.0204 & z_{2}=z_{1}+\left(0.01 \mathrm{~T}_{1}-0.2\right)(2)=15.4173 \\
T_{3}=T_{2}+z_{2}(2)=127.8550 & z_{3}=z_{2}+\left(0.01 \mathrm{~T}_{2}-0.2\right)(2)=16.6577 \\
\mathrm{~T}_{4}=T_{3}+\mathrm{z}_{3}(2)=161.7704 & \mathrm{z}_{4}=z_{3}+\left(0.01 \mathrm{~T}_{3}-0.2\right)(2)=19.1148 \\
T_{5}=T_{4}+z_{4}(2)=200.0000 & \mathrm{z}_{5}=\mathrm{z}_{4}+\left(0.01 \mathrm{~T}_{4}-0.2\right)(2)=21.9502
\end{array}
$$



- Note that we got $\mathrm{T}(10)=200$ exactly. This is because the ODE that we are solving is linear.

Therefore the linear interpolation we performed with the first two guesses was good enough to get $\mathrm{T}(10)$ exactly.

- $T(10)$ being exact does not mean that the intermediate $T$ values are exact. They are not.
- For this linear ODE, three trials was enough. For a nonlinear ODE it is not this simple. You may need to combine the first three guesses with a $2^{\text {nd }}$ order interpolation to get a fourth guess, and so on (Read page 755 for details).

Exercise 52: Solve the following BVP with the shooting mehod.

$$
u^{\prime \prime}-\left(1-\frac{x}{5}\right) u u^{\prime}=x \quad u(1)=2 \quad u(3)=-1
$$

## Finite Difference Method

- The idea is to replace the derivatives in the ODE with finite divided differences.

Example 48: Consider the same BVP.

$$
\begin{array}{rl}
\frac{d^{2} T}{d x^{2}}=0.01 T-0.2 & T(0)
\end{array}=40
$$

Approximating the second derivative with centered differences, ODE becomes

$$
\left.\frac{d^{2} \mathbf{T}}{d x^{2}}\right|_{i} \approx \frac{T_{i+1}-2 T_{i}+T_{i-1}}{h^{2}} \quad \rightarrow \quad \frac{T_{i+1}-2 T_{i}+T_{i-1}}{h^{2}}=0.01 T_{i}-0.2
$$

For $h=\Delta x=2$ we will have four points at which we need to determine $T$.


Rearrange the above difference equation and write it for each unknown point.

$$
\begin{array}{ll}
\text { General: } & -T_{i-1}+2.04 T_{i}-T_{i+1}=0.8 \\
i=1: & -T_{0}+2.04 T_{1}-T_{2}=0.8 \quad\left(T_{0}=40 \text { is known }\right) \\
i=2: & -T_{1}+2.04 T_{2}-T_{3}=0.8 \\
i=3: & -T_{2}+2.04 T_{3}-T_{4}=0.8 \\
i=4: & -T_{3}+2.04 T_{4}-T_{5}=0.8 \quad\left(T_{5}=200 \text { is known }\right)
\end{array}
$$

## Example 48 (cont'd):

This is $4 \times 4$ system of linear equations. Solve it with one of the methods that we learned.

$$
\left[\begin{array}{cccc}
2.04 & -1 & 0 & 0 \\
-1 & 2.04 & -1 & 0 \\
0 & -1 & 2.04 & -1 \\
0 & 0 & -1 & 2.04
\end{array}\right]\left\{\begin{array}{l}
\mathbf{T}_{1} \\
T_{2} \\
T_{3} \\
T_{4}
\end{array}\right\}=\left\{\begin{array}{c}
40.8 \\
0.8 \\
0.8 \\
200.8
\end{array}\right\} \quad \rightarrow \quad\left\{\begin{array}{l}
T_{1} \\
T_{2} \\
T_{3} \\
T_{4}
\end{array}\right\}=\left\{\begin{array}{c}
65.97 \\
93.78 \\
124.54 \\
159.48
\end{array}\right\}
$$

- Note that this is a tridiagonal system. There are very efficient algorithms specially designed to solve such systems. See page 286 for details.
- More accurate results can be obtained by using
- Higher order derivative approximations. This will increase the bandwidth of the coefficient matrix.
- Smaller step size. This will result in a larger matrix.
- If we use higher order approximations, we may need to use forward or backward differences at the points close to the boundaries.

Exercise 53: Solve the previous problem with $\mathrm{h}=0.1$. Write a computer program that will generate the system of equations and solve them using an iterative method. Compare the answers with the exact solution (See page 753).

