2021 Spring MAS 365
Chapter 5: Initial-Value Problems for Ordinary Differential Equations

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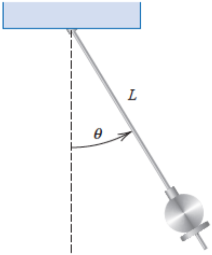
Introduction

- The motion of a swinging pendulum under certain simplifying assumptions is described by the second-order differential equation

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\sin\theta = 0, .$$



- If, in addition, we specify the position of the pendulum when the motion begins, $\theta(t_0) = \theta_0$, and its velocity at that point, $\theta'(t_0) = \theta'_0$, we have what is called an *initial-value problem*.

Introduction (cont'd)

- For small values of θ, the approximation $\theta \approx \sin\theta$ can be used to simplify this problem to the linear initial-value problem

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\theta = 0, \quad \theta(t_0) = \theta_0, \quad \theta'(t_0) = \theta_0'.$$

- This can be solved by a standard differential-equation technique.

- For larger values of θ, the assumption that $\theta \approx \sin\theta$ is not reasonable, so approximation methods must be used.

- In practice, few of the problems originating from the study of physical phenomena can be solved exactly...

Introduction (cont'd)

- The first part of this chapter studies approximating the solution $y(t)$ to a problem of the form

$$\frac{dy}{dt} = f(t, y), \quad \text{for } a \le t \le b,$$

subject to an initial condition $y(a) = \alpha$.

Introduction (cont'd)

- Later in the chapter, we study its extension to a **system** of first-order differential equations in the form

$$\frac{dy_1}{dt} = f_1(t, y_1, y_2, \ldots, y_n), \quad \ldots, \quad \frac{dy_n}{dt} = f_n(t, y_1, y_2, \ldots, y_n),$$

for $a \le t \le b$, subject to the initial conditions

$$y_1(a) = \alpha_1, \quad y_2(a) = \alpha_2, \quad \ldots, \quad y_n(a) = \alpha_n.$$

- We also consider the general n**th-order** initial value problem of the form

$$y^{(n)} = f(t, y, y', y'', \ldots, y^{(n-1)}),$$

for $a \le t \le b$, subject to the initial conditions

$$y(a) = \alpha_1, \quad y'(a) = \alpha_2, \quad \ldots, \quad y^{(n-1)}(a) = \alpha_n.$$

Initial-Value Problems

- Differential equations are used to model problems in science and engineering that involve the change of some variables with respect to another.
- Most of these problems require the solution of an *initial-value problem*, that is, the solution to a differential equation that satisfies a given initial condition.

1. Simplify the differential equation that can be solved exactly.
2. (This chapter) Approximate the solution of the original problem at certain specified points.

- This section studies the theory of ordinary differential equations before studying their approximations.

Lipschitz Condition and Convexity

Definition 1

A function $f(t, y)$ is said to satisfy a **Lipschitz condition** *in the variable y on a set $D \subset \mathbb{R}^2$ if a constant $L > 0$ exists with*

$$|f(t, y_1) - f(t, y_2)| \leq L|y_1 - y_2|,$$

whenever (t, y_1) and (t, y_2) are in D. The constant L is called a **Lipschitz constant** *for f.*

Ex. Show that $f(t, y) = t|y|$ satisfies a Lipschitz condition on the interval $D = \{(t, y) \mid 1 \leq t \leq 2 \text{ and } -3 \leq y \leq 4\}$.

Lipschitz Condition and Convexity (cont'd)

Definition 2

A set $D \subset \mathbb{R}^2$ is said to be **convex** *if whenever (t_1, y_1) and (t_2, y_2) belong to D, then $((1-\lambda)t_1 + \lambda t_2, (1-\lambda)y_1 + \lambda y_2)$ also belongs to D for every λ in $[0, 1]$.*

Theorem 1

Suppose $f(t, y)$ is defined on a convex set $D \subset \mathbb{R}^2$. If a constant $L > 0$ exists with

$$\left|\frac{\partial f}{\partial y}(t, y)\right| \leq L, \quad \text{for all } (t, y) \in D,$$

then f satisfies a Lipschitz condition on D in the variable y with Lipschitz constant L.

Lipschitz Condition and Convexity (cont'd)

Proof Let (t, y_1) and (t, y_2) be in D. Define $g(y) = f(t, y)$ with t fixed. Suppose $y_1 < y_2$. Since the line passing through (t, y_1) and (t, y_2) lies in D, and f is continuous on D, we have $g \in C[y_1, y_2]$.

Using MVT on g, there exists a number ξ between y_1 and y_2 with

$$g(y_2) - g(y_1) = g'(\xi)(y_2 - y_1).$$

Existence and Uniqueness for Initial-Value Problem

Theorem 2

Suppose that $D = \{(t, y) \mid a \le t \le b \text{ and } -\infty < y < \infty\}$ and that $f(t, y)$ is continuous on D. If f satisfies a Lipschitz condition on D in the variable y, then the initial-value problem

$$y'(t) = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

has a unique solution $y(t)$ for $a \le t \le b$.

Existence and Uniqueness for Initial-Value Problem

Ex. Show that there is a unique solution to the initial-value problem

$$y' = 1 + t\sin(ty), \quad 0 \le t \le 2, \quad y(0) = 0.$$

Well-Posed Problems

- In addition to the uniqueness, we want to know whether small changes in the statement of the problem introduce correspondingly small changes in the solution.
- This is because the initial-value problems obtained by observing physical phenomena generally only approximate the true situation.
- This is also important because of the introduction of round-off error.

Well-Posed Problems (cont'd)

Definition 3

The initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$$

is said to be a **well-posed problem** *if*

- *a unique solution , $y(t)$, to the problem exists, and*
- *there exist constants $\epsilon_0 > 0$ and $k > 0$ such that for any ϵ, with $\epsilon_0 > \epsilon > 0$, whenever $\delta(t)$ is continuous with $|\delta(t)| < \epsilon$ for all t in $[a, b]$, and when $|\delta_0| < \epsilon$, the initial-value (perturbed) problem*

  $$\frac{dz}{dt} = f(t, z) + \delta(t), \quad a \le t \le b, \quad z(a) = \alpha + \delta_0,$$

  has a unique solution $z(t)$ that satisfies

  $$|z(t) - y(t)| < k\epsilon \quad \text{for all } t \text{ in } [a, b].$$

Well-Posed Problems (cont'd)

Theorem 3

Suppose $D = \{(t, y) \mid a \le t \le b \text{ and } -\infty < y < \infty\}$*. If* f *is continuous and satisfies a Lipschitz condition in the variable* y *on the set* D*, then the initial-value problem*

$$\frac{dy}{dt} = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha$$

is well-posed.

Ex. Show that the initial-value problem

$$\frac{dy}{dt} = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5$$

is well-posed on $D = \{(t, y) \mid 0 \le t \le 2 \text{ and } -\infty < y < \infty\}$.

Well-Posed Problems (cont'd)

- Consider the solution to the perturbed problem

$$\frac{dz}{dt} = z - t^2 + 1 + \delta, \quad 0 \le t \le 2, \quad z(0) = 0.5 + \delta_0,$$

where δ and δ_0 are constants. The solution to the original and perturbed problems are

$$y(t) = (t+1)^2 - 0.5e^t \quad \text{and} \quad z(t) = (t+1)^2 + (\delta + \delta_0 - 0.5)e^t - \delta,$$

respectively.

Suppose that ϵ is a positive number. If $|\delta| < \epsilon$ and $|\delta_0| < \epsilon$, then

$$|y(t) - z(t)| =$$

for all t. This implies that the original problem is well-posed with $k =$ for all $\epsilon > 0$.

Euler's Method

- The object of Euler's methods is to obtain approximations to the well-posed initial-value problem

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

- Approximations to y will be generated at various values, called **mesh points**, in the interval $[a, b]$.

Euler's Method (cont'd)

- Consider the equally distributed mesh points

$$t_i = a + ih, \quad \text{for each } i = 0, 1, 2, \ldots, N.$$

  The common distance between the points $h = (b-a)/N = t_{i+1} - t_i$ is called the **step size**.

- Consider Taylor's Theorem with assumption that the unique solution $y(t)$ is twice continuously differentiable, so that

$$y(t_{i+1}) = y(t_i) + (t_{i+1} - t_i)y'(t_i) + \frac{(t_{i+1} - t_i)^2}{2} y''(\xi_i)$$

  for some number ξ_i in (t_i, t_{i+1}).

Euler's Method (cont'd)

- Because $h = t_{i+1} - t_i$, we have

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\xi_i),$$

and using the differential equation we have

$$y(t_{i+1}) =$$

Euler's Method (cont'd)

- Euler's method constructs $w_i \approx y(t_i)$, for each $i = 1, 2, \ldots, N$, by deleting the remainder term.

- The Euler's method is

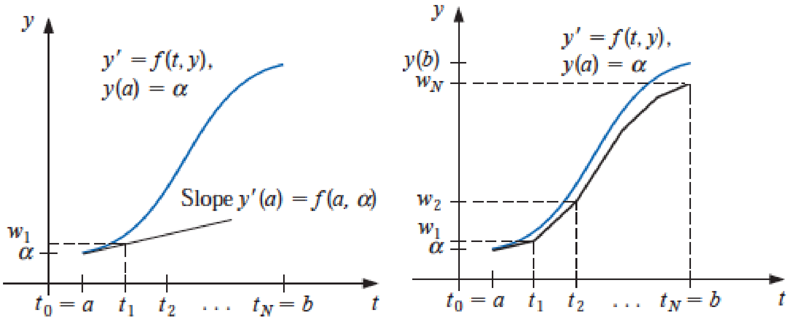
$$
\begin{aligned}
w_0 &= \alpha, \\
w_{i+1} &= w_i + hf(t_i, w_i), \quad \text{for each } i = 0, 1, \ldots, N-1.
\end{aligned}
$$

This is called the **difference equation** associated with Euler's method.

Euler's Method (cont'd)

- When $w_i \approx y(t_i)$, the well-posedness implies that

$$f(t_i, w_i) \approx y'(t_i) = f(t_i, y(t_i)).$$



Euler's Method (cont'd)

Ex. Use Euler's method with $h = 0.5$ to approximate the solution to

$$y' = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5,$$

at $t = 2$.

Euler's Method (cont'd)

Ex. Use Euler's method with $h = 0.2$ to approximate the solution to

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5,$$

and compare with the exact values given by $y(t) = (t+1)^2 - 0.5e^t$.

t_i	w_i	$y_i = y(t_i)$	$\lvert y_i - w_i \rvert$
0.0	0.5000000	0.5000000	0.0000000
0.2	0.8000000	0.8292986	0.0292986
0.4	1.1520000	1.2140877	0.0620877
0.6	1.5504000	1.6489406	0.0985406
0.8	1.9884800	2.1272295	0.1387495
1.0	2.4581760	2.6408591	0.1826831
1.2	2.9498112	3.1799415	0.2301303
1.4	3.4517734	3.7324000	0.2806266
1.6	3.9501281	4.2834838	0.3333557
1.8	4.4281538	4.8151763	0.3870225
2.0	4.8657845	5.3054720	0.4396874

Error Bounds for Euler's Method

Lemma 1

If s *and* t *are positive real numbers,* $\{a_i\}_{i=0}^{k}$ *is a sequence satisfying* $a_0 \geq -t/s$, *and*

$$a_{i+1} \leq (1+s)a_i + t, \quad \textit{for each } i = 0, 1, 2, \ldots, k-1,$$

then

$$a_{i+1} \leq e^{(i+1)s}\left(a_0 + \frac{t}{s}\right) - \frac{t}{s}.$$

Error Bounds for Euler's Method (cont'd)

Theorem 4

Suppose f is continuous and satisfies a Lipschitz condition in the second variable with constant L on

$$D = \{(t, y) \mid a \le t \le b \text{ and } -\infty < y < \infty\},$$

and that a constant M exists with

$$|y''(t)| \le M, \quad \text{for all } t \in [a, b],$$

where $y(t)$ denotes the unique solution ot the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha.$$

Let $w_0, w_1, \ldots, w_N$ be the approximations generated by Euler's method for some positive integer N. Then, for each $i = 0, 1, 2, \ldots, N$,

$$|y(t_i) - w_i| \le \frac{hM}{2L}[e^{L(t_i - a)} - 1].$$

Error Bounds for Euler's Method (cont'd)

Proof When $i = 0$ the result is true. We have

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2}y''(\xi_i),$$

for $i = 0, 1, \ldots, N-1$, and

$$w_{i+1} = w_i + hf(t_i, w_i).$$

Using the notation $y_i = y(t_i)$, subtracting the two equations leads to

$$y_{i+1} - w_{i+1} = y_i - w_i + h[f(t_i, y_i) - f(t_i, w_i)] + \frac{h^2}{2}y''(\xi_i).$$

Hence,

$$|y_{i+1} - w_{i+1}| \leq |y_i - w_i| + h|f(t_i, y_i) - f(t_i, w_i)| + \frac{h^2}{2}|y''(\xi_i)|.$$

Error Bounds for Euler's Method (cont'd)

Proof Since f satisfies a Lipschitz condition in the second variable with constant L, and $|y''(t)| \leq M$, we have

$$|y_{i+1} - w_{i+1}| \leq$$

Using Lemma 1 with

Error Bounds for Euler's Method (cont'd)

- Theorem 4 requires the bound for the second derivative of the solution...
- If $\frac{\partial f}{\partial t}$ and $\frac{\partial f}{\partial y}$ both exist, the chain rule implies that

$$y''(t) = \frac{dy'}{dt}(t) = \frac{df}{dt}(t, y(t)) = \frac{\partial f}{\partial t}(t, y(t)) + \frac{\partial f}{\partial y}(t, y(t)) \ \cdot \ f(t, y(t)),$$

so an error bound could be obtained without explicitly knowing $y(t)$.

Error Bounds for Euler's Method (cont'd)

Ex. Find error bounds for approximating the following initial-value problem

$$y' = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

by Euler's method, and compare these with the actual errors from $y(t) = (t+1)^2 - 0.5e^t$.

t_i	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6	1.8	2.0
Actual Error	0.02930	0.06209	0.09854	0.13875	0.18268	0.23013	0.28063	0.33336	0.38702	0.43969
Error Bound	0.03752	0.08334	0.13931	0.20767	0.29117	0.39315	0.51771	0.66985	0.85568	1.08264

Error Bounds for Euler's Method (cont'd)

- Further consider the effect of round-off error:

$$u_0 = \alpha + \delta_0,$$
$$u_{i+1} = u_i + hf(t_i, u_i) + \delta_{i+1}, \quad \text{for each } i = 0, 1, \ldots, N-1, \tag{1}$$

where δ_i denotes the round-off error associated with u_i.

Error Bounds for Euler's Method (cont'd)

Theorem 5

Let $y(t)$ denote the unique solution to the initial-value problem

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha \tag{2}$$

and $u_0, u_1, \ldots, u_N$ be the approximations obtained using (1). If $|\delta_i| < \delta$ for each $i = 0, 1, \ldots, N$ and the hypotheses of Theorem 4 hold for (2), then

$$|y(t_i) - u_i| \le \frac{1}{L}\left(\frac{hM}{2} + \frac{\delta}{h}\right)[e^{L(t_i-a)} - 1] + |\delta_0| e^{L(t_i-a)}$$

for each $i = 0, 1, \ldots, N$.

Error Bounds for Euler's Method (cont'd)

- The error bound is no longer linear in h, and

$$\lim_{h\to 0}\left(\frac{hM}{2}+\frac{\delta}{h}\right)=\infty.$$

- Letting $E(h)=\frac{hM}{2}+\frac{\delta}{h}$, one can find that the minimum value of $E(h)$ occurs when

$$h=\sqrt{\frac{2\delta}{M}}.$$

Local Truncation Error

Definition 4

The difference method

$$w_0 = \alpha$$
$$w_{i+1} = w_i + h\phi(t_i, w_i), \quad \textit{for each } i = 0, 1, \ldots, N-1,$$

has **local truncation error**

$$\tau_{i+1}(h) = \frac{y_{i+1} - (y_i + h\phi(t_i, y_i))}{h} = \frac{y_{i+1} - y_i}{h} - \phi(t_i, y_i)$$

for each $i = 0, 1, \ldots, N-1$, *where* y_i *and* y_{i+1} *denote the solution at* t_i *and* t_{i+1}, *respectively.*

Local Truncation Error (cont'd)

- Euler's method has local truncation error at the ith step

$$\tau_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - f(t_i, y_i), \quad \text{for each } i = 0, 1, \ldots, N-1.$$

- We previously learned that

$$\tau_{i+1}(h) = \qquad\qquad \text{for some } \xi \text{ in } (t_i, t_{i+1}).$$

When $y''(t)$ is bounded by a constant M on $[a, b]$, this implies

$$|\tau_{i+1}(h)| \leq$$

Taylor Method of Order n

- Suppose the solution $y(t)$ to the initial-value problem

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha,$$

has $(n+1)$ continuous derivatives.

- Expand $y(t)$ in terms of its nth Taylor polynomial about t_i and evaluate at t_{i+1}, for some ξ_i in (t_i, t_{i+1}):

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \cdots + \frac{h^n}{n!}y^{(n)}(t_i) + \frac{h^{n+1}}{(n+1)!}y^{(n+1)}(\xi_i),$$

- Using $y^{(k)}(t) = f^{(k-1)}(t, y(t))$ for $k = 1, \ldots, n+1$, we have

$$y(t_{i+1}) =$$

Taylor Method of Order n (cont'd)

- Taylor method of order n is

$$w_0 = \alpha$$
$$w_{i+1} = w_i + hT^{(n)}(t_i, w_i), \quad \text{for each } i = 0, 1, \ldots, N-1,$$

where

$$T^{(n)}(t_i, w_i) = \ f(t_i, w_i) +$$

- Euler's method is Taylor's method of order one.

Taylor Method of Order n (cont'd)

Theorem 6

If Taylor's method of order n is used to approximate the solution to

$$y'(t) = f(t, y(t)), \quad a \le t \le b, \quad y(a) = \alpha,$$

with step size h and if $y \in C^{n+1}[a,b]$, then the local truncation error is $O(h^n)$.

Proof The local truncation error is

$$\tau_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - T^{(n)}(t_i, y_i) = \frac{h^n}{(n+1)!} f^{(n)}(\xi_i, y(\xi_i)),$$

for each $i = 0, 1, \ldots, N-1$. Since $y \in C^{n+1}[a,b]$, we have $y^{(n+1)}(t) = f^{(n)}(t, y(t))$ bounded on $[a,b]$ and thus $\tau_i(h) = O(h^n)$, for each $i = 1, 2, \ldots, N$. □

Taylor Method of Order n (cont'd)

Ex. Apply Taylor's method of order two with $N = 10$ to the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \leq t \leq 2, \quad y(0) = 0.5.$$

Taylor Method of Order n (cont'd)

Ex. Apply Taylor's method of orders two and four with $N = 10$ to the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

t_i	Taylor Order 2 w_i	Error $\lvert y(t_i) - w_i \rvert$
0.0	0.500000	0
0.2	0.830000	0.000701
0.4	1.215800	0.001712
0.6	1.652076	0.003135
0.8	2.132333	0.005103
1.0	2.648646	0.007787
1.2	3.191348	0.011407
1.4	3.748645	0.016245
1.6	4.306146	0.022663
1.8	4.846299	0.031122
2.0	5.347684	0.042212

t_i	Taylor Order 4 w_i	Error $\lvert y(t_i) - w_i \rvert$
0.0	0.500000	0
0.2	0.829300	0.000001
0.4	1.214091	0.000003
0.6	1.648947	0.000006
0.8	2.127240	0.000010
1.0	2.640874	0.000015
1.2	3.179964	0.000023
1.4	3.732432	0.000032
1.6	4.283529	0.000045
1.8	4.815238	0.000062
2.0	5.305555	0.000083

Interpolation on Taylor Method

Ex. Determine an approximation to an intermediate point in the table, for example, at $t = 1.25$ for the problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Interpolation on Taylor Method (cont'd)

- The divided-difference formula gives

1.2	3.1799640			
		2.7399640		
1.2	3.1799640		0.1118825	
		2.7623405		−0.3071225
1.4	3.7324321		0.0504580	
		2.7724321		
1.4	3.7324321			

- The cubic Hermite polynomial is

$$\begin{aligned} y(t) \approx 3.1799640 + (t-1.2)2.7399640 + (t-1.2)^2 0.1118825 \\ + (t-1.2)^2(t-1.4)(-0.3071225), \end{aligned}$$

so

$$y(1.25) \approx 3.1799640 + 0.1369982 + 0.0002797 + 0.0001152 = 3.3173571,$$

a result that is accurate to within 0.0000286.

Runge-Kutta Methods

- Taylor methods have the high-order local truncation error, but also the disadvantage of requiring the computation and evaluation of the derivatives of $f(t, y)$.
- Runge-Kutta methods
- We first need Taylor's Theorem in two variables.

Taylor's Theorem in Two Variables

Theorem 7 (Taylor's Theorem in Two Variables)

Suppose that $f(t,y)$ and all its partial derivatives of order less than or equal to $n+1$ are continuous on $D = \{(t,y) \mid a \le t \le b,\ c \le y \le d\}$, and let $(t_0, y_0) \in D$. For every $(t,y) \in D$, there exists ξ between t and t_0 and μ between y and y_0 with

$$f(t,y) = P_n(t,y) + R_n(t,y), \quad \textit{where}$$

$$P_n(t,y) = f(t_0,y_0) + \left[(t-t_0)\frac{\partial f}{\partial t}(t_0,y_0) + (y-y_0)\frac{\partial f}{\partial y}(t_0,y_0)\right]$$

$$+ \left[\frac{(t-t_0)^2}{2}\frac{\partial^2 f}{\partial t^2}(t_0,y_0) + (t-t_0)(y-y_0)\frac{\partial^2 f}{\partial t \partial y}(t_0,y_0) + \frac{(y-y_0)^2}{2}\frac{\partial^2 f}{\partial y^2}(t_0,y_0)\right]$$

$$+ \cdots + \left[\frac{1}{n!}\sum_{j=0}^{n}\binom{n}{j}(t-t_0)^{n-j}(y-y_0)^j \frac{\partial^n f}{\partial t^{n-j}\partial y^j}(t_0,y_0)\right],$$

$$R_n(t,y) = \frac{1}{(n+1)!}\sum_{j=0}^{n+1}\binom{n+1}{j}(t-t_0)^{n+1-j}(y-y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j}\partial y^j}(\xi,\mu).$$

Taylor's Theorem in Two Variables (cont'd)

Ex Determine $P_2(t, y)$, the second Taylor polynomial about $(2, 3)$ for the function

$$f(t, y) = \exp\left[-\frac{(t-2)^2}{4} - \frac{(y-3)^2}{4}\right]\cos(2t + y - 7)\,.$$

Sol To determine $P_2(t, y)$, we need the values of f and its first and second partial derivatives at $(2, 3)$. Then, we have

$$\begin{aligned}
P_2(t, y) &= f(2,3) + \left[(t-2)\frac{\partial f}{\partial t}(2,3) + (y-3)\frac{\partial f}{\partial y}(2,3)\right] \\
&\quad + \left[\frac{(t-2)^2}{2}\frac{\partial^2 f}{\partial t^2}(2,3) + (t-2)(y-3)\frac{\partial^2 f}{\partial t \partial y}(2,3) + \frac{(y-3)}{2}\frac{\partial^2 f}{\partial y^2}(2,3)\right] \\
&= 1 - \frac{9}{4}(t-2)^2 - 2(t-2)(y-3) - \frac{3}{4}(y-3)^2
\end{aligned}$$

Runge-Kutta Method of Order Two

- Determine values for a_1, α_1 and β_1 with the property that $a_1 f(t+\alpha_1, y+\beta_1)$ approximates

$$T^{(2)}(t,y) = f(t,y) + \frac{h}{2} f'(t,y),$$

with error no greater than $O(h^2)$.

Runge-Kutta Method of Order Two

- Since

$$f'(t,y) = \frac{df}{dt}(t,y) = \frac{\partial f}{\partial t}(t,y) + \frac{\partial f}{\partial y}(t,y) \cdot y'(t) \quad \text{and} \quad y'(t) = f(t,y),$$

we have

$$T^{(2)}(t,y) = f(t,y) + \frac{h}{2}\frac{\partial f}{\partial t}(t,y) + \frac{h}{2}\frac{\partial f}{\partial y}(t,y) \cdot f(t,y).$$

Runge-Kutta Method of Order Two (cont'd)

- Expanding $f(t+\alpha_1, y+\beta_1)$ in its Taylor polynomial of degree one about (t, y) gives

$$\begin{aligned} a_1 f(t+\alpha_1, y+\beta_1) = a_1 f(t,y) &+ a_1\alpha_1 \frac{\partial f}{\partial t}(t,y) \\ &+ a_1\beta_1 \frac{\partial f}{\partial y}(t,y) + a_1 \cdot R_1(t+\alpha_1, y+\beta_1), \end{aligned}$$

where

$$R_1(t+\alpha_1, y+\beta_1) = \frac{\alpha_1^2}{2}\frac{\partial^2 f}{\partial t^2}(\xi,\mu) + \alpha_1\beta_1 \frac{\partial^2 f}{\partial t \partial y}(\xi,\mu) + \frac{\beta_1^2}{2}\frac{\partial^2 f}{\partial y^2}(\xi,\mu),$$

for some ξ between t and $t+\alpha_1$, and some μ between y and $y+\beta_1$.

Runge-Kutta Method of Order Two (cont'd)

- The parameters a_1, α_1, and β_1 are

$$a_1 = \qquad \alpha_1 = \qquad \text{and} \quad \beta_1 =$$

Runge-Kutta Method of Order Two (cont'd)

- We then have

$$T^{(2)}(t,y) = f\left(t+\frac{h}{2}, y+\frac{h}{2}f(t,y)\right) - R_1\left(t+\frac{h}{2}, y+\frac{h}{2}f(t,y)\right)$$

  and

$$R_1\left(t+\frac{h}{2}, y+\frac{h}{2}f(t,y)\right) = \frac{h^2}{8}\frac{\partial^2 f}{\partial t^2}(\xi,\mu) + \frac{h^2}{4}f(t,y)\frac{\partial^2 f}{\partial t}\partial y(\xi,\mu) + \frac{h^2}{8}(f(t,y))^2\frac{\partial^2 f}{\partial y^2}(\xi,\mu).$$

- If all the second-order partial derivatives of f are bounded, then $R_1\left(t+\frac{h}{2}, y+\frac{h}{2}f(t,y)\right)$is $O(h^2)$.

Runge-Kutta Method of Order Two (cont'd)

- The difference-equation method resulting from replacing $T^{(2)}(t, y)$ in Taylor's method of order two by $f(t + (h/2), y + (h/2)f(t, y))$ is a specific Runge-Kutta method known as the Midpoint method:

$$
\begin{aligned}
w_0 &= \alpha, \\
w_{i+1} &= w_i + hf\left(t_i + \frac{h}{2}, w_i + \frac{h}{2}f(t_i, w_i)\right), \quad \text{for } i = 0, 1, \ldots, N-1.
\end{aligned}
$$

- How about $T^{(3)}$?

Runge-Kutta Method of Order Two (cont'd)

- Consider approximating

$$T^{(3)}(t,y) = f(t,y) + \frac{h}{2}f'(t,y) + \frac{h^2}{6}f''(t,y)$$

by

$$a_1 f(t,y) + a_2 f(t+\alpha_2, y+\delta_2 f(t,y)).$$

This has insufficient flexibility to match the term

$$\frac{h^2}{6}\left[\frac{\partial f}{\partial y}(t,y)\right]^2 f(t,y),$$

resulting from the expansion of $(h^2/6)f''(t,y)$.

Runge-Kutta Method of Order Two (cont'd)

- Modified Euler Method with $O(h^2)$ for $a_1 = a_2 = \frac{1}{2}$ and $\alpha_2 = \delta_2 = h$:

$$w_0 = \alpha,$$
$$w_{i+1} = w_i + \frac{h}{2}[f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))], \quad \text{for } i = 0, 1, \ldots, N-1.$$

Higher-Order Runge-Kutta Methods

- The term $T^{(3)}(t, y)$ can be approximated with error $O(h^3)$ by

$$f(t + \alpha_1, y + \delta_1 f(t + \alpha_2, y + \delta_2 f(t, y))).$$

- The most common $O(h^3)$ is Heun's method, given by

$$\begin{aligned} w_0 &= \alpha \\ w_{i+1} &= w_i + \frac{h}{4}\left(f(t_i, w_i) + 3f\left(t_i + \frac{2h}{3}, w_i + \frac{2h}{3} f\left(t_i + \frac{h}{3}, w_i + \frac{h}{3} f(t_i, w_i)\right)\right)\right) \\ & \text{for } i = 0, 1, \ldots, N-1. \end{aligned}$$

Runge-Kutta Order Four

- The most common Runge-Kutta method in use is of order four in difference-equation form, given by

$$\begin{aligned}
w_0 &= \alpha, \\
k_1 &= hf(t_i, w_i), \\
k_2 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_1\right), \\
k_3 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_2\right), \\
k_4 &= hf(t_{i+1}, w_i + k_3), \\
w_{i+1} &= w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),
\end{aligned}$$

  for each $i = 0, 1, \ldots, N-1$.

- This has local truncation error $O(h^4)$, provided the solution $y(t)$ has five continuous derivatives.

Computational Comparisons

Evaluations per step	2	3	4	$5 \le n \le 7$	$8 \le n \le 9$	$10 \le n$
Best possible local truncation error	$O(h^2)$	$O(h^3)$	$O(h^4)$	$O(h^{n-1})$	$O(h^{n-2})$	$O(h^{n-3})$

Computational Comparisons (cont'd)

Ex. For the problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5,$$

compare Euler's method with $h = 0.025$, the Midpoint method with $h = 0.05$, and the Runge-Kutta fourth-order method with $h = 0.1$ at the common mesh points 0.1,0.2,0.3,0.4 and 0.5.

Sol.

t_i	Exact	Euler $h = 0.025$	Modified Euler $h = 0.05$	Runge-Kutta Order Four $h = 0.1$
0.0	0.5000000	0.5000000	0.5000000	0.5000000
0.1	0.6574145	0.6554982	0.6573085	0.6574144
0.2	0.8292986	0.8253385	0.8290778	0.8292983
0.3	1.0150706	1.0089334	1.0147254	1.0150701
0.4	1.2140877	1.2056345	1.2136079	1.2140869
0.5	1.4256394	1.4147264	1.4250141	1.4256384

One-Step Methods

- One-step methods: Approximation for the mesh point t_{i+1} involves information from only one of the previous mesh points, t_i.

- Heun's method

$$w_0 = \alpha,$$

$$w_{i+1} = w_i + \frac{h}{4}\left(f(t_i, w_i) + 3f\left(t_i + \frac{2h}{3}, w_i + \frac{2h}{3}f\left(t_i + \frac{h}{3}, w_i + \frac{h}{3}f(t_i, w_i)\right)\right)\right)$$

- How about using more accurate previous data when approximating the solution at t_{i+1}?

Multistep Methods

Definition 5

An m-**step multistep method** *for solving the initial-value problem*

$$y' = f(t, y), \quad a \le t \le b, \quad y(a) = \alpha,$$

has a difference equation for finding the approximation w_{i+1} *at the mesh point* t_{i+1} *represented by the following equation, where* m *is an integer greater than* 1*:*

$$\begin{aligned} w_{i+1} = {} & a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ & + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})] \end{aligned}$$

for $i = m-1, m, \ldots, N-1$*, where* $h = (b-a)/N$*, the* $a_0, a_1, \ldots, a_{m-1}$ *and* $b_0, b_1, \ldots, b_m$ *are constants, and the starting values*

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad \ldots, \quad w_{m-1} = \alpha_{m-1}$$

are specified.

Multistep Methods (cont'd)

- An m-step multistep method:

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})]$$

- When $b_m = 0$, it is called **explicit**, or **open**, because we have w_{i+1} explicitly in terms of previously determined values.

- When $b_m \neq 0$, it is called **implicit**, or **closed**, because w_{i+1} is specified only implicitly.

Multistep Methods (cont'd)

- Fourth-order Adams-Bashforth technique:

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2, \quad w_3 = \alpha_3,$$
$$w_{i+1} = w_i + \frac{h}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]$$

for each $i = 3, 4, \ldots, N-1$.

- Fourth-order Adams-Moulton technique:

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$
$$w_{i+1} = w_i + \frac{h}{24}[9f(t_{i+1}, w_{i+1}) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})],$$

for each $i = 2, 3, \ldots, N-1$.

Multistep Methods (cont'd)

- Initialization: assume $w_0 = \alpha$ and use a Runge-Kutta or Taylor method.
- Implicit methods are generally more accurate than the explicit methods.
- Implicit methods must solve the implicit equation for w_{i+1}, which is not always possible.

Example of Multistep Methods

Ex. Use the fourth-order Adams-Bashforth method to approximate the solutions to the initial value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Sol. We previously used the Runge-Kutta method of order four with $h = 0.2$ to approximate the solutions to the initial value problem, where the first four approximations were found to be $y(0) = w_0 = 0.5$ and

$$y(0.2) \approx w_1 = 0.829293, \quad y(0.4) \approx w_2 = 1.214076, \quad y(0.6) \approx w_3 = 1.648922.$$

Then for the fourth-order Adams-Bashforth we have

Derivation of Multistep Methods

- Consider the initial-value problem

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

- The solution has the property that

$$y(t_{i+1}) - y(t_i) = \int_{t_i}^{t_{i+1}} y'(t)dt = \int_{t_i}^{t_{i+1}} f(t, y(t))dt,$$

and thus

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t))dt.$$

Derivation of Multistep Methods (cont'd)

- Approximate $f(t, y(t))$ by an interpolating polynomial $P(t)$ determined by some of the previous data points $(t_0, w_0), (t_1, w_1), \ldots, (t_i, w_i)$.

- When we further assume that $y(t_i) \approx w_i$, we have

$$y(t_{i+1}) \approx w_i + \int_{t_i}^{t_{i+1}} P(t)dt.$$

Derivation of Multistep Methods (cont'd)

- Among many, it is most convenient to use the Newton backward-difference formula:

$$P_n(x) = f[x_n] + \sum_{k=1}^{n} (-1)k \binom{-s}{k} \nabla^k f(x_n)$$

where $\nabla p_n = p_n - p_{n-1}$ and $\nabla^k p_n = \nabla(\nabla^{k-1} p_n)$, because this form more easily incorporates the most recently calculated data.

Derivation of Adams-Bashforth Explicit m-step Technique

- Form the backward-difference polynomial $P_{m-1}(t)$ through

$$(t_i, f(t_i, y(t_i))), \quad (t_{i-1}, f(t_{i-1}, y(t_{i-1}))), \quad \ldots, \quad (t_{i+1-m}, f(t_{i+1-m}, y(t_{i+1-m})))$$

- There exists some number ξ_i in (t_{i+1-m}, t_i) with

$$f(t, y(t)) = P_{m-1}(t) + \frac{f^{(m)}(\xi_i, y(\xi_i))}{m!}(t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m}).$$

Derivation of Adams-Bashforth Explicit m-step (cont'd)

- Introducing the variable substitution $t = t_i + sh$, with $dt = h\,ds$, yields

$$\begin{aligned}
\int_{t_i}^{t_{i+1}} f(t, y(t))dt &= \int_{t_i}^{t_{i+1}} \sum_{k=0}^{m-1} (-1)^k \binom{-s}{k} \nabla^k f(t_i, y(t_i))dt \\
&\quad + \int_{t_i}^{t_{i+1}} \frac{f^{(m)}(\xi, y(\xi))}{m!} (t - t_i)(t - t_{i-1}) \cdots (t - t_{i+1-m})dt \\
&= \sum_{k=0}^{m-1} \nabla^k f(t_i, y(t_i)) h (-1)^k \int_0^1 \binom{-s}{k} ds \\
&\quad + \frac{h^{m+1}}{m!} \int_0^1 s(s+1) \cdots (s+m-1) f^{(m)}(\xi, y(\xi))ds.
\end{aligned}$$

Derivation of Adams-Bashforth Explicit m-step (cont'd)

- Consequently, we have

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt = h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\right]$$
$$+ \frac{h^{m+1}}{m!}\int_0^1 s(s+1)\cdots(s+m-1)f^{(m)}(\xi_i, y(\xi_i))ds.$$

Derivation of Adams-Bashforth Explicit m-step (cont'd)

- Because $s(s+1)\cdots(s+m-1)$ does not change sign on $[0,1]$, the Weighted MVT for Integrals can be used to deduce that for some number μ_i, where $t_{i+1-m} < \mu_i < t_{i+1}$, the error term becomes

$$\begin{aligned}
&\frac{h^{m+1}}{m!}\int_0^1 s(s+1)\cdots(s+m-1)f^{(m)}(\xi_i, y(\xi_i))ds \\
&= \frac{h^{m+1}f^{(m)}(\mu_i, y(\mu_i))}{m!}\int_0^1 s(s+1)\cdots(s+m-1)ds \\
&= h^{m+1}f^{(m)}(\mu_i, y(\mu_i))(-1)^m\int_0^1 \binom{-s}{m}ds.
\end{aligned}$$

Derivation of Adams-Bashforth Explicit m-step (cont'd)

- We finally have

$$y(t_{i+1}) = y(t_i) + h\left[f(t_i, y(t_i)) + \frac{1}{2}\nabla f(t_i, y(t_i)) + \frac{5}{12}\nabla^2 f(t_i, y(t_i)) + \cdots\right]$$
$$+ h^{m+1} f^{(m)}(\mu_i, y(\mu_i))(-1)^m \int_0^1 \binom{-s}{m} ds.$$

Derivation of Adams-Bashforth Explicit m-step (cont'd)

Ex. Derive the three-step Adams-Bashforth technique.

Local Truncation Error of Multistep Methods

Definition 6

If $y(t)$ is the solution to the initial-value problem

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha,$$

and

$$\begin{aligned} w_{i+1} = {} & a_{m-1} w_i + a_{m-2} w_{i-1} + \cdots + a_0 w_{i+1-m} \\ & + h[b_m f(t_{i+1}, w_{i+1}) + b_{m-1} f(t_i, w_i) + \cdots + b_0 f(t_{i+1-m}, w_{i+1-m})] \end{aligned}$$

is the $(i+1)$st step in a multistep method, the **local truncation error** *at this step is*

$$\begin{aligned} \tau_{i+1}(h) = {} & \frac{y(t_{i+1}) - a_{m-1} y(t_i) - \cdots - a_0 y(t_{i+1-m})}{h} \\ & - [b_m f(t_{i+1}, y(t_{i+1})) + \cdots + b_0 f(t_{i+1-m}, y(t_{i+1-m})], \end{aligned}$$

for each $i = m-1, m, \ldots, N-1$.

Local Truncation Error of Multistep Methods (cont'd)

Ex. Determine the local truncation error for the three-step Adams-Bashforth method.

Adams-Bashforth Explicit Methods

- Adams-Bashforth Two-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1,$$
$$w_{i+1} = w_i + \frac{h}{2}[3f(t_i, w_i) - f(t_{i-1}, w_{i-1})],$$

where $i = 1, 2, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{5}{12}y'''(\mu_i)h^2$, for some $\mu_i \in (t_{i-1}, t_{i+1})$.

- Adams-Bashforth Three-Step Explicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1, \quad w_2 = \alpha_2,$$
$$w_{i+1} = w_i + \frac{h}{12}[23f(t_i, w_i) - 16f(t_{i-1}, w_{i-1}) + 5f(t_{i-2}, w_{i-2})],$$

where $i = 2, 3, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = \frac{3}{8}y^{(4)}(\mu_i)h^3$, for some $\mu_i \in (t_{i-2}, t_{i+1})$.

Adams-Moulton Implicit Methods

- Use $(t_{i+1}, f(t_{i+1}, y(t_{i+1})))$ as an additional interpolation node in the approximation of the integral

$$\int_{t_i}^{t_{i+1}} f(t, y(t))dt.$$

- Adams-Moulton Two-Step Implicit Method

$$w_0 = \alpha, \quad w_1 = \alpha_1,$$
$$w_{i+1} = w_i + \frac{h}{12}[5f(t_{i+1}, w_{i+1}) + 8f(t_i, w_i) - f(t_{i-1}, w_{i-1})],$$

where $i = 1, 2, \ldots, N-1$. The local truncation error is $\tau_{i+1}(h) = -\frac{1}{24}y^{(4)}(\mu_i)h^3$, for some $\mu_i \in (t_{i-1}, t_{i+1})$.

Explicit and Implicit Multistep Methods

- m-step Adams-Bashforth explicit method
  vs. $(m-1)$-step Adams-Moulton implicit method
- Both involve m evaluations of f per step, and have the terms $y^{(m+1)}(\mu_i)h^m$ in their local truncation errors.
- In general, the coefficients of the terms in the local truncation error are smaller for the implicit methods than for the explicit methods.
- Implicit methods thus has greater stability and smaller round-off errors.

Explicit and Implicit Multistep Methods (cont'd)

Ex. Consider the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

State the implicit Adams-Moulton two-step method with $h = 0.2$.

Explicit and Implicit Multistep Methods (cont'd)

Ex. For the given problem, use the exact values given from $y(t) = (t+1)^2 - 0.5e^t$ as starting values and $h = 0.2$ to compare the approximations from by (a) the explicit Adams-Bashforth four-step method and (b) the implicit Adams-Moulton three-step method.

t_i	Exact	Adams-Bashforth w_i	Error	Adams-Moulton w_i	Error
0.0	0.5000000				
0.2	0.8292986				
0.4	1.2140877				
0.6	1.6489406			1.6489341	0.0000065
0.8	2.1272295	2.1273124	0.0000828	2.1272136	0.0000160
1.0	2.6408591	2.6410810	0.0002219	2.6408298	0.0000293
1.2	3.1799415	3.1803480	0.0004065	3.1798937	0.0000478
1.4	3.7324000	3.7330601	0.0006601	3.7323270	0.0000731
1.6	4.2834838	4.2844931	0.0010093	4.2833767	0.0001071
1.8	4.8151763	4.8166575	0.0014812	4.8150236	0.0001527
2.0	5.3054720	5.3075838	0.0021119	5.3052587	0.0002132

Implicit Adams-Moulton Method

- Consider the initial value problem

$$y' = e^y, \quad 0 \le t \le 0.25, \quad y(0) = 1.$$

- The three-step Adams-Moulton method has

$$w_{i+1} = w_i + \frac{h}{24}[9e^{w_{i+1}} + 19e^{w_i} - 5e^{w_{i-1}} + e^{w_{i-2}}]$$

  as its difference equation.

Predictor-Corrector Methods

- Consider the combination of an explicit method to predict and an implicit to improve the prediction.

- Calculate an approximation, w_{4p}, to $y(t_4)$ using the explicit Adams-Bashforth method as a **predictor**:

$$w_{4p} = w_3 + \frac{h}{24}[55f(t_3, w_3) - 59f(t_2, w_2) + 37f(t_1, w_1) - 9f(t_0, w_0)].$$

- This approximation is improved by inserting w_{4p} in the right side of the three-step implicit Adams-Moulton method and using that method as a **corrector**:

$$w_4 = w_3 + \frac{h}{24}[9f(t_4, w_{4p}) + 19f(t_3, w_3) - 5f(t_2, w_2) + f(t_1, w_1)].,$$

  which requires only one additional function evaluation.

Predictor-Corrector Methods (cont'd)

Ex. Apply the Adams fourth-order predictor-corrector method with $h = 0.2$ and starting values from the Runge-Kutta fourth order method to the initial-value problem

$$y' = y - t^2 + 1, \quad 0 \le t \le 2, \quad y(0) = 0.5.$$

Sol. The fourth-order Adams-Bashforth method gives

$$\begin{aligned} y(0.8) \approx w_{4p} &= w_3 + \frac{0.2}{24}[55f(0.6, w_3) - 59f(0.4, w_2) + 37f(0.2, w_1) - 9f(0, w_0)] \\ &= 2.1272892. \end{aligned}$$

We then use w_{4p} as the predictor of the approximation to $y(0.8)$ and determine the corrected value w_4, from the implicit Adams-Moulton method, which is

$$\begin{aligned} y(0.8) \approx w_4 &= w_3 + \frac{0.2}{24}[9f(0.8, w_{4p}) + 19f(0.6, w_3) - 5f(0.4, w_w) + f(0.2, w_1)] \\ &= 2.127056. \end{aligned}$$

Higher-Order Systems

- An m**th-order system** of first-order initial-value problems has the form

$$\begin{aligned} \frac{du_1}{dt} &= f_1(t, u_1, u_2, \ldots, u_m), \\ \frac{du_2}{dt} &= f_2(t, u_1, u_2, \ldots, u_m), \\ &\vdots \\ \frac{du_m}{dt} &= f_m(t, u_1, u_2, \ldots, u_m), \end{aligned} \tag{3}$$

for $a \leq t \leq b$, with the initial conditions

$$u_1(a) = \alpha_1, \quad u_2(a) = \alpha_2, \quad \ldots, \quad u_m(a) = \alpha_m. \tag{4}$$

Higher-Order Systems (cont'd)

Definition 7

The function $f(t, y_1, \ldots, y_m)$, *defined on the set*

$$D = \{(t, u_1, \ldots, u_m) \mid a \le t \le b \text{ and } -\infty < u_i < \infty \text{ for each } i = 1, 2, \ldots, m\}$$

is said to satisfy a **Lipschitz condition** *on* D *in the variables* $u_1, u_2, \ldots, u_m$ *if a constant* $L > 0$ *exists with*

$$|f(t, u_1, \ldots, u_m) - f(t, z_1, \ldots, z_m)| \le L \sum_{j=1}^{m} |u_j - z_j|,$$

for all $(t, u_1, \ldots, u_m)$ *and* $(t, z_1, \ldots, z_m)$ *in* D.

Higher-Order Systems (cont'd)

- By using the MVT, it can be shown that if f and its first partial derivatives are continuous on D and if

$$\left| \frac{\partial f(t, u_1, \ldots, u_m)}{\partial u_i} \right| \le L,$$

for each $i = 1, 2, \ldots, m$ and all $(t, u_1, \ldots, u_m)$ in D, then f satisfies a Lipschitz condition on D with Lipschitz constant L.

Higher-Order Systems (cont'd)

Theorem 8

Suppose that

$$D = \{(t, u_1, \ldots, u_m) \mid a \le t \le b \text{ and } -\infty < u_i < \infty \text{ for each } i = 1, 2, \ldots, m\}$$

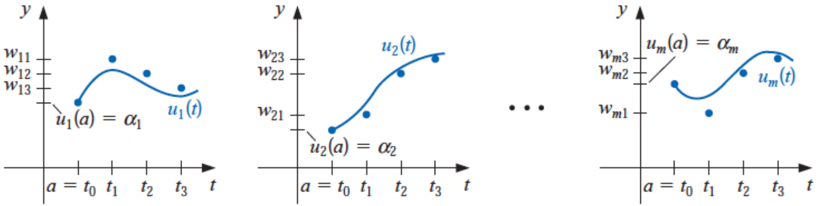
and let $f_i(t, u_1, \ldots, u_m)$, for each $i = 1, 2, \ldots, m$, be continuous and satisfy a Lipschitz condition on D. The system of first-order differential equations (3)*, subject to the initial conditions* (4) *has a unique solution $u_1(t), \ldots, u_m(t)$, for $a \le t \le b$.*

Higher-Order Systems (cont'd)

- Methods to solve systems of first-order differential equations are generalizations of the methods for a single first-order equation.

- Use the notation w_{ij}, for each $j = 0, 1, \ldots, N$ and $i = 1, 2, \ldots, m$ to denote an approximation to $u_i(t_j)$.
- For the initial conditions, set

$$w_{1,0} = \alpha_1, \quad w_{2,0} = \alpha_2, \quad \ldots, \quad w_{m,0} = \alpha_m.$$



Higher-Order Systems (cont'd)

- Recall: Runge-Kutta method of order four

$$
\begin{aligned}
k_1 &= hf(t_i, w_i),\\
k_2 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_1\right),\\
k_3 &= hf\left(t_i + \frac{h}{2}, w_i + \frac{1}{2}k_2\right),\\
k_4 &= hf(t_{i+1}, w_i + k_3),\\
w_{i+1} &= w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).
\end{aligned}
$$

Higher-Order Systems (cont'd)

- Runge-Kutta method of order four for the system is as follows.
- Suppose that the values $w_{1,j}, w_{2,j}, \ldots, w_{m,j}$ have been computed. We then compute, for each $i = 1, 2, \ldots, m$,

$$
\begin{aligned}
k_{1,i} &= hf_i(t_j, w_{1,j}, w_{2,j}, \ldots, w_{m,j}), \\
k_{2,i} &= hf_i\left(t_j + \frac{h}{2}, w_{1,j} + \frac{1}{2}k_{1,1}, w_{2,j} + \frac{1}{2}k_{1,2}, \ldots, w_{m,j} + \frac{1}{2}k_{1,m}\right), \\
k_{3,i} &= hf_i\left(t_j + \frac{h}{2}, w_{1,j} + \frac{1}{2}k_{2,1}, w_{2,j} + \frac{1}{2}k_{2,2}, \ldots, w_{m,j} + \frac{1}{2}k_{2,m}\right), \\
k_{4,i} &= hf_i(t_j + h, w_{1,j} + k_{3,1}, w_{2,j} + k_{3,2}, \ldots, w_{m,j} + k_{3,m}).
\end{aligned}
$$

- Finally, we have

$$w_{i,j+1} = w_{i,j} + \frac{1}{6}(k_{1,i} + 2k_{2,i} + 2k_{3,i} + k_{4,i}).$$

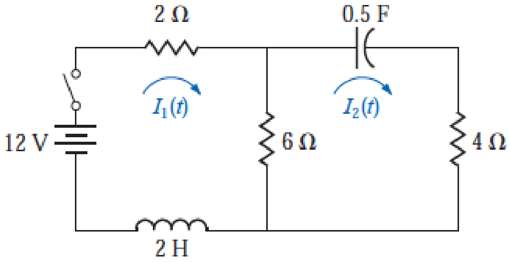
Higher-Order Systems (cont'd)

Note. Kirchoff's Voltage Law states that the sum of all instantaneous voltage changes around a closed circuit is zero. This law implies that the current $I(t)$ in a closed circuit containing a resistance of R ohms, a capacitance of C farads, an inductance of L henries, and a voltage source of $E(t)$ volts satisfies the equation

$$LI'(t) + RI(t) + \frac{1}{C}\int I(t)dt = E(t).$$

Higher-Order Systems (cont'd)

Ex. Find the current $I_1(t)$ and $I_2(t)$ of the system of equations of the circuit:



- That is

$$2I_1(t) + 6[I_1(t) - I_2(t)] + 2I_1'(t) = 12,$$

$$\frac{1}{0.5}\int_0^t I_2(t)dt + 4I_2(t) + 6[I_2(t) - I_1(t)] = 0.$$

- Assume that the switch is closed at time $t = 0$. Then, we have initial conditions $I_1(0) = 0$ and $I_2(0) = 0$.

Higher-Order Systems (cont'd)

Ex Find the system of equations, and apply the Runge-Kutta method of order four with $h = 0.1$, $w_{1,0} = I_1(0) = 0$ and $w_{2,0} = I_2(0) = 0$.

The first step yields

$$k_{1,1} = hf_1(t_0, w_{1,0}, t_{2,0}) = 0.1f_1(0,0,0) = 0.1(-4(0) + 3(0) + 6) = 0.6,$$
$$k_{1,2} = hf_2(t_0, w_{1,0}, t_{2,0}) = 0.1f_2(0,0,0) = 0.1(-2.4(0) + 1.6(0) + 3.6) = 0.36,$$

and the second step yields

$$\begin{aligned} k_{2,1} &= hf_1\left(t_0 + \frac{1}{2}h, w_{1,0} + \frac{1}{2}k_{1,1}, w_{2,0} + \frac{1}{2}k_{1,2}\right) = 0.2f_1(0.05, 0.3, 0.18) \\ &= 0.1(-4(0.3) + 3(0.18) + 6) = 0.534, \\ k_{2,2} &= hf_2\left(t_0 + \frac{1}{2}h, w_{1,0} + \frac{1}{2}k_{1,1}, w_{2,0} + \frac{1}{2}k_{1,2}\right) = 0.1f_2(0.05, 0.3, 0.18) \\ &= 0.1(-2.4(0.3) + 1.6(0.18) + 3.6) = 0.3168, \end{aligned}$$

Higher-Order Systems (cont'd)

- Remaining steps yield

$$k_{3,1} = 0.54072, \quad k_{3,2} = 0.321264, \quad k_{4,1} = 0.4800912, \quad k_{4,2} = 0.28162944.$$

- So, we have

$$I_1(0.1) \approx w_{1,1} = w_{1,0} + \frac{1}{6}(k_{1,1} + 2k_{2,1} + 2k_{3,1} + k_{4,1}) = 0.5382552,$$
$$I_2(0.1) \approx w_{2,1} = w_{2,0} + \frac{1}{6}(k_{1,2} + 2k_{2,2} + 2k_{3,2} + k_{4,2}) = 0.3196263.$$

t_j	$w_{1,j}$	$w_{2,j}$	$\lvert I_1(t_j) - w_{1,j}\rvert$	$\lvert I_2(t_j) - w_{2,j}\rvert$
0.0	0	0	0	0
0.1	0.5382550	0.3196263	0.8285×10^{-5}	0.5803×10^{-5}
0.2	0.9684983	0.5687817	0.1514×10^{-4}	0.9596×10^{-5}
0.3	1.310717	0.7607328	0.1907×10^{-4}	0.1216×10^{-4}
0.4	1.581263	0.9063208	0.2098×10^{-4}	0.1311×10^{-4}
0.5	1.793505	1.014402	0.2193×10^{-4}	0.1240×10^{-4}

Higher-Order Differential Equations

- Consider a general mth-order initial-value problem

$$y^{(m)}(t) = f(t, y, y', \ldots, y^{(m-1)}), \quad a \le t \le b,$$

with initial conditions $y(a) = \alpha_1,\ y'(a) = \alpha_2,\ \ldots,\ y^{(m-1)}(a) = \alpha_m$

- Let's convert it into a m-th order system of first-order initial value problems. How?

Higher-Order Differential Equations (cont'd)

- Let $u_1(t) = y(t),\ u_2(t) = y'(t),\ \ldots$, and $u_m(t) = y^{(m-1)}(t)$.
- This produces the first-order system

with initial conditions

$$u_1(a) = y(a) = \alpha_1, \quad u_2(a) = y'(a) = \alpha_2, \quad \ldots, \quad u_m(a) = y^{(m-1)}(a) = \alpha_m.$$

Higher-Order Differential Equations (cont'd)

Ex. Transform the second-order initial-value problem

$$y'' - 2y' + 2y = e^{2t} \sin t, \quad \text{for } 0 \le t \le 1, \quad \text{with } y(0) = -0.4,\ y'(0) = -0.6$$

into a system of first order initial-value problems. (Then, apply the Runge-Kutta method.)

Properties of One-Step Methods

Definition 8

A one-step difference equation method with local truncation error $\tau_i(h)$ *at the* i*th step is said to be* **consistent** *with the differential equation it approximates if*

$$\lim_{h \to 0} \max_{1 \le i \le N} |\tau_i(h)| = 0.$$

Properties of One-Step Methods (cont'd)

Definition 9

A one-step difference-equation method is said to be **convergent** *with respect to the differential equation it approximates if*

$$\lim_{h \to 0} \max_{1 \leq i \leq N} |w_i - y(t_i)| = 0,$$

where $y(t_i)$ denotes the exact value of the solution of the differential equation and w_i is the approximation obtained from the difference method at the ith step.

Properties of One-Step Methods (cont'd)

Ex. Show that Euler's method is (a) consistent and (b) convergent under the hypothesis of Theorem 4.

Stability of One-Step Methods

- In practice, there is the round-off error.

- A method is **stable** when small changes or perturbations in the initial conditions produce correspondingly small changes in the subsequent approximations.
- A method is **stable** when the results depend continuously on the initial data.

- The concept of **stability** of a one-step difference equation is somewhat analogous to the condition of a differential equation being **well-posed**, so the Lipschitz condition appears here.

Stability of One-Step Methods (cont'd)

Theorem 9

Suppose that the initial-value problem is approximated by a one-step difference method in the form

$$w_0 = \alpha, \quad w_{i+1} = w_i + h\phi(t_i, w_i, h).$$

Suppose also that $h_0 > 0$ exists and that $\phi(t, w, h)$ is continuous and satisfies a Lipschitz condition in the variable w with Lipschitz constant L on the set

$$D = \{(t, w, h) \mid a \le t \le b \text{ and } -\infty < w < \infty,\ 0 \le h \le h_0\}.$$

Then

(1) *The method is stable;*

(2) *The difference method is convergent if and only if it is consistent, i.e.,*

$$\phi(t, y, 0) = f(t, y), \quad \text{for all } a \le t \le b;$$

(3) *If a function τ exists and, for each $i = 1, 2, \ldots, N$, the local truncation error $\tau_i(h)$ satisfies $|\tau_i(h)| \le \tau(h)$ whenever $0 \le h \le h_0$, then*

$$|y(t_i) - w_i| \le \frac{\tau(h)}{L} e^{L(t_i - a)}.$$

Stability of One-Step Methods (cont'd)

Ex. The Modified Euler method is given by $w_0 = \alpha$,

$$w_{i+1} = w_i + \frac{h}{2}[f(t_i, w_i) + f(t_{i+1}, w_i + hf(t_i, w_i))], \text{ for } i = 0, 1, \ldots, N-1.$$

Verify that this method is stable.

Sol. With $\phi(t, w, h) = \frac{1}{2}f(t, w) + \frac{1}{2}f(t + h, w + hf(t, w))$, we have

Properties of Multistep Methods

- For multistep methods, the problems involved with consistency, convergence, and stability are compounded because of the number of approximations involved at each step.
- A multistep method is **convergent** if the solution to the difference equation approaches the solution to the differential equation as the step size approaches zero. This means that

$$\lim_{h\to 0} \max_{0\le i\le N} |w_i - y(t_i)| = 0.$$

Properties of Multistep Methods (cont'd)

- A multistep method is **consistent** if

$$\lim_{h\to 0} |\tau_i(h)| = 0, \quad \text{for all } i = m, m+1, \ldots, N, \quad \text{and}$$
$$\lim_{h\to 0} |\alpha_i - y(t_i)| = 0, \quad \text{for all } i = 1, 2, \ldots, m-1.$$

Stability of Multistep Methods

- Associated with the multistep difference equation

$$
\begin{aligned}
w_0 = \alpha, \quad w_1 = \alpha_1, \ldots, w_{m-1} = \alpha_{m-1} \\
w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\
+ hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m})
\end{aligned}
$$

  is a polynomial, called the **characteristic polynomial** of the method, given by

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_1\lambda - a_0 = 0.$$

- The **stability** of a multistep method with respect to round-off error is dictated by **the magnitudes of the zeros of the characteristic polynomial**. Why?

Stability of Multistep Methods (cont'd)

- Consider the trivial (homogeneous) initial-value problem

$$y' \equiv 0, \quad y(a) = \alpha, \quad \text{where } \alpha \neq 0,$$

which has the exact solution $y(t) = \alpha$.

- The standard form of the difference equation becomes

$$w_{i+1} = a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \tag{5}$$

- Suppose λ is one of the zeros of the characteristic polynomial. Then $w_n = \lambda^n$ is a solution to (5) since

$$\begin{aligned} &\lambda^{i+1} - a_{m-1}\lambda^i - a_{m-2}\lambda^{i-1} - \cdots - a_0\lambda^{i+1-m} \\ = &\lambda^{i+1-m}[\lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_0] = 0. \end{aligned}$$

Stability of Multistep Methods (cont'd)

- If $\lambda_1, \lambda_2, \ldots, \lambda_m$ are distinct zeros of the characteristic polynomial, it can be shown that *every* solution can be expressed in the form

$$w_n = \sum_{i=1}^{m} c_i \lambda_i^n,$$

for some unique collection of constants $c_1, c_2, \ldots, c_m$. (See the textbook when the multiple zeros occur.)

Stability of Multistep Methods (cont'd)

- The choice $w_n = \alpha$ for all n is a solution, so

  $$0 = \alpha - \alpha a_{m-1} - \alpha a_{m-2} - \cdots - \alpha a_0 = \alpha[1 - a_{m-1} - a_{m-2} - \cdots - a_0],$$

  which implies that $\lambda = 1$ is a zero of $P(\lambda)$.

- Then, all the solutions are expressed as

  $$w_n = \alpha + \sum_{i=2}^{m} c_i \lambda_i^n.$$

- If all the calculations were exact, all the constants $c_2, c_3, \ldots, c_m$ would be zero. In practice they are not zero due to round-off error.

Stability of Multistep Methods (cont'd)

- Although we have considered only the special case of approximating the trivial (homogeneous) initial-value problem

$$y' \equiv 0, \quad y(a) = \alpha, \quad \text{where } \alpha \neq 0, ,$$

the stability characteristics for this equation determine the stability for the situation when $f(t, y)$ is not identically zero.

- This is because the solution to the trivial (homogeneous) equation is embedded in the solution to any equation.

Stability of Multistep Methods (cont'd)

Definition 10

Let $\lambda_1, \lambda_2, \ldots, \lambda_m$ denote the (not necessarily distinct) roots of the characteristic equation

$$P(\lambda) = \lambda^m - a_{m-1}\lambda^{m-1} - \cdots - a_1\lambda - a_0 = 0$$

associated with the multistep difference method

$$\begin{aligned} w_0 = \alpha, \quad w_1 &= \alpha_1, \ldots, w_{m-1} = \alpha_{m-1} \\ w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\ &\quad + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m}). \end{aligned}$$

If $|\lambda_i| \leq 1$, for each $i = 1, 2, \ldots, m$, and all roots with absolute value 1 are simple roots, then the difference method is said to satisfy the **root condition**.

Stability of Multistep Methods (cont'd)

Definition 11

- *Methods that satisfy the root condition and have $\lambda = 1$ as the only root of the characteristic equation with magnitude one are called* **strongly stable**.
- *Methods that satisfy the root condition and have more than one distinct root with magnitude one are called* **weakly stable**.
- *Methods that do not satisfy the root condition are called* **unstable**.

- Consistency and convergence of a multistep method are closely related to the round-off stability of the method.

Stability of Multistep Methods (cont'd)

Theorem 10

A multistep method of the form

$$
\begin{aligned}
w_0 = \alpha, \quad w_1 &= \alpha_1, \ldots, w_{m-1} = \alpha_{m-1} \\
w_{i+1} &= a_{m-1}w_i + a_{m-2}w_{i-1} + \cdots + a_0 w_{i+1-m} \\
&\quad + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i+1-m}).
\end{aligned}
$$

is **stable** *if and only if it satisfies the* **root condition**. *Moreover, if the difference method is* **consistent** *with the differential equation, then the method is* **stable** *if and only if it is* **convergent**.

Stability of Multistep Methods (cont'd)

Ex. The fourth-order Adams-Bashforth method can be expressed as

$$w_{i+1} = w_i + hF(t_i, h, w_{i+1}, w_i, \ldots, w_{i-3}),$$

where

$$\begin{aligned} & F(t_i, h, w_{i+1}, \ldots, w_{i-3}) \\ = & \frac{1}{24}[55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})]; \end{aligned}$$

Show that this method is strongly stable.

Stability of Multistep Methods (cont'd)

Ex. Show that the fourth-order Milne's method, the explicit multistep method given by

$$w_{i+1} = w_{i-3} + \frac{4h}{3}[2f(t_i, w_i) - f(t_{i-1}, w_{i-1}) + 2f(t_{i-2}, w_{i-2})]$$

satisfies the root condition, but it is only weakly stable.

Example of Stiff Differential Equation

Ex. The system of initial-value problems

$$u_1' = 9u_1 + 24u_2 + 5\cos t - \frac{1}{3}\sin t, \quad u_1(0) = \frac{4}{3},$$
$$u_2' = -24u_1 - 51u_2 - 9\cos t + \frac{1}{3}\sin t, \quad u_2(0) = \frac{2}{3}$$

has the unique solution

$$u_1(t) = 2e^{-3t} - e^{-39t} + \frac{1}{3}\cos t, \quad u_2(t) = -e^{-3t} + 2e^{-39t} - \frac{1}{3}\cos t.$$

Example of Stiff Differential Equation

- Applying the Runge-Kutta fourth-order method gives the following table.

t	$u_1(t)$	$w_1(t)$ $h = 0.05$	$w_1(t)$ $h = 0.1$
0.1	1.793061	1.712219	−2.645169
0.2	1.423901	1.414070	−18.45158
0.3	1.131575	1.130523	−87.47221
0.4	0.9094086	0.9092763	−934.0722
0.5	0.7387877	9.7387506	−1760.016
0.6	0.6057094	0.6056833	−7848.550
0.7	0.4998603	0.4998361	−34989.63
0.8	0.4136714	0.4136490	−155979.4
0.9	0.3416143	0.3415939	−695332.0
1.0	0.2796748	0.2796568	−3099671.

Stiff Differential Equation

- When the magnitude of the derivative increases but the solution does not, the error can dominate the calculations.
- Initial-value problems for which this is likely to occur are called **stiff equations**.

- The exact solution of stiff equation has term of the form e^{-ct}, where c is a large positive constant, called the **transient** solution. The more important portion of the solution is called the **steady-state** solution.

- The transient portion will rapidly decay to zero as t increases, but since the nth derivative has magnitude $c^n e^{-ct}$, the derivative does not decay as quickly.

Stiff Differential Equation (cont'd)

- A particular numerical method applied to a stiff system can be predicted by examining the error produced when the method is applied to a simple *test equation*,

$$y' = \lambda y, \quad y(0) = \alpha, \quad \text{where } \lambda < 0,$$

which has the solution $y(t) = \alpha e^{\lambda t}$ with a zero steady-state solution.

Euler's Method on Stiff Equation

- Let $h = (b-a)/N$ and $t_j = jh$ for $j = 0, 1, \ldots, N$. Euler's method is

$$w_0 = \alpha, \quad \text{and} \quad w_{j+1} = w_j + h(\lambda w_j) = (1 + h\lambda)w_j,$$

so

$$w_{j+1} = (1+h\lambda)^{j+1} w_0 = (1+h\lambda)^{j+1}\alpha, \quad \text{for } j = 0, 1, \ldots, N-1.$$

- The absolute error is

$$|y(t_j) - w_j| = |e^{jh\lambda} - (1+h\lambda)^j|\,|\alpha| = |(e^{h\lambda})^j - (1+h\lambda)^j|\,|\alpha|.$$

- When $\lambda < 0$, the exact solution $(e^{h\lambda})^j$ decays to 0 as j increases.

Euler's Method on Stiff Equation (cont'd)

- Suppose a round-off error δ_0 is introduced in the initial condition

$$w_0 = \alpha + \delta_0.$$

At the jth step the round-off error is

$$\delta_j = (1 + h\lambda)^j \delta_0,$$

which will be under control when $|1 + h\lambda| < 1$.

- Euler's method is expected to be stable for

$$y' = \lambda y, \quad y(0) = \alpha, \quad \text{where } \lambda < 0,$$

only if the step size h is less than $2/|\lambda|$.

One-step Method on Stiff Equation

- In general, a function Q exists with the property that the difference method, when applied to the test equation, gives

$$w_{i+1} = Q(h\lambda)w_i.$$

- The accuracy of the method depends on how well $Q(h\lambda)$ approximates $e^{h\lambda}$, and the error will grow without bound if $|Q(h\lambda)| > 1$.

- nth-order Taylor method will have stability with regard to both the growth of round-off error and absolute error, provided that h is chosen to satisfy

$$|?| < 1$$

Multistep Method on Stiff Equation

- A multistep method to the test equation:

$$\begin{aligned} w_{j+1} =& a_{m-1}w_j + \cdots + a_0 w_{j+1-m} \\ &+ h\lambda(b_m w_{j+1} + b_{m-1}w_j + \cdots + b_0 w_{j+1-m}), \end{aligned}$$

  can be rewritten as

$$(1 - h\lambda b_m)w_{j+1} - (a_{m-1} + h\lambda b_{m-1})w_j - \cdots - (a_0 + h\lambda b_0)w_{j+1-m} = 0.$$

- The associated characteristic polynomial is

$$Q(z, h\lambda) = (1 - h\lambda b_m)z^m - (a_{m-1} + h\lambda b_{m-1})z^{m-1} - \cdots - (a_0 + h\lambda b_0).$$

- Let $\beta_1, \ldots, \beta_m$ be distinct zeros of $Q(z, h\lambda)$. Then $c_1, \ldots, c_m$ exist with

$$w_j = \sum_{k=1}^{m} c_k(\beta_k)^j, \quad j = 0, \ldots, N.$$

The Region R of Absolute Stability

Definition 12

The **region** R **of absolute stability**
for a one-step method is $R = \{h\lambda \in \mathcal{C} \mid |Q(h\lambda)| < 1\}$,
and for a multistep method, it is
$R = \{h\lambda \in \mathcal{C} \mid |\beta_k| < 1, \text{ for all zeros } \beta_k \text{ of } Q(z, h\lambda)\}$.