Today’s discussion is an illustration of a general concept: if you have special structure consider using it.

Consider the second order equation
\[ y'' = f(x, y, y'). \]

We can, of course, convert it to a first order system, and consider the problem solved:
\[
\begin{align*}
    z' &= f(x, y, z) \\
    y' &= z
\end{align*}
\]

However, there are applications where the first derivative does not occur explicitly:
\[
y'' = f(x, y), \quad y(a) = y_0, \quad y'(a) = \bar{y}_0. \tag{1}
\]

This kind of problem occurs, for example, in Celestial Mechanics: acceleration, the second derivative of location, and proportional to force, depends on location (and perhaps time), but not on your current velocity.
• It may be worthwhile to develop special techniques for this problem.

• Indeed, one might even build special hardware for some purposes.

• Consider the modified linear multistep method

\[
\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f_{n+j} \tag{2}
\]

where

\[
\alpha_k = 1 \quad \text{and} \quad |\alpha_0| + |\beta_0| > 0.
\]

• The \( \beta \)'s are of course different from those we used for first order problems.

• Again, we define the first and second characteristic polynomials by

\[
\rho(r) = \sum_{j=0}^{k} \alpha_j r^j \quad \text{and} \quad \sigma(r) = \sum_{j=0}^{k} \beta_j r^j.
\]

• The following discussion parallels part of our earlier discussion for first order problems.

• We define the local truncation error of the method (2) by

\[
\text{LTE} = \sum_{j=0}^{k} \alpha_j y(x_{n+j}) - h^2 \sum_{j=0}^{k} \beta_j y''(x_{n+j})
\]

\[
= \sum_{j=0}^{\infty} C_j h^j y^{(j)}(x_n)
\]
• One can easily work out (as we did in the first order case) that

\[ C_0 = \sum_{j=0}^{k} \alpha_j = \rho(1) \]

\[ C_1 = \sum_{j=1}^{k} j \alpha_j = \rho'(1) \]

\[ C_2 = \frac{1}{2} \sum_{j=1}^{k} j^2 \alpha_j - \sum_{j=0}^{k} \beta_j \]

\[ \vdots \]

\[ C_q = \frac{1}{q!} \sum_{j=1}^{k} j^q \alpha_j - \frac{1}{(q-2)!} \sum_{j=1}^{k} j^{q-2} \beta_j, \quad q > 2 \]

• We say that the method is of order \( p \) if

\[ C_0 = C_1 = \ldots = C_P = C_{P+1} = 0, \quad C_{P+2} \neq 0 \]

\[ y' = f(x, y), \quad C_0 = C_1 = \ldots = C_P = 0, \quad C_{P+1} \neq 0 \]

• The linear multistep method (2) is zero-stable if no root of \( \rho \) has absolute value greater than 1, and those of absolute value equal to 1 have multiplicity no greater than 2.

• The linear multistep method (2) is consistent if it has order at least 1.

• As before, consistency and zero-stability are equivalent to convergence.
$$
\begin{align*}
L T E &= \sum_{j=0}^{k} a_{j} y(x_{u+j}) - h \sum_{j=0}^{k} \beta_{j} y^{(j)}(x_{u+j}) \\
&= \sum_{j=0}^{k} a_{j} \sum_{i=0}^{\infty} \frac{(j h)^{i}}{i!} y^{(i)}(x_{u+j}) - h \sum_{j=0}^{k} \beta_{j} \sum_{i=0}^{\infty} \frac{(j h)^{i}}{i!} y^{(i)}(x_{u+j}) \\
&= \sum_{i=0}^{\infty} C_{i} h^{i} y^{(i)}(x_{u+j}) \\
C_{0} &= k \sum_{j=0}^{a_{j}} = g(1) \\
C_{1} &= k \sum_{j=0}^{a_{j} j} = \sum_{j=1}^{k} j a_{j} = g^{'}(1) \\
C_{q} &= k \sum_{j=0}^{a_{j} j q} - q \sum_{j=0}^{a_{j} j} + q \sum_{j=0}^{a_{j}} = \frac{k}{q!} \sum_{j=0}^{a_{j} j q+2} \beta_{j}
\end{align*}$$
• For details see Chapter 6 of Peter Henrici, Discrete Variable Methods in Ordinary Differential Equations, Wiley and Sons, 1962.

Query: How does the solution of (1) by (2) depend on $\bar{y}_0$, the initial value of the derivative?
• Consistency requires that $k \geq 2$. Thus we need a separate technique to get $y_1$. Supposing that we have the starting procedure

$$y_j = \eta_j(h), \quad j = 0, 1, \ldots, k$$

it turns out that convergence requires

$$\lim_{h \to 0} \frac{\eta_j(h) - \eta_0(h)}{jh} = \bar{y}_0,$$

in addition to

$$\lim_{h \to 0} \eta_j(h) = y_0.$$

### Examples of Explicit Methods

$k = 2$, $p = 2$, $C_4 = \frac{1}{12}$

$$y_{n+2} - 2y_{n+1} + y_n = h^2 f_{n+1}.$$  

Do you recognize this formula?

$k = 3$, $p = 3$, $C_5 = \frac{1}{12}$

$$y_{n+3} - 2y_{n+2} + y_{n+1} = h^2 \left( \frac{13}{12} f_{n+2} - \frac{1}{6} f_{n+1} + \frac{1}{12} f_n \right).$$

$k = 4$, $p = 4$, $C_6 = \frac{19}{240}$

$$y_{n+4} - 2y_{n+3} + y_{n+2} = h^2 \left( \frac{7}{6} f_{n+3} - \frac{5}{12} f_{n+2} + \frac{1}{3} f_{n+1} - \frac{1}{12} f_n \right).$$
Examples of Implicit Methods

\( k = 2, \ p = 4, \ C_6 = -\frac{1}{240} \)

\[ y_{n+2} - 2y_{n+1} + y_n = h^2 \left( \frac{1}{12} f_{n+2} + \frac{5}{6} f_{n+1} + \frac{1}{12} f_n \right). \]

This method is known as Numerov's Method, or, somewhat extravagantly, as the Royal Road Formula

\( k = 3, \ p = 4, \ C_6 = -\frac{1}{240} \)

\[ y_{n+3} - 2y_{n+2} + y_{n+1} = h^2 \left( \frac{1}{12} f_{n+3} + \frac{5}{6} f_{n+2} + \frac{1}{12} f_{n+1} \right). \]

\( k = 4, \ p = 5, \ C_7 = -\frac{1}{240} \)

\[ y_{n+4} - 2y_{n+3} + y_{n+2} = h^2 \left( \frac{19}{240} f_{n+4} + \frac{17}{20} f_{n+3} + \frac{7}{120} f_{n+2} + \frac{1}{60} f_{n+1} - \frac{1}{240} f_n \right). \]

- One way to obtain starting values is by a Taylor expansion, which, however, would require partial derivatives of \( f \), as in, for example,

\[ y_1 = y(a) + hy'(a) + \frac{h^2}{2} y''(a) + \frac{h^3}{6} y'''(a) \]

\[ = y_0 + hy_0 + \frac{h^2}{2} f(a, y_0) + \frac{h^3}{6} \left( f_x(a, y_0) + f_y(a, y_0) y_0 \right). \]
\[ y'' = f(x, y(x)) \]

\[ y'' = f_x(x, y(x)) + f_y(x, y(x)) y'(x) \]

- Absolute stability works similarly as in the first order case.

\[ y''' = f_{xx} + f_{xy} y' + (f_{yx} + f_{yy} y'') y' + f_y y' \]

- However, the test equation becomes

\[ y'' = \lambda y \]

and the stability polynomial becomes

\[ \pi(r, h^2 \lambda) = \rho(r) - h^2 \lambda \sigma(r). \]

- The method (2) is absolutely stable for given \( h^2 \lambda \) if all roots of \( \pi(\cdot, h^2 \lambda) \) have an absolute value less than 1.

**Exercise:** Think about matching the behavior of the numerical solution with that of the analytical solution.

**Exercise:** Think about the design of predictor corrector type formulas.

**Boundary Value Problem**

- Suppose we apply Numerov’s Method to the Boundary Value Problem

\[ y'' = f(x, y), \quad y(a) = \alpha, \quad y(b) = \beta. \]

- Let

\[ h = \frac{b - a}{N} \quad \text{and} \quad x_n = a + nh. \]
For example, you might consider the design of a trip from Earth to Mars.

We obtain a **nonlinear system** of $N - 1$ equations in $N - 1$ unknowns $y_1, y_2, y_3, \ldots, y_{N-1}$

\[
Ay = Bf - c
\]

where

\[
A = \begin{bmatrix}
-2 & 1 & 0 & 0 & \ldots & 0 & 0 \\
1 & -2 & 1 & 0 & \ldots & 0 & 0 \\
0 & 1 & -2 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & 1 & -2 \\
\end{bmatrix},
\]

\[
B = \frac{h^2}{12} \begin{bmatrix}
10 & 1 & 0 & 0 & \ldots & 0 & 0 \\
1 & 10 & 1 & 0 & \ldots & 0 & 0 \\
0 & 1 & 10 & 1 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \ldots & 1 & 10 \\
\end{bmatrix},
\]

\[
y = [y_1, y_2, \ldots, y_{N-1}]^T,
\]

\[
f = [f_1, f_2, \ldots, f_{N-1}]^T,
\]

and

\[
c = \left[ y_0 - \frac{h^2}{12} f_0, \ 0, \ \ldots, \ 0, \ y_N - \frac{h^2}{12} f_N \right]^T.
\]

\[\text{This is a **nonlinear system** of equations!}\]

It can be solved, for example, by Newton’s Method, which requires an expression for $f_y$. Every step of Newton’s Method requires the solution of a tridiagonal linear system.