Example from Chemistry

The chemical reaction involving the combination of two chemicals C_1 and C_2, to yield a product C_3 is represented by,

$$C_1 + C_2 \underset{K_1}{\overset{K_2}{\rightleftharpoons}} C_3 \quad .$$

We can model this chemical reaction with the system of 3 ODEs, where $y_1(x) = [C_1]$ the concentration of C_1 (at time x), $y_2(x) = [C_2]$ and $y_3(x) = [C_3]$. The resulting system of IVPs whose solution for $x \in [a, b]$ describes the change in concentrations over time as the reaction takes place is,

$$\begin{aligned} y_1' &= K_1 y_3 - K_2 y_1 y_2, \\ y_2' &= K_1 y_3 - K_2 y_1 y_2, \\ y_3' &= K_2 y_1 y_2 - K_1 y_3. \end{aligned}$$

Second Order ODEs

- Often physical or biological systems are best described by second or higher-order ODEs. That is, second or higher order derivatives appear in the mathematical model of the system.

  For example, from physics we know that Newtons laws of motion describe trajectory or gravitational problems in terms of relationships between velocities, accelerations and positions. These can often be described as IVPs, where the ODE has the form,

$$y''(x) = f(x, y)$$

  or

$$y''(x) = f(x, y, y').$$

Second Order ODEs (cont)

A Second-order scalar ODE can be reduced to an equivalent system of first-order ODEs as follows: With $y^{''} = f(x, y, y')$ we let $Z(x)$ be defined by,

$$Z(x) = [z_1(x), z_2(x)]^T,$$

where $z_1(x) \equiv y(x)$ and $z_2(x) \equiv y'(x)$. It is then clear that $Z(x)$ is the solution of the first order system of IVPs:

$$\begin{aligned} Z' &= \begin{bmatrix} z_1'(x) \\ z_2'(x) \end{bmatrix} = \begin{bmatrix} y'(x) \\ y''(x) \end{bmatrix} \\ &= \begin{bmatrix} z_2(x) \\ f(x, y, y') \end{bmatrix} = \begin{bmatrix} z_2(x) \\ f(x, z_1, z_2) \end{bmatrix} \\ &\equiv F(x, Z). \end{aligned}$$

Observations re 2^{nd}-order ODEs

- Note that in solving this 'equivalent' system for $Z(x)$, we determine an approximation to $y'(x)$ as well as to $y(x)$. This has implications for numerical methods as, when working with this equivalent system, we will also be trying to accurately approximate $y'(x)$ and this may be more difficult than just approximating $y(x)$.
- Note also that to determine a unique solution to our problem we must prescribe initial conditions for $Z(a)$, that is for both $y(a)$ and $y'(a)$.
- Second order systems of ODEs can be reduced to first order systems similarly (doubling the number of equations).
- Higher order equations can be reduced to first order systems in a similar way.

Numerical Methods for IVPs

Taylor Series Methods:

If $f(x, y)$ is sufficiently differentiable wrt x and y then we can determine the Taylor series expansion of the unique solution $y(x)$ to

$$y' = f(x, y), \;\; y(a) = y_0,$$

by differentiating the ODE at the point $x_0 = a$. That is, for x near $x_0 = a$ we have,

$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x - x_0)^2}{2}y''(x_0) + \cdots,$$

Taylor Series Methods (cont)

To generate the TS coefficients, $y^{(n)}(x_0)/n!$, we differentiate the ODE and evaluate at $x = x_0 = a$. The first few terms are computed from the expressions,

$$
\begin{aligned}
y'(x) = f(x,y) &= f, \\
y''(x) = \frac{d}{dx} f(x,y) &= f_x + f_y y' \quad = f_x + f_y f, \\
y'''(x) = \frac{d}{dx}[y''(x)] &= (f_{xx} + f_{xy} f) + (f_{yx} + f_{yy} f) f + f_y (f_x + f_y f) \\
&= f_{xx} + 2 f_{xy} f + f_{yy} f^2 + f_y f_x + f_y^2 f.
\end{aligned}
$$

Key Observation for TS Methods

- In general, if $f(x, y)$ is sufficiently differentiable, we can use the first ($k+1$) terms of the Taylor series as an approximation to $y(x)$ for $|(x - x_0)|$ 'small'. That is, we can approximate $y(x)$ by $\hat{z}_{k,0}(x)$,

$$\hat{z}_{k,0}(x) \equiv y_0 + (x - x_0)y_0' + \cdots + \frac{(x - x_0)^k}{k!} y_0^k.$$

Note that the derivatives of y become quite complicated so one usually chooses a small value of k ($k \leq 6$ or 7).

Key Observation for TS (cont)

- One can use $\hat{z}_{k,0}(x_1)$ as an approximation, y_1, to $y(x_1)$. We can then evaluate the derivatives of $y(x)$ at $x = x_1$ to define a new polynomial $\hat{z}_{k,1}(x)$ as an approximation to $y(x)$ for $|(x - x_1)|$ 'small' and repeat the procedure.

  Note:

  - The resulting $\hat{z}_{k,j}(x)$ for $j = 0, 1, \cdots$ define a piecewise polynomial approximation to $y(x)$ that is continuous on $[a, b]$.
  - How do we choose $h_j = (x_j - x_{j-1})$ and k?