Module 6 : Solving Ordinary Differential Equations - Initial Value Problems (ODE-IVPs)

Section 1 : Introduction

1 Introduction

In this module, we develop solution techniques for numerically solving ordinary differential equations (ODE) of the form

$$\frac{d\mathbf{x}}{d\eta} = F(\mathbf{x}, \eta) \qquad \text{-----(1)}$$

$$\mathbf{x}(0) = \mathbf{x}_0 \qquad \text{-----(2)}$$

where $\mathbf{x} \in R^n$, $F(.,.) \; : R^n \rightarrow R^n$ represents function vector, $\mathbf{x}(0)$ denotes the initial condition and η denotes independent variable such as time or space. The problem at hand is to develop numerical approximation for solution over $[0, \eta]$, which can be expressed as the following integral equation

$$x(\eta) = x_0^* + \int_0^{\eta} F[x(\tau), \tau] d\tau$$

There are two basic approaches to solving ODE-IVPs numerically:

- Taylor series expansion, which forms the basis of Runge - Kutta class of methods
- Polynomial interpolation, which forms the basis of multi-step (or predictor - corrector) methods and orthogonal collocations

In this module, we describe these methods in detail. In the remaining part of this module, we use t as the independent variable. While it is convention to use this variable to denote time, the algorithm developed are general and can be applied even when the independent variable represents spatial dimension.

It may appear that the form given by equations (ODEs-IV) is somewhat restrictive or a special class of the set of ODEs as the L.H.S. involves only the first order derivatives. In practice, not all models appear as first order ODEs. In general, one can get an m'th order ODE of the type:

$$\frac{d^m y}{dt^m} = f[y, \frac{dy}{dt}, \frac{d^2 y}{dt^2}, \ldots\ldots, \frac{d^{m-1} y}{dt^{m-1}}, t] \qquad \text{-----(3)}$$

$$\text{Given } y(0), \ldots\ldots \frac{d^{m-1} y}{dt^{m-1}}(0) \qquad \text{-----(4)}$$

Now, do we develop separate methods for each order? It turns out that such a exercise in unnecessary as a m'th order ODE can be converted to m first order ODEs. Thus, we can define auxiliary variables

$$\begin{aligned} x_1(t) &= y(t) \\ x_2(t) &= \frac{dy}{dt} \\ &\ldots\ldots. \qquad \text{-----(5)} \\ &\ldots\ldots. \\ x_m(t) &= \frac{d^{m-1} y}{dt^{m-1}} \end{aligned}$$

Using these variables, the original mth order ODE can be converted to m first order ODE's as,

$$\begin{aligned}
\frac{dx_1}{dt} &= x_2 \\
\frac{dx_2}{dt} &= x_3 \\
&\ldots\ldots\ldots \\
\frac{dx_{m-1}}{dt} &= x_m \\
\frac{dx_m}{dt} &= f[x_1, x_2, x_3, \ldots, x_m, t]
\end{aligned} \qquad \text{-----(6)}$$

Defining function vector

$$F(\mathbf{x}) = \begin{bmatrix} x_2 \\ \ldots\ldots \\ x_m \\ f[x_1, x_2, x_3, .., x_m, t] \end{bmatrix} \qquad \text{-----(7)}$$

we can write the above set of

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{x}, t) \qquad \text{-----(8)}$$

$$\mathbf{x}(0) = \begin{bmatrix} y(0) & \frac{dy}{dt}(0) \ldots\ldots & \frac{d^{m-1}y}{dt^{m-1}}(0) \end{bmatrix}^T \qquad \text{-----(9)}$$

Thus, it is sufficient to study only the solution methods for solving n first order ODE's of the form (ODEs-IV). Any set of higher order ODEs can be reduced to a set of first order ODEs. Also, forced systems (non-homogeneous systems) can be looked upon as unforced systems (homogenous systems) with time varying parameters. For example, consider a system of ODEs

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{x}, u(t)) \qquad \text{-----(10)}$$

$$\mathbf{x}(0) = \mathbf{x}_0 \qquad \text{-----(11)}$$

where $u \in R$ represents system input, such as inlet flow to a reactor or inlet temperature. A typical simulation problem is to investigate system dynamics when the independent input $u(t)$ is specified, say $u(t) = \sin(\omega t)$ for $t > 0$. With the input $u(t)$ specified, the ODE can be represented as follows

$$\frac{d\mathbf{x}}{dt} = F(\mathbf{x}, \sin(wt)) = F_T(\mathbf{x}, t) \qquad \text{-----(12)}$$

$$\mathbf{x}(0) = \mathbf{x}_0 \qquad \text{-----(13)}$$

where $F_T(\mathbf{x}, t)$ is a function of states and time. Thus, it is sufficient to study the solution methods for homogenous set of equations of the type (ODEs-IV).

6 Existence of Solutions and Convergence of Iterative Methods [12]

If we critically view the methods presented for solving equation (2), it is clear that this problem, in general, cannot solved in its original form. To generate a numerical approximation to the solution of equation (2), this equation is further transformed to formulate an iteration sequence as follows

$$\mathbf{x}^{(k+1)} = \mathbf{G}\left[\mathbf{x}^{(k)}\right] \ ; \ k = 0,1,2,...... \qquad \text{-------(52)}$$

where $\left\{\mathbf{x}^{(k)} : k = 0,1,2,......\right\}$ is sequence of vectors in vector space under consideration. The iteration equation is formulated in such a way that the solution $\mathbf{x}^*$ of equation **(**52**)** also solves equation **(2),** i.e.

$$\mathbf{x}^* = \mathbf{G}[\mathbf{x}^*] \Rightarrow \mathbf{F}(\mathbf{x}^*) = \overline{\mathbf{0}}$$

For example, in the Newton's method, we have

$$\mathbf{G}[\mathbf{x}] \leftrightarrow \mathbf{F}(\mathbf{x}) - \left[\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right]^{-1} \mathbf{F}(\mathbf{x})$$

Thus, we concentrate on the existence and (local) uniqueness of solutions of $\mathbf{x}^* = \mathbf{G}[\mathbf{x}^*]$ rather than that of $\mathbf{F}(\mathbf{x})$.

Contraction mapping theorem develops sufficient conditions for convergence of general nonlinear iterative equation (5). Consider general nonlinear iteration equation of the form

$$\mathbf{x}^{(k+1)} = \mathbf{G}(\mathbf{x}^{(k)}) \qquad \text{-------(53)}$$

which defines a mapping from a Banach space $\mathbf{X}$ into itself, i.e. $\mathbf{G}(.) : X \to X$.

Definition 4 (Contraction Mapping): An operator $\mathbf{G} : X \to X$ given by equation (5), mapping a Banach space X into itself, is called a contraction mapping of closed ball $U(\mathbf{x}^{(0)}, r) = \left\{\mathbf{x} \in X : \left\|\mathbf{x} - \mathbf{x}^{(0)}\right\| \leq r\right\}$, if there exists a real number θ $(0 \leq \theta < 1)$ such that

$$\left\| \mathbf{G}\left(\mathbf{x}^{(1)}\right) - \mathbf{G}\left(\mathbf{x}^{(2)}\right) \right\| \leq \theta \left\| \mathbf{x}^{(1)} - \mathbf{x}^{(2)} \right\|$$

for all $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in U(\mathbf{x}^{(0)}, r)$. The quantity θ is called contraction constant of $\mathbf{G}$ on $U(\mathbf{x}^{(0)}, r)$.

In other words, a function $\mathbf{x} = \mathbf{G}(\mathbf{x})$ is said to be a contraction mapping with respect to a norm $\|.\|$ on a closed region $\mathbf{S}$ if

Definition 5

- $\mathbf{x} \in \mathbf{S}$ implies that $\mathbf{G}(\mathbf{x}) \in \mathbf{S}$, i.e. $\mathbf{G}$ maps $\mathbf{S}$ onto itself
- $\|\mathbf{G}(\mathbf{x}) - \mathbf{G}(\overline{\mathbf{x}})\| \leq \theta \|\mathbf{x} - \overline{\mathbf{x}}\|$ with $0 \leq \theta < 1$ for all $\mathbf{x}, \overline{\mathbf{x}} \in \mathbf{S}$

When the map $\mathbf{G}(.)$ is differentiable, an exact characterization of the contraction property can be developed.

Lemma 6 Let the operator $\mathbf{G}(.)$ on a Banach space X be differentiable in $U(\mathbf{x}^{(0)},r)$. Operator $\mathbf{G}(.)$ is a contraction of $U(\mathbf{x}^{(0)},r)$ if and only if

$$\left\| \frac{\partial \mathbf{G}}{\partial \mathbf{x}} \right\| \leq \theta < 1 \quad \textit{for every } \mathbf{x} \in U(\mathbf{x}^{(0)},r)$$

where $\|.\|$ is any induced operator norm.

The contraction mapping theorem is stated next. Here, $\mathbf{x}^{(0)}$ refers to the initial guess vector in the iteration process given by equation (53).

Theorem 7 [12,9] If $\mathbf{G}(.)$ maps $U(\mathbf{x}^{(0)},r)$ into itself and $\mathbf{G}(.)$ is a contraction mapping on the set with contraction constant θ, for

$$r \geq r_0$$
$$r_0 = \frac{1}{1-\theta} \left\| \mathbf{G}\left[\mathbf{x}^{(0)}\right] - \mathbf{x}^{(0)} \right\|$$

then:

1. $\mathbf{G}(.)$ has a fixed point $\mathbf{x}^*$ in $U(\mathbf{x}^{(0)},r_0)$ such that $\mathbf{x}^* = \mathbf{G}(\mathbf{x}^*)$
2. $\mathbf{x}^*$ is unique in $U(\mathbf{x}^{(0)},r)$
3. The sequence $\mathbf{x}^{(k)}$ generated by equation $\mathbf{x}^{(k+1)} = \mathbf{G}\left[\mathbf{x}^{(k)}\right]$ converges to $\mathbf{x}^*$ with

$$\left\| \mathbf{x}^{(k)} - \mathbf{x}^* \right\| \leq \theta^k \left\| \mathbf{x}^{(0)} - \mathbf{x}^* \right\|$$

4. Furthermore, the sequence $\overline{\mathbf{x}}^{(k)}$ generated by equation

$$\overline{\mathbf{x}}^{(k+1)} = \mathbf{G}\left[\overline{\mathbf{x}}^{(k)}\right] \quad \textit{starting from any initial guess } \overline{\mathbf{x}}^{(0)} \in U(\mathbf{x}^{(0)},r_0)$$

converges to $\mathbf{x}^*$ with

$$\left\| \overline{\mathbf{x}}^{(k)} - \mathbf{x}^* \right\| \leq \theta^k \left\| \overline{\mathbf{x}}^{(0)} - \mathbf{x}^* \right\|$$

The proof of this theorem can be found in Rall Rall[12] and Linz [9].

Example 8 [9] Consider simultaneous nonlinear equations

$$z + \frac{1}{4}y^2 = \frac{1}{16} \qquad \text{-------(54)}$$
$$\frac{1}{3}\sin(z) + y = \frac{1}{2} \qquad \text{-------(55)}$$

We can form an iteration sequence

$$z^{(k+1)} = \frac{1}{16} - \frac{1}{4}\left(y^{(k)}\right)^2 \qquad \text{-------(56)}$$
$$y^{(k+1)} = \frac{1}{2} - \frac{1}{3}\sin(z^{(k)}) \qquad \text{-------(57)}$$

Using $\infty-$norm In the unit ball $U(\mathbf{x}^{(0)} = \overline{0}, 1)$ in the neighborhood of origin, we have

$$\left\|\mathbf{G}\left(\mathbf{x}^{(i)}\right)-\mathbf{G}\left(\mathbf{x}^{(j)}\right)\right\|_{\infty} = \max\left(\frac{1}{4}\left|\left(y^{(i)}\right)^2-\left(y^{(j)}\right)^2\right|, \frac{1}{3}\left|\sin(x^{(i)})-\sin(x^{(j)})\right|\right) \qquad \text{-------(58)}$$

$$\leq \max\left(\frac{1}{4}\left|y^{(i)}-y^{(j)}\right|, \frac{1}{3}\left|x^{(i)}-x^{(j)}\right|\right) \qquad \text{-------(59)}$$

$$\leq \frac{1}{2}\left\|\mathbf{x}^{(i)}-\mathbf{x}^{(j)}\right\|_{\infty} \qquad \text{-------(60)}$$

Thus, $\mathbf{G}(.)$ is a contraction map with $\theta = 1/2$ and the system of equation has a unique solution in the unit ball $U(\mathbf{x}^{(0)} = \overline{0}, 1)$ i.e. $-1 \leq x \leq 1$ and $-1 \leq y \leq 1.$ The iteration sequence converges to the solution.

Example 9 [9] Consider system

$$x - 2y^2 = -1 \qquad \text{-------(61)}$$

$$3x^2 - y = 2 \qquad \text{-------(62)}$$

which has a solution (1,1). The iterative method

$$x^{(k+1)} = 2\left(y^{(k)}\right)^2 - 1 \qquad \text{-------(63)}$$

$$y^{(k+1)} = 3\left(x^{(k)}\right)^2 - 2 \qquad \text{-------(64)}$$

is not a contraction mapping near (1,1) and the iterations do not converge even if we start from a value close to the solution. On the other hand, the rearrangement

$$x(k+1) = \sqrt{(y^{(k)} + 2)/3} \qquad \text{-------(65)}$$

$$y^{(k+1)} = \sqrt{(x^{(k)} + 1)/2} \qquad \text{-------(66)}$$

is a contraction mapping and solution converges if the starting guess is close to the solution.

6.1 Convergence of Successive Substitution Schemes [4]

Either by successive substitution approach or Newton's method, we generate an iteration sequence

$$\mathbf{x}^{(k+1)} = \mathbf{G}(\mathbf{x}^{(k)}) \qquad \text{-------(67)}$$

which has a fixed point

$$\mathbf{x}^* = \mathbf{G}(\mathbf{x}^*) \qquad \text{-------(68)}$$

at solution of $\mathbf{F}(\mathbf{x}^*) = \overline{0}.$ Defining error

$$\mathbf{e}^{(k+1)} = \mathbf{x}^{(k+1)} - \mathbf{x}^* = \mathbf{G}(\mathbf{x}^{(k)}) - \mathbf{G}(\mathbf{x}^*) \qquad \text{-------(69)}$$

and using Taylor series expansion, we can write

$$\mathbf{G}(\mathbf{x}^*) = \mathbf{G}[\mathbf{x}^{(k)} - (\mathbf{x}^{(k)} - \mathbf{x}^*)] \qquad \text{-------(70)}$$

$$\simeq \mathbf{G}(\mathbf{x}^{(k)}) - \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{x=x^{(k)}} (\mathbf{x}^{(k)} - \mathbf{x}^*) \qquad \text{-------(71)}$$

Substituting in (69)

-------(72)

$$\mathbf{e}^{(k+1)} = \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{x=x^{(k)}} \mathbf{e}^{(k)}$$

where

$$\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \mathbf{x}^*$$

and using definition of induced matrix norm, we can write

$$\frac{\|\mathbf{e}^{(k+1)}\|}{\|\mathbf{e}^{(k)}\|} < \left\| \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{x=x^{(k)}} \right\| \qquad \text{-------(73)}$$

It is easy to see that the successive errors will reduce in magnitude if the following condition is satisfied at each iteration i.e.

$$\left\| \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right]_{x=x^{(k)}} \right\| < 1 \text{ for } k = 1, 2, ... \qquad \text{-------(74)}$$

Applying *contraction mapping theorem* (refer to Appendix A for details), a sufficient condition for convergence of iterations in the neighborhood $\mathbf{x}^*$ can be stated as

$$\left\| \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right] \right\|_1 \le \theta_1 < 1$$

or

$$\left\| \left[\frac{\partial \mathbf{G}}{\partial \mathbf{x}}\right] \right\|_\infty \le \theta_\infty < 1$$

Note that this is only a sufficient conditions. If the condition is not satisfied, then the iteration scheme may or may not converge. Also, note that introduction of step length parameter $\lambda^{(k)}$ in Newton's step as

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \lambda^{(k)} \Delta \mathbf{x}^{(k)} \qquad \text{-------(75)}$$

such that $\left\| \mathbf{F}^{(k+1)} \right\| < \left\| \mathbf{F}^{(k)}) \right\|$ ensures that $\mathbf{G}(\mathbf{x})$ is a contraction map and ensures convergence.

Consider equation of type $\mathbf{x} = \mathbf{G}(\mathbf{x})$ where $\mathbf{x} \in \mathbf{R}^n$ and $\mathbf{G}(\mathbf{x})$ represents a function vector of type

$$\mathbf{G}(\mathbf{x}) = \left[\begin{array}{cccc} \mathbf{g}_1(\mathbf{x}) & \mathbf{g}_2(\mathbf{x}) & .... & \mathbf{g}_n(\mathbf{x}) \end{array}\right]^T$$

Let us suppose that $\partial G/\partial x_i$ are continuous in some region $\mathbf{S}$. Let us define a matrix $\mathbf{J}$ such that (i.j)'th element of $\mathbf{J}$ is defined as follows

$$\mathbf{J}_{i,j} = \sup_{x \in S} \left| \frac{\partial \mathbf{g}_i(\mathbf{x})}{\partial x_j} \right|$$

Then, it can be shown that

$$\|\mathbf{G}(\mathbf{x}) - \mathbf{G}(\widetilde{\mathbf{x}})\|_p \le \|\mathbf{J}\|_p \|\mathbf{x} - \widetilde{\mathbf{x}}\|_p$$

and if $\|\mathbf{J}\|_p < 1$ holds in the region of interest, then $\mathbf{G}(.)$ is a contraction mapping with $L = \|\mathbf{J}\|_p$. Also, note that, for 2 norm, the following inequality can be used

$$\|\mathbf{G}(\mathbf{x}) - \mathbf{G}(\widetilde{\mathbf{x}})\|_2 \le \|\mathbf{J}\|_{FRO}\|\mathbf{x} - \widetilde{\mathbf{x}}\|_2$$

$$\|\mathbf{J}\|_{FRO} = \left[\sum_{i,j}(\mathbf{J}_{i,j})^2\right]^{1/2}$$

where $\|\mathbf{J}\|_{FRO}$ is called as *Frobenius norm* of matrix $\mathbf{J}$.

Example 10 Consider the following system of equations

$$x_1 = \frac{1}{12}(-1 + \sin(x_2) + \sin(x_3))$$
$$x_2 = \frac{1}{3}(x_1 - \sin(x_2) + \sin(x_3))$$
$$x_3 = \frac{1}{12}(1 - \sin(x_1) + x_2)$$

which is of the form, $\mathbf{x} = \mathbf{G}(\mathbf{x}),$ in the closed and bounded region $\mathbf{S}$ defined as $-1 \le x_1, x_2, x_3 \le 1.$ Then, the matrix $\mathbf{J}$ can be shown to be

$$\mathbf{J} = \frac{1}{12}\begin{bmatrix} 0 & 1 & 1 \\ 4 & 4 & 4 \\ 1 & 1 & 0 \end{bmatrix}$$

Further, $\|\mathbf{J}\|_1 = \frac{1}{2},$ $\|\mathbf{J}\|_\infty = 1$ and $\|\mathbf{J}\|_{FRO} = \sqrt{13}/6.$ The $\mathbf{G}(.)$ is a contraction mapping for norms $\|.\|_1$ and $\|.\|_2$ in region $\mathbf{S}.$ From contraction mapping theorem, it follows that the system of equations $\mathbf{x} = \mathbf{G}(\mathbf{x})$ has a unique solution in region $\mathbf{S}.$

6.2 Convergence of Newton's Method

Sufficient conditions for the convergence of Newton's method have been established by Kantorovic' Theorem.

Theorem 11 (Kantorovic'): Consider equation $\mathbf{F}(\mathbf{x}) = \overline{\mathbf{0}}$ where operator $\mathbf{F} : R^n \to R^n$ is twice differentiable and the following conditions hold

- There is a $\mathbf{x}^{(0)} \in R^n$ such that $\left[\frac{\partial \mathbf{F}(\mathbf{x}^{(0)})}{\partial \mathbf{x}}\right]^{-1}$ exists with

$$\left\| \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}}\right]^{-1} \right\| = \beta_0 \; and \; \left\| \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}}\right]^{-1} \mathbf{F}\left(\mathbf{x}^{(0)}\right) \right\| \le \eta_0$$

- $\left\| \left[\frac{\partial^2 \mathbf{F}(\mathbf{x}^{(0)})}{\partial \mathbf{x}^2}\right] \right\| \le \kappa$ in a closed ball $U(\mathbf{x}^{(0)}, 2\eta_0)$
- $h_0 = \beta_0 \eta_0 \kappa < 1/2$

Then the sequence

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(k)}\right)}{\partial \mathbf{x}} \right]^{-1} \mathbf{F}\left(\mathbf{x}^{(k)}\right) \qquad \text{-------(76)}$$

exists for all $k \geq 0$ and converges to the solution of $\mathbf{F}(\mathbf{x}) = \overline{\mathbf{0}}$, which exists and is unique in $U(\mathbf{x}^{(0)}, 2\eta_0)$.

Proof Proof of this theorem can be found in Demidovich[6]

Economou [10] has given an interesting interpretation of this theorem. Using multivariable Taylor series expansion of $\left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right]$ in the neighborhood of $\mathbf{x}^{(0)}$, we have

$$\left\| \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right\| \leq \sup_{0 \leq \lambda \leq 1} \left\| \frac{\partial^2 \mathbf{F}\left(\lambda \mathbf{x} + (1-\lambda)\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}^2} \right\| \left\| \mathbf{x} - \mathbf{x}^{(0)} \right\|$$

$$\leq \kappa \left\| \mathbf{x} - \mathbf{x}^{(0)} \right\|$$

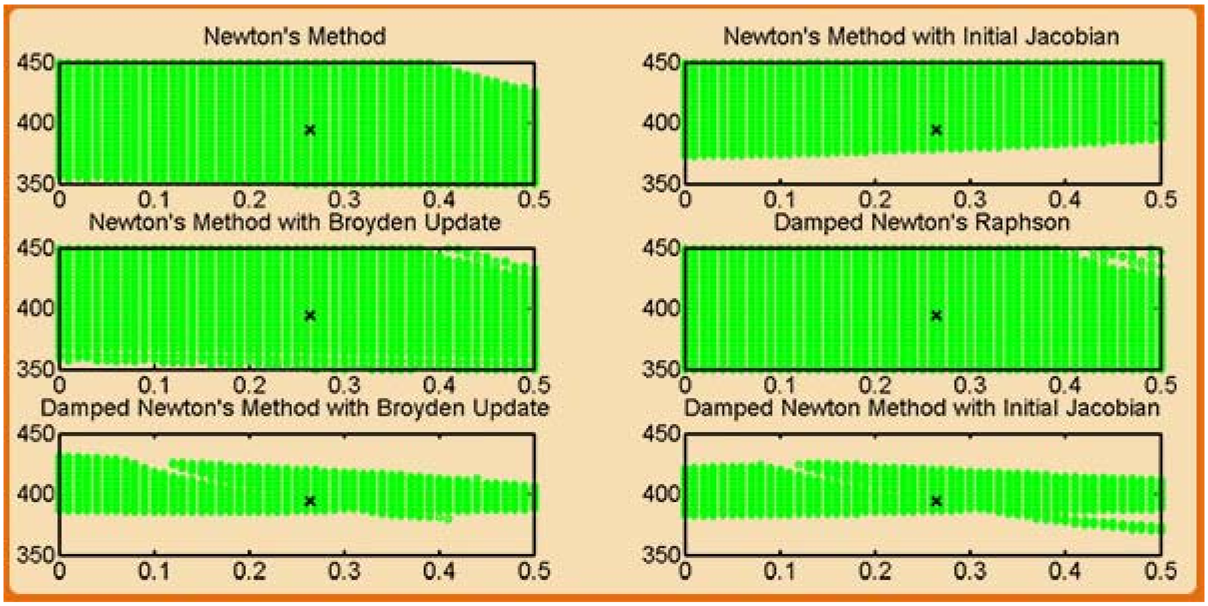

Figure 5 :CSTR Example: Basins of convergence for different variants of Newton's method. Green dots represent initial conditions that lead to convergence of iterations while the black cross represents the solution.

Multiplying by $\left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right]^{-1}$ on both the sides, we have

$$\left\| \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right]^{-1} \right\| \left\| \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right\| \leq \left\| \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right]^{-1} \right\| \kappa \left\| \mathbf{x} - \mathbf{x}^{(0)} \right\|$$

When conditions of the Kantorovic' theorem are satisfied, it follows that

$$\left\| \left[\frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right]^{-1} \right\| \left\| \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}} - \frac{\partial \mathbf{F}\left(\mathbf{x}^{(0)}\right)}{\partial \mathbf{x}} \right\| \leq 2\beta_0 \eta_0 \kappa < 1$$

The term on the L.H.S. of the inequality represents the magnitude of relative change in the Jacobian of operator $\mathbf{F}(.)$ in ball $U(\mathbf{x}^{(0)}, 2\eta_0)$. The Kantorovic' theorem asserts that Newton's method converges if the relative change of the Jacobian in ball $U(\mathbf{x}^{(0)}, 2\eta_0)$ is less than 100%.

Example 12 Basins of Attraction for CSTR Example: The CSTR system described in Example 2 was studied for understanding convergence behavior of variants of Newton's method. Iterations were started from various initial conditions in a box around the steady state solution and progress of iterations towards the solutions was recorded. Figure 5 compares sets of initial conditions starting from which the respective methods converge to the solution. In each box, green dots represent initial conditions that lead to convergence of iterations. As evident from this figure, Newton's method with the initial Jacobian has a smaller basin of convergence. Damped Newton's method appears to have largest basin of convergence.