NUMERICAL METHODS
Chapter 5: Iterative Methods for System of Nonlinear Equations

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The objectives of this chapter are

- ★ To calculate the Jacobian of a vector valued function;
- ★ To solve a small system of nonlinear equations using Newton method;
- ★ To use finite differencing to approximate the Jacobian of a vector valued function;

System of Nonlinear Equations

The main objective is to find the root of x such that

$$f(x) = 0,$$

Question: What is the solution x of $f(x) = 0$?.

For example, consider the function $f(x)$ given as follows:

$$\begin{aligned} x_1^2 + x_2^2 - 1 &= 0, \\ x_1^2 - x_2^2 &= 0. \end{aligned}$$

How can you find the solution x to this function? How many solutions you can have for this function?.

A quick answer to that questions can be answered by producing the graph of that given function. As shown in Figure 1, there are four solutions for that function.

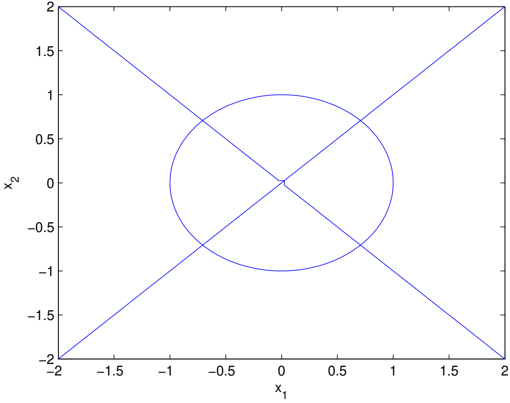

Figure: Nonlinear system

To check whether these are solutions to that function, just plug in the values for x_1 and x_2 into the two components of $f(x)$ and simplify. You should get zero for both components.

Example

Let $f(x) = 0$ be defined as

$$x_1^2 + x_2^2 - 1 = 0,$$
$$x_1^2 - x_2^2 = 0.$$

Given $x^{(k)} = [x_1^{(k)}, x_2^{(k)}]^T$, use a linear approximation to find δx such that $f(x^{(k)} + \delta) \approx 0$.
Note: δ often known as the rate of change. In this case the rate of change $\delta = x^{(k)} - x^{(k-1)}$.

Solution

The superscript (k) *are dropped and replaced* δx *by* δ *to simplify the notation.*

$$f(x) = \begin{bmatrix} x_1^2 + x_2^2 - 1. \\ x_1^2 - x_2^2 \end{bmatrix}.$$

Solution

$$
\begin{aligned}
f(x+\delta) &= \begin{bmatrix} (x_1+\delta_1)^2+(x_2+\delta_2)^2-1 \\ (x_1+\delta_1)^2-(x_2+\delta_2)^2 \end{bmatrix}, \\
&= \begin{bmatrix} x_1^2+x_2^2-1+2(x_1\delta_1+x_2\delta_2)+(\delta_1^2+\delta_2^2) \\ x_1^2-x_2^2+2(x_1\delta_1-x_2\delta_2)+(\delta_1^2-\delta_2^2) \end{bmatrix}, \\
&= \begin{bmatrix} x_1^2+x_2^2-1 \\ x_1^2-x_2^2 \end{bmatrix} + 2\begin{bmatrix} x_1+x_2 \\ x_1-x_2 \end{bmatrix}\begin{bmatrix} \delta_1 \\ \delta_2 \end{bmatrix} + O(\delta_1^2,\delta_2^2), \\
&= f(x)+J(x)\delta+O(\delta_1^2,\delta_2^2),
\end{aligned}
$$

Jacobian Matrix

$J(x)$ is called the Jacobian (see below for a general definition). A linear approximation is formed to the right hand side by omitting the δ_1^2 and δ_2^2 terms. This gives

$$f(x+\delta) \approx f(x) + J(x)\delta.$$

To find δ such that $f(x+\delta) \approx 0$, set the right hand side of the above equation to zero and solve for δ. This gives

$$\begin{aligned} f(x) + J(x)\delta &= 0, \\ J(x)\delta &= -f(x). \end{aligned}$$

Since $J(x)$ is a matrix, you cannot divide by $J(x)$. In order to simplify this term, multiply front left with $[J(x)]^{-1}$ since any matrices multiply by its inverse gives the identity I such that $A^{-1}A = I$ provided A is a non singular matrix.

This yields

$$\begin{aligned}[J(x)]^{-1}J(x)\delta &= -[J(x)]^{-1}f(x),\\ \delta &= -[J(x)]^{-1}f(x).\end{aligned}$$

Thus,

$$x^{(k)} - x^{(k-1)} = -[J(x^{(k-1)})]^{-1}f(x^{(k-1)}).$$

Then the new value, $x^{(k)}$, is therefore given by

$$x^{(k)} = x^{(k-1)} - [J(x^{(k-1)})]^{-1}f(x^{(k-1)}).$$

This equation is known as the Newton iteration.

Jacobian Matrix

The Jacobian matrix is needed in order to use the Newton method. Jacobian matrix is the matrix of all first-order partial derivatives of a vector-valued function. The matrix must be a square matrix. The definition of Jacobian matrix is given in Definition 4.

Definition

The Jacobian of $f(x)$ where $f(x) : \mathbb{R}^n \to \mathbb{R}^n$ is defined as

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \vdots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \cdots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

To understand the Jacobian matrix definition, consider Example 5.

Example

Write down the Jacobian for the following system

$$
\begin{aligned}
5x_1^2 - e^{x_1 x_2} &= 0, \ \rightarrow f_1, \\
x_1 x_2 + 2\cos(x_2) &= 0, \ \rightarrow f_2.
\end{aligned}
$$

Solution

The above systems involves the variables x_1 *and* x_2. *By the Definition 4,*

$$\frac{\partial f_1}{\partial x_1} = 10x_1 - x_2 e^{x_1 x_2}.$$
$$\frac{\partial f_1}{\partial x_2} = -x_1 e^{x_1 x_2}.$$
$$\frac{\partial f_2}{\partial x_1} = x_2.$$
$$\frac{\partial f_2}{\partial x_2} = x_1 - 2\sin(x_2).$$

Solution

Thus, the Jacobian is given by

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 10x_1 - x_2 e^{x_1 x_2} & -x_1 e^{x_1 x_2} \\ x_2 & x_1 - 2\sin(x_2) \end{bmatrix}.$$

Example

Given the system of nonlinear equations

$$4x_1^2 - 15x_1 + x_2^2 + 8 = 0,$$
$$\frac{1}{4}x_1x_2^2 + 2x_1 - 5x_2 + 2 = 0.$$

Find the Jacobian of that system.

Solution

The variables involves are x_1 and x_2. The size of Jacobian is 2×2.

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 8x_1 - 15 & 2x_2 \\ \frac{1}{4}x_2^2 + 2 & \frac{1}{2}x_1x_2 - 5 \end{bmatrix}.$$

Example

Find the Jacobian of this function

$$f(x, y) = 4x^2 - 15x\sin(y) + y^2.$$

Solution

By inspection, there are two variables x and y so the Jacobian is a 2×2 matrix.

$$\frac{\partial f}{\partial x} = 8x - 15\sin(y).$$
$$\frac{\partial f}{\partial y} = -15x\cos(y) + 2y.$$

Solution

The Jacobian is therefore given by

$$\begin{bmatrix} \frac{\partial f_x}{\partial x} & \frac{\partial f_x}{\partial y} \\ \frac{\partial f_y}{\partial x} & \frac{\partial f_y}{\partial y} \end{bmatrix} = \begin{bmatrix} 8 & -15\cos(y) \\ -15\cos(y) & 15x\sin(y)+2 \end{bmatrix}.$$

The above Jacobian often regarded as the **Hessian**.

Newton-Raphson Method

Newton method is one of famous method to solve system of nonlinear equations. To solve ordinary differential equations using Runge-Kutta methods, Newton method is needed to solve the implicit equations. The method is also known as the **Newton-Raphson method**, that is named after Isaac Newton and Joseph Raphson. It is a method for finding successively better approximations to the roots (or zeroes) of a real-valued function.

Definition

Newton's equation for $f(x) = 0$ where $f(x) : \mathbb{R}^n \to \mathbb{R}^n$ is defined as

$$x^{(k)} = x^{(k-1)} - [J(x^{(k-1)})]^{-1} f(x^{(k-1)}).$$

Example

Apply two iterations of Newton-Raphson's method to

$$x_1^2 + x_2^2 - 1 = 0,$$
$$x_1^2 - x_2^2 = 0.$$

Start with the initial estimate $x^{(0)} = [3/4, 3/4]^T$.

Solution

First, find the Jacobian matrix. By inspection, the Jacobian is given by

$$J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{bmatrix} = \begin{bmatrix} 2x_1 & 2x_2 \\ 2x_1 & -2x_2 \end{bmatrix}.$$

Solution

First Iteration

Given $x^{(0)} = [3/4, 3/4]^T$ *such that* $x_1^{(0)} = 3/4$ *and* $x_2^{(0)} = 3/4$.

$$x^{(1)} = x^{(0)} - [J(x^{(0)})]^{-1} f(x^{(0)}).$$

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} x_1^{(0)} \\ x_2^{(0)} \end{bmatrix} - \begin{bmatrix} 2x_1^{(0)} & 2x_2^{(0)} \\ 2x_1^{(0)} & -2x_2^{(0)} \end{bmatrix}^{-1} \begin{bmatrix} (x_1^{(0)})^2 + (x_2^{(0)})^2 - 1 \\ (x_1^{(0)})^2 - (x_2^{(0)})^2 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{3}{4} \\ \frac{3}{4} \end{bmatrix} - \begin{bmatrix} 2(\frac{3}{4}) & 2(\frac{3}{4}) \\ 2(\frac{3}{4}) & -2(\frac{3}{4}) \end{bmatrix}^{-1} \begin{bmatrix} (\frac{3}{4})^2 + (\frac{3}{4})^2 - 1 \\ (\frac{3}{4})^2 - (\frac{3}{4})^2 \end{bmatrix}$$

Solution

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} \frac{3}{4} \\ \frac{3}{4} \end{bmatrix} - \begin{bmatrix} \frac{3}{2} & \frac{3}{2} \\ \frac{3}{2} & -\frac{3}{2} \end{bmatrix}^{-1} \begin{bmatrix} \frac{9}{16} + \frac{9}{16} - 1 \\ 0 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{3}{4} \\ \frac{3}{4} \end{bmatrix} - \begin{bmatrix} \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & -\frac{1}{3} \end{bmatrix} \begin{bmatrix} \frac{1}{8} \\ 0 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{3}{4} \\ \frac{3}{4} \end{bmatrix} - \begin{bmatrix} \frac{1}{24} \\ \frac{1}{24} \end{bmatrix} = \begin{bmatrix} \frac{17}{24} \\ \frac{17}{24} \end{bmatrix},$$

$$= \begin{bmatrix} 0.7083 \\ 0.7083 \end{bmatrix}.$$

Solution

Second Iteration

Now $x^{(1)} = [17/24, 17/24]^T$ *such that* $x_1^{(1)} = 17/24$ *and* $x_2^{(1)} = 17/24$.

$$x^{(2)} = x^{(1)} - [J(x^{(1)})]^{-1} f(x^{(1)}).$$

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} - \begin{bmatrix} 2x_1^{(1)} & 2x_2^{(1)} \\ 2x_1^{(1)} & -2x_2^{(1)} \end{bmatrix}^{-1} \begin{bmatrix} (x_1^{(1)})^2 + (x_2^{(1)})^2 - 1 \\ (x_1^{(1)})^2 - (x_2^{(1)})^2 \end{bmatrix}$$

Solution

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{17}{24} \\ \frac{17}{24} \end{bmatrix} - \begin{bmatrix} 2(\frac{17}{24}) & 2(\frac{17}{24}) \\ 2(\frac{17}{24}) & -2(\frac{17}{24}) \end{bmatrix}^{-1} \begin{bmatrix} (\frac{17}{24})^2 + (\frac{17}{24})^2 - 1 \\ (\frac{17}{24})^2 - (\frac{17}{24})^2 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{17}{24} \\ \frac{17}{24} \end{bmatrix} - \begin{bmatrix} \frac{17}{12} & \frac{17}{12} \\ \frac{17}{12} & -\frac{17}{12} \end{bmatrix}^{-1} \begin{bmatrix} \frac{1}{288} \\ 0 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{17}{24} \\ \frac{17}{24} \end{bmatrix} - \begin{bmatrix} \frac{6}{17} & \frac{6}{17} \\ \frac{6}{17} & -\frac{6}{17} \end{bmatrix} \begin{bmatrix} \frac{1}{288} \\ 0 \end{bmatrix},$$

$$= \begin{bmatrix} \frac{17}{24} \\ \frac{17}{24} \end{bmatrix} - \begin{bmatrix} \frac{1}{816} \\ \frac{1}{816} \end{bmatrix} = \begin{bmatrix} \frac{577}{816} \\ \frac{577}{816} \end{bmatrix} = \begin{bmatrix} 0.7071 \\ 0.7071 \end{bmatrix}.$$

Example

Apply two iterations of Newton-Raphson's method to

$$5x_1^2 - e^{x_1 x_2} = 0,$$
$$x_1 x_2 + 2\cos(x_2) = 0.$$

Start with the initial estimate $x^{(0)} = [1, 0]^T$.

Solution

The Jacobian matrix is given by

$$\begin{bmatrix} 10x_1 - x_2 e^{x_1 x_2} & -x_1 e^{x_1 x_2} \\ x_2 & x_1 - 2\sin(x_2) \end{bmatrix}.$$

Solution

First Iteration
Given $x^{(0)} = [1, 0]^T$ *such that* $x_1^{(0)} = 1$ *and* $x_2^{(0)} = 0$.

$$
\begin{aligned}
x^{(1)} &= x^{(0)} - [J(x^{(0)})]^{-1} f(x^{(0)}). \\
&= \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 10(1) - 0 & -1e^0 \\ 0 & 1 - 2\sin(0) \end{bmatrix}^{-1} \begin{bmatrix} 5(1)^2 - e^0 \\ (1)(0) + 2\cos(0) \end{bmatrix}, \\
&= \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 10 & -1 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 5 - 1 \\ 0 + 2 \end{bmatrix}, \\
&= \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \begin{bmatrix} 0.1 & 0.1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 4 \\ 2 \end{bmatrix} = \begin{bmatrix} 0.4 \\ -2 \end{bmatrix}.
\end{aligned}
$$

Thus, $x^{(1)} = [0.4000, -2.0000]^T$.

Solution

Second Iteration
From the first iteration, $x^{(1)} = [0.4000, -2.0000]^T$ *such that* $x_1^{(1)} = 0.4000$ *and* $x_2^{(1)} = -2.0000$.

$$\begin{bmatrix} x_1^{(2)} \\ x_2^{(2)} \end{bmatrix} = \begin{bmatrix} 0.4 \\ -2 \end{bmatrix} - \begin{bmatrix} 4.8987 & -0.1797 \\ -2 & 2.2186 \end{bmatrix}^{-1} \begin{bmatrix} 0.3507 \\ -1.6323 \end{bmatrix},$$

$$= \begin{bmatrix} 0.4 \\ -2 \end{bmatrix} - \begin{bmatrix} 0.2111 & 0.0171 \\ 0.1903 & 0.4661 \end{bmatrix} \begin{bmatrix} 0.3507 \\ -1.6323 \end{bmatrix},$$

$$= \begin{bmatrix} 0.4 \\ -2 \end{bmatrix} - \begin{bmatrix} 0.04611 \\ -0.6942 \end{bmatrix} = \begin{bmatrix} 0.3539 \\ -1.3058 \end{bmatrix}.$$

This gives $x^{(2)} = [0.3539, -1.3058]^T$.

Example

Consider the system of nonlinear equations

$$\begin{aligned} x_1(x_2^2+1)+\sin(x_1)-2+x_2 &= 0,\\ x_2+x_2^3+\cos(x_1)-3 &= 0. \end{aligned}$$

(a) Give the Jacobian of the system at $[0,0]^T$.

(b) Apply one iteration of Newton-Raphson's method using the initial estimate $x^{(0)}=[0,0]^T$.

Solution

(a) *Give the Jacobian of the system at* $[0,0]^T$.

$$J(x) = \begin{bmatrix} x_2^2 + 1 + \cos(x_1) & 2x_1x_2 + 1 \\ -\sin(x_1) & 1 + 3x_2^2 \end{bmatrix}.$$

Solution

(b) *Apply one iteration of Newton-Raphson's method using the initial estimate $x^{(0)} = [0,0]^T$.*

$$x^{(1)} = x^{(0)} - [J(x^{(0)})]^{-1} f(x^{(k-1)}).$$

$$\begin{bmatrix} x_1^{(1)} \\ x_2^{(1)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 2 & 1 \\ 0 & 1 \end{bmatrix}^{-1} \begin{bmatrix} -2 \\ -2 \end{bmatrix},$$

$$= \begin{bmatrix} 0 \\ 0 \end{bmatrix} - \begin{bmatrix} 0.5 & -0.5 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -2 \\ -2 \end{bmatrix},$$

$$= \begin{bmatrix} 0 \\ 2 \end{bmatrix}.$$

The formulas for the Newton-Raphson method is summarized as follows:
If it is a **scalar nonlinear equation** then use

$$x^{(k)} = x^{(k-1)} - \frac{f(x^{(k-1)})}{f'(x^{(k-1)})}.$$

If you are give a **system of nonlinear equation**, then you need to use the following equation

$$x^{(k)} = x^{(k-1)} - [J(x^{(k-1)})]^{-1} f(x^{(k-1)}).$$