Part 5. Numerical Analysis

Newton's Method for Solving Systems of Equations

5.1 Note: A system of n equations in n variables given by

$$f_1(x_1,x_2,\cdots,x_n)=0\ ,\ f_2(x_1,x_2,\cdots,x_n)=0\ ,\ \cdots\ ,\ f_n(x_1,x_2,\cdots,x_n)=0$$

where each function $f_k:U\subseteq\mathbb{R}^n\to\mathbb{R}$, can be written as a single equation $F(x)=0$ where $F:U\subseteq\mathbb{R}^n\to\mathbb{R}^n$. A point $x=a\in\mathbb{R}^n$ is a **solution** when $F(a)=0$. We can approximate a solution $x=a$ to the equation $F(x)=0$ numerically using the following method, which is called **Newton's method**, or the **Newton-Raphson method**. We start with an initial estimate $a_0\cong a$. Having found an estimate a_k, we let a_{k+1} be the solution to the equation $L(x)=0$ where $L(x)$ is the linearization of $F(x)$ at the point a_k. We have $L(x)=F(a_k)+DF(a_k)(x-a_k)$, so $L(x)=0$ when $DF(a_k)(x-a_k)=-F(a_k)$, that is when $x=a_k-DF(a_k)^{-1}F(a_k)$. Thus a_{k+1} is obtained from a_k using the formula

$$a_{k+1}=a_k-DF(a_k)^{-1}F(a_k).$$

5.2 Exercise: Let $F(x,y)=\begin{pmatrix}x^2-y^2+x+1\\2xy+y\end{pmatrix}$. Find all $a=\binom{x}{y}\in\mathbb{R}^2$ such that $F(a)=0$. Starting with $a_0=\binom{x_0}{y_0}=\binom{0}{1}$, find the first and second estimates $a_1=\binom{x_1}{y_1}$ and $a_2=\binom{x_2}{y_2}$ obtained using Newton's method.

Numerical Methods for Evaluating Definite Integrals

5.3 Definition: There are a number of methods that can be used to approximate the value of a definite integral $\int_a^b f(x)\,dx$, where $f:[a,b]\to\mathbb{R}$ is continuous (or piecewise continuous), and finding such an approximation is known as **numerical integration** or **numerical quadrature**. A **Newton-Cotes quadrature** rule is obtained by selecting points x_k with $a\le x_0<x_1<\cdots<x_n\le b$ and making the approximation

$$\int_a^b f(x)\,dx\cong I_n(f)=\int_a^b p(x)\,dx$$

where $p(x)$ is the polynomial of degree at most n with $p(x_k)=f(x_k)$ for all $0\le k\le n$. This polynomial is given by

$$p(x)=\sum_{k=0}^n f(x_k)g_k(x)\ ,\ \text{where}\ \ g_k(x)=\frac{\prod_{i\neq k}(x-x_i)}{\prod_{i\neq k}(x_k-x_i)},$$

so the approximation rule is given by

$$\int_a^b f(x)\,dx=I_n(f)=\int_a^b\sum_{k=0}^n f(x_k)g_k(x)\,dx=\sum_{k=0}^n w_k\,f(x_k)\ \ ,\ \text{where}\ \ w_k=\int_a^b g_k(x)\,dx.$$

The **closed Newton-Cotes quadrature** rule is obtained by choosing the points x_k to be evenly spaced with $a=x_0<x_1<\cdots<x_n=b$ (dividing the interval into n subintervals) so the points are given by $x_k=a+k\,\frac{b-a}{n}$. The **open Newton-cotes quadrature** rule is obtained by choosing the points $a<x_0<x_1<\cdots<x_n<b$ to be evenly spaced (dividing the interval into $n+2$ subintervals), so the points x_k are given by $x_k=a+(k+1)\,\frac{b-a}{n+2}$. **Composite Newton-Cotes quadrature** involves first dividing the interval $[a,b]$ into subintervals and then applying a Newton-Cotes quadrature rule in each subinterval.

5.4 Exercise: Show that when $n = 0$, the open Newton-Cotes quadrature rule is the midpoint rule, and when $n = 1$, the closed Newton-Cotes quadrature rule is the trapezoidal rule, and when $n = 2$, the closed Newton-Cotes quadrature rule is Simpson's rule.

5.5 Exercise: Show that when $n = 1$, the open Newton-Cotes rule is given by

$$I_1^o(f) = \tfrac{b-a}{2}\big(f(x_0) + f(x_1)\big) \quad \text{, where } \; x_k = a + (k+1)\tfrac{b-a}{3}.$$

5.6 Exercise: Show that when $n = 3$, the closed Newton-Cotes rule is given by

$$I_3^c(f) = \tfrac{b-a}{8}\big(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\big) \quad \text{, where } \; x_k = a + k\,\tfrac{b-a}{3}.$$

5.7 Definition: Given $n \in \mathbb{Z}^+$, the n^{th} **Gaussian quadrature** is given by

$$\int_a^b f(x)\,dx \cong I_n^g(f) = \sum_{k=1}^{n} w_k f(x_k)$$

where the n points x_k with $a \le x_1 < x_2 < \cdots < x_n \le b$ and the weights $w_1, w_2, \cdots, w_n$ are chosen such that

$$\int_a^b p(x)\,dx = \sum_{k=1}^{n} w_k\, p(x_k)$$

for all polynomials $p(x)$ of degree less than $2n$, or equivalently when $p(x)$ is equal to each of the polynomials $1, x, x^2, \cdots, x^{2n-1}$.

5.8 Exercise: Show that when $n = 1$, the Gaussian quadrature rule is the midpoint rule.

5.9 Exercise: Show that when $n = 2$, the Gaussian quadrature on the interval $[-1, 1]$ is given by

$$\int_{-1}^1 f(x)\,dx \cong I_2^g(f) = f\big(-\tfrac{1}{\sqrt{3}}\big) + f\big(\tfrac{1}{\sqrt{3}}\big)$$

and that, on the general interval $[a, b]$, it is given by

$$\int_a^b f(x)\,dx \cong I_2^g(f) = \tfrac{b-a}{2}\Big(f\big(\tfrac{a+b}{2} - \tfrac{b-a}{2\sqrt{3}}\big) + f\big(\tfrac{a+b}{2} + \tfrac{b-a}{2\sqrt{3}}\big)\Big).$$

5.10 Exercise: Approximate the value of $\ln 2$ by approximating the value of $\int_1^2 \frac{1}{x}\,dx$ using the trapezoidal rule, the midpoint rule, Simpson's rule, the open Newton-Cotes quadrature rule for $n = 1$, the closed Newton-cotes quadrature rule for $n = 3$, and the Gaussian quadrature rule for $n = 2$.

Numerical Methods for Solving First Order IVPs

5.11 Note: Recall that we can approximate the solution $y = y(x)$ to the IVP given by $y' = f(x, y)$ with $y(x_0) = y_0$ using **Euler's method**: choose a small step size $h = \Delta x$, start at (x_0, y_0) then, having found (x_n, y_n), let $x_{n+1} = x_n + h$ and $y_{n+1} = y_n + f(x_n, y_n)\,h$. Euler's method is related to the fact that the solution $y = y(x)$ with $y(x_n) = y_n$ can be approximated by the linearization of $y(x)$ at x_n, which is given by

$$L(x) = y(x_n) + y'(x_n)(x - x_n) = y_n + f(x_n, y_n)(x - x_n).$$

It follows that when h is small and $x_{n+1} = x_n + h$ we have

$$y(x_{n+1}) = y(x_n + h) \cong L(x_n + h) = y_n + f(x_n, y_n)h = y_{n+1}.$$

5.12 Definition: Let us use a similar argument to obtain a more accurate method, called the **second-order Taylor method**. When $y = y(x)$ is a solution to the DE $y' = f(x, y)$, we have $y'(x) = f(x, y(x))$ for all x so that, by the chain rule,

$$y''(x) = \tfrac{\partial f}{\partial x}(x, y(x)) + \tfrac{\partial f}{\partial y}(x, y(x))y'(x) = \tfrac{\partial f}{\partial x}(x, y(x)) + \tfrac{\partial f}{\partial y}(x, y(x))f(x, y(x)).$$

When $y = y(x)$ is the solution with $y(x_n) = y_n$, we have $y'(x_n) = f(x_n, y_n)$ and

$$y''(x_n) = \tfrac{\partial f}{\partial x}(x_n, y_n) + \tfrac{\partial f}{\partial y}(x_n, y_n)f(x_n, y_n),$$

so the second Taylor polynomial of $y(x)$ at $x = x_n$ is given by

$$\begin{aligned} T_2(x) &= y(x_n) + y'(x_n)(x - x_n) + \tfrac{1}{2}y''(x_n)(x - x_n)^2 \\ &= y_n + f(x_n, y_n)(x - x_n) + \tfrac{1}{2}\Big(\tfrac{\partial f}{\partial x}(x_n, y_n) + \tfrac{\partial f}{\partial y}(x_n, y_n)f(x_n, y_n)\Big)(x - x_n)^2 \\ T_2(x_n + h) &= y_n + f(x_n, y_n)h + \tfrac{1}{2}\Big(\tfrac{\partial f}{\partial x}(x_n, y_n) + \tfrac{\partial f}{\partial y}(x_n, y_n)f(x_n, y_n)\Big)h^2. \end{aligned}$$

Thus we approximate the solution $y = y(x)$ to the IVP given by $y' = f(x, y)$ with $y(x_0) = y_0$ as follows: choose a small step size $h = \Delta x$, start at the point (x_0, y_0) then, having found (x_n, y_n), let $x_{n+1} = x_n + h$ and

$$y_{n+1} = y_n + f(x_n, y_n)h + \tfrac{1}{2}\Big(\tfrac{\partial f}{\partial x}(x_n, y_n) + \tfrac{\partial f}{\partial y}(x_n, y_n)f(x_n, y_n)\Big)h^2.$$

5.13 Definition: A **second-order Runga-Kutta method** for solving $y' = f(x, y)$ with $y(x_0) = y_0$, is a method in which we choose a small step size $h = \Delta x$, we start at (x_0, y_0) then, having found (x_n, y_n) we let $x_{n+1} = x_n + h$ and we let y_{n+1} be obtained using a formula of the form

$$y_{n+1} = y_n + r\, m_1 h + s\, m_2 h$$

where

$$\begin{aligned} m_1 &= f(x_n, y_n) \\ m_2 &= f\big((x_n, y_n) + t(h, m_1 h)\big) \end{aligned}$$

for some $r, s, t \in \mathbb{R}$ with $r + s = 1$ and $0 \leq t \leq 1$.

5.14 Example: When $r = 1$ and $s = 0$ we obtain Euler's method. When $r = 0$ and $s = 1$ and $t = \frac{1}{2}$, the resulting method is called the **modified Euler**, or **midpoint method**. When $r = s = \frac{1}{2}$ and $t = 1$, the resulting method is called the **Heun method**. When $r = \frac{1}{4}$ and $s = \frac{3}{4}$ and $t = \frac{2}{3}$, the resulting method is called the **optimal RK2 method**.

5.15 Definition: The **classical fourth-order Runga-Kutta method**, also called the **RK4 method**, for solving $y' = f(x, y)$ with $y(x_0) = y_0$ is performed as follows: We choose a small step size $h = \Delta x$, we start at (x_0, y_0) then, having found (x_n, y_n), we let $x_{n+1} = x_n + h$ and

$$y_{n+1} = y_n + \tfrac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4)\, h$$

where

$$\begin{aligned} m_1 &= f(x_n, y_n) \\ m_2 &= f\big((x_n, y_n) + \tfrac{1}{2}(h, m_1 h)\big) \\ m_3 &= f\big((x_n, y_n) + \tfrac{1}{2}(h, m_2 h)\big) \\ m_4 &= f\big((x_n, y_n) + (h, m_3 h)\big). \end{aligned}$$

5.16 Exercise: Consider the IVP given by $y' = 1 + \frac{y}{x}$ with $y(1) = 1$. Find the exact solution $y = y(x)$ and the exact value of $y(2)$. Approximate the value of $y(2)$ using Euler's method with $h = \frac{1}{4}$, then again using the second-order Taylor method with $h = \frac{1}{2}$, then again using RK4 with $h = 1$.