2072U Computational Science I
Winter 2022

Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. Newton-Raphson iteration
2. Pseudo-code
3. Trivial test

Newton iteration can be generalized to n equations with n unknowns.
Alternative derivation in 1D:

$$f(x+\delta x) \approx f(x) + f'(x)\delta x = 0 \quad \Rightarrow \quad \delta x = -\frac{f(x)}{f'(x)}$$

Now in 2D. We want to find x_1 and x_2 such that

$$f_1(x_1, x_2) = 0$$
$$f_1(x_1, x_2) = 0$$

Note that, in general, we need the same number of equations and unknowns to find (isolated) solutions...

$$f_1(x_1+\delta x_1, x_2+\delta x_2) \approx f_1(x_1,x_2) + \frac{\partial f_1}{\partial x_1}(x_1,x_2)\delta x_1 + \frac{\partial f_1}{\partial x_2}(x_1,x_2)\delta x_2$$
$$f_2(x_1+\delta x_1, x_2+\delta x_2) \approx f_2(x_1,x_2) + \frac{\partial f_2}{\partial x_1}(x_1,x_2)\delta x_1 + \frac{\partial f_2}{\partial x_2}(x_1,x_2)\delta x_2$$

In matrix form:

$$\begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x_1,x_2) & \frac{\partial f_1}{\partial x_2}(x_1,x_2) \\ \frac{\partial f_2}{\partial x_1}(x_1,x_2) & \frac{\partial f_2}{\partial x_2}(x_1,x_2) \end{pmatrix} \begin{pmatrix} \delta x_1 \\ \delta x_2 \end{pmatrix} = -\begin{pmatrix} f_1(x_1,x_2) \\ f_2(x_1,x_2) \end{pmatrix}$$

Problem statement: *given a function* $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$ *and an initial guess* $\mathbf{x}^{(0)} \in \mathbb{R}^n$*, find an approximate solution to* $\mathbf{f}(\mathbf{x}) = 0$*.*
The derivation of the iterative method is similar to that of Newton iteration:

$$f(x+\delta x) \approx f(x)+f'(x)\delta x = 0 \;\Rightarrow\; \delta x = -\frac{f(x)}{f'(x)} \text{ for } f(x),\, x,\, \delta x \in \mathbb{R}$$

becomes

$$\mathbf{f}(\mathbf{x}+\delta\mathbf{x}) \approx \mathbf{f}(\mathbf{x})+D\mathbf{f}\delta\mathbf{x} = 0 \;\Rightarrow\; D\mathbf{f}\delta\mathbf{x} = -\mathbf{f}(\mathbf{x}) \text{ for } \mathbf{f}(\mathbf{x}),\, \mathbf{x},\, \delta\mathbf{x} \in \mathbb{R}^n$$

That is, the update $\delta\mathbf{x}$ is found from the linear system:

$$D\mathbf{f}\delta\mathbf{x} = \begin{pmatrix} \partial_{x_1} f_1(\mathbf{x}) & \partial_{x_2} f_1(\mathbf{x}) & \cdots & \partial_{x_n} f_1(\mathbf{x}) \\ \partial_{x_1} f_2(\mathbf{x}) & \partial_{x_2} f_2(\mathbf{x}) & \cdots & \partial_{x_n} f_2(\mathbf{x}) \\ \vdots & \vdots & & \vdots \\ \partial_{x_1} f_n(\mathbf{x}) & \partial_{x_2} f_n(\mathbf{x}) & \cdots & \partial_{x_n} f_n(\mathbf{x}) \end{pmatrix} \begin{pmatrix} \delta x_1 \\ \delta x_2 \\ \vdots \\ \delta x_n \end{pmatrix} = -\begin{pmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_n(\mathbf{x}) \end{pmatrix}$$

Function NewtonSystem

Input:

Output:

Initializations:

1.
2. For $k =$

   Evaluate the residual vector:

   a.

   Evaluate the Jacobian:

   b.

   Solve the linear system:

   c.

   Update the solution:

   d.

   Check for convergence:

   e.

end for

First test problem:

$$f_1(x_1, x_2) = 2\exp(x_1 x_2) - 2x_1 + 2x_2 - 2 = 0$$
$$f_2(x_1, x_2) = x_1^5 + x_1 x_2^5 - 2x_2 = 0$$

with the exact solution $\mathbf{x}^* = (0,0)^t$. In matrix form:

$$J = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}$$

$$J =$$