MAE 306 Notes

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Fall 2025

Contents

Introduction

This document contains notes taken for the class MAE 306: Mathematics in Engineering II at Princeton University, taken in the Spring 2025 semester. These notes are primarily based on lectures by Professor Mikko Haataja. This class covers finite-difference, finite-element, and spectral methods for numerical solutions to the wave and heat equations. Since these notes were primarily taken live, they may contains typos or errors.

Chapter 1

Numerical Solving

An important application of numerical methods is the computation of solution sets of various kinds of equations. Here we cover methods that may be used for algebraic equations and linear equations.

1.1 Algebraic Equations

We first consider methods which may be used to solve algebraic equations; namely finding values of x such that

$$f(x) = 0$$

for an algebraic function f. An algebraic function is a polynomial with roots in a particular field (here, $\mathbb{R}$).

Example 1.1

Consider a sphere of radius R which falls through a fluid under the force of gravity. Suppose we wish to determine its terminal velocity. The drag force is given by

$$F_D = \frac{1}{2} C_D \rho V^2 \pi R^2$$

where C_D is the drag coefficient. C_D can be empirically approximated by

$$C_D = \left[0.63 + \frac{4.9}{\sqrt{\mathrm{Re}}} \right]^2$$

with Re denoting the Reynolds number, given by

$$\mathrm{Re} = \frac{\rho V R}{\eta(V)}$$

1.1.1 Successive Substitution

One method for finidng roots of algebraic equations is the method of **successive substitution**. To do this, we rewrite the equation $f(x) = 0$ as $x = g(x)$ for an appropriate function g. We can then pick a starting "guess" x_0 and consider the sequence $x_0 = x_0, x_{n+1} = g(x_n)$. For sufficiently nice g, this sequence should converge to a fixed point x^* of g, which is a root of f.

Example 1.2

Consider the function

$$f(x) = x^3 + 2x + 2 - 10\exp(-2x^2) = 0$$

We can rearrange this to the equivalent equation

$$x = \sqrt{-\frac{1}{2}\ln\left(\frac{x^3+2x+2}{10}\right)} = g(x)$$

We then make a starting guess and calculate $g(x), g(g(x)), g(g(g(x))), \ldots$.

To study its convergence, we can apply a taylor expansion to g around the root x^*, writing

$$x_{n+1} = g(x_n) = g(x^*) + g'(x^*)(x_n - x^*) + O((x_n - x^*)^2)$$

The order 1 approximation is given by

$$x_{n+1} \approx g(x^*) + g'(x^*)(x_n - x^*) = x^* + g'(x^*)(x_n - x^*)$$

Rearranging, we have

$$x_{n+1} - x^* \approx g'(x^*)(x_n - x^*)$$

Thus, we see that successive iterations have error ε_n which approximately scale geometrically with rate $|g'(x^*)|$. Thus the successive substitution method will converge to x^* when $g'(x^*) < 1$, but it diverges when $g'(x^*) > 1$.

We perform this analysis without resorting to order 1 approximations by adding and subtracting $g(x^*)$:

$$x_{n+1} = g(x_n) + g(x^*) - g(x^*)$$
$$\implies x_{n+1} - x^* = g(x_n) - g(x^*)$$

We write

$$g(x_n) = g(x^*) + \int_{x^*}^{x_n} g'(y)\,\mathrm{d}y$$

so

$$x_{n+1} - x^* = \int_{x^*}^{x_n} g'(y)\,\mathrm{d}y$$

This gives the bound

$$|x_{n+1} - x^*| \leq \int_{x^*}^{x_n} |g'(y)| \, \mathrm{d}y \leq |x_n - x^*| \sup_{y \in [x^*, x_n]} |g'(y)|$$

This implies that if $x_0 - x^* = \delta$ and $|g'(y)| < 1$ for all $y \in [x^* - \delta, x^* + \delta]$, the successive substitution method converges exponentially.

This gives us a convenient criterion for guaranteed exponential convergence of successive substitution; however, this criterion is not too useful in practice. This is not too surprising since the assumption that iterated evaluation leads to a fixed point is only really justified for contractions.

1.1.2 Newton-Raphson and Wegstein's Method

We can improve on successive substitution by using higher order terms in the Taylor expansion around x_n in order to interpolate more efficiently. If x_{n+1} is a fixed point, then

$$x_{n+1} = g(x_{n+1}) = g(x_n) + g'(x_n)(x_{n+1} - x_n) + O((x_{n+1} - x_n)^2)$$

Thus we define a new iterative algorithm which takes into account the linear term, defined by

$$x_{n+1} = \frac{g(x_n) - g'(x_n)x_n}{1 - g'(x_n)}$$

This is essentially Newton's method for root-finding. We can make a slight modification to this to avoid calculating derivatives, which gives the **secant method**, also known as **Wegstein's method**. To do this, we use the linear approximation of the derivative as

$$g'(x_n) \approx \frac{g(x_n) - g(x_{n-1})}{x_n - x_{n-1}}$$

which can be combined to give the rule

$$x_{n+1} = \frac{x_n g(x_{n-1}) - x_{n-1} g(x_n)}{x_n - g(x_n) - x_{n-1} + g(x_{n-1}))}$$

Note that in this case, two starting iterates are required. The second iterate could be calculated simply using successive substitution as $g(x_0)$, if desired.

We observe that due to the $1 - g'(x_n)$ term in the denominator, the Newton-Raphson method has convergence issues when g' is close to 1. This is intuitively explained by the fact that g is near linear with slope 1, and we are trying to calculate its intersection with $y = x$, so this becomes very difficult. While computation of derivatives for Newton-Raphson is computationally expensive, it does allow quadratic convergence.

1.1.3 Convergence Analysis of Iterated Schemes

In this section we quantify orders of convergence for iterative approximation schemes.

Suppose that $\{x_n\}$ is a sequence of points generated by some iterative approximation method, and x^* is the target value. Then we define:

$$\begin{cases} \varepsilon_n = x_n - x^* \\ p_n = -\ln|\varepsilon_n| \end{cases}$$

If $x_n \to x^*$, then $p_n \to \infty$. We then define the **order of convergence** by

$$\rho = \lim \frac{p_{n+1}}{p_n}$$

when the limit exists. If $\rho = 1$ then we say the error decreases "linearly". For $\rho = 2$ ("quadratic convergence") it is even stronger. (Compare this to order of growth for entire functions). Note that geometric decay has order one convergence.

We can now demonstrate what it means to say that Newton-Raphson converges quadratically. In its general form, Newton-Raphson can be written to find a root of a function f using the iteration

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

Then

$$\begin{aligned} \varepsilon_{n+1} = x_{n+1} - x^* = x_n - x^* - \frac{f(x_n)}{f'(x_n)} &= \varepsilon_n - \frac{f(x_n)}{f'(x_n)} \\ \implies f'(x_n)\varepsilon_{n+1} &= f'(x_n)\varepsilon_n - f(x_n) \qquad (*) \end{aligned}$$

Taylor series expanding f around x^*, we have

$$\begin{aligned} f(x_n) &= \underbrace{f(x^*)}_{=0} + f'(x^*)(x_n - x^*) + \frac{1}{2}f''(x^*)(x_n - x^*)^2 + O((x_n - x^*)^3) \\ &= f'(x^*)\varepsilon_n + \frac{1}{2}f''(x^*)\varepsilon_n^2 + O(\varepsilon_n^3) \qquad (1) \end{aligned}$$

We similarly expand f' as

$$\begin{aligned} f'(x_n) &= f'(x^*) + f''(x^*)(x_n - x^*) + \frac{1}{2}f'''(x^*)(x_n - x^*)^2 + O((x_n - x^*)^3) \\ &= f'(x^*) + f''(x^*)\varepsilon_n + O(\varepsilon_n^2) \qquad (2) \end{aligned}$$

Notice that we approximated f and f' to different orders; this is because we care about the quantity $\varepsilon_n f' - f$.

Substituting (1) and (2) into $(*)$ and cancelling terms, we have

$$[f'(x^*) + f''(x^*)\varepsilon_n + O(\varepsilon_n^2)]\varepsilon_{n+1} = \frac{1}{2}f''(x^*)\varepsilon_n^2 + O(\varepsilon_n^3)$$

Thus

$$\varepsilon_{n+1} = \frac{\frac{1}{2}f''(x^*)\varepsilon_n^2 + O(\varepsilon_n^3)}{f'(x^*) + f''(x^*)\varepsilon_n + O(\varepsilon_n^2)}$$

If the Newton-Raphson method converges, then $\varepsilon \to 0$. Thus we discard the ε_n terms in the denominator (here we see that we need $f'(x^*) \neq 0$) to approximate this for large n as

$$\varepsilon_{n+1} \approx \frac{f''(x^*)\varepsilon_n^2}{f'(x^*)} = C\varepsilon_n^2$$

Taking logarithms, we see that the convergence is quadratic.

Note that the secant method has order of convergence somewhat slower than Newton-Raphson, which is ϕ.

Definitions