Computational Notes

Closed root finding (week 2/3)

- Closed root finding methods find a root within a closed interval bound by two points and will always converge to a solution if the roots are within the chosen interval
- Bisection (bracketing) method:
    - Choose lower and upper guesses, estimate the root in between
    - Check whether root is greater or lower than guess and change boundaries until root is found
    - Error can be calculated from old and new root and code ends once an acceptable error is achieved
- False position
    - Creates two triangles and estimates the root from common point of triangles, change boundaries from root estimation
    - Generally converges on root much faster than bisection
    - Can be slower to converge depending on the shape of the function, can be modified to half the function after getting stuck at a certain number of steps
- Incremental search
    - Chooses a point at either end of interval and evaluate at increments in one direction until a root within the required error tolerance is found
    - If roots are too close, a large step can miss the groups of root

Open Root Finding (week 2/3)

- Open root finding only requires one initial starting point and may not converge to a root but if they do, they are far more efficient than closed methods
- Fixed Point Iteration
    - Rearranges the equation and iterates new estimates of x until the difference between successive estimates is less than a defined error
- Newton Raphson
    - Calculates a new root from the current root subtracted by function and derivative of function at that root by visually projecting a line to the x axis
    - Cannot solve asymptotic functions, multiple minima, periodic functions
    - Error directly calculated from the function at the root
- Secant/False position
    - Similar to newton but approximates the derivative instead
    - False position sets the right bound of the line as the new root estimate while secant cuts the curve directly above with the new estimate
    - False position guaranteed to find the root
- Muller's technique
    - Similar to secant but projects a parabola instead of a line to the x axis

Roots of system of equations (week 3)

- The system of equations can be rewritten in the Taylor series expansion and rearranged, with the partial derivatives in the series calculated using Newton Raphson

Polynomial Division (week 3)

- Polynomial division can be performed by using a nested polynomial to reduce multiplications and additions performed

Regression (week 4)

- Polynomials can fit data better than a linear approach by setting the sum of residuals as a polynomial, setting the derivatives equal to zero and rearranging for unknown coefficients
- Nonlinear models can used to fit data in different cases such as an exponential function, with the coefficients found using optimisation methods

Interpolation (week 4)

- Intermediate values can be estimated between data points with different orders of interpolation, although more estimation points are required for higher orders
- Spline interpolation fits low degree polynomials to subsets of the values and avoids oscillatory behaviour from fitting a single high order polynomial instead

Linear Algebra (week 5)

- Cramer's rule (matrix determinant) can be used to solve systems of linear equations
    - It always finds a solution where it exists is not efficient to solve systems with more than three equations
- Gauss Elimination uses forward elimination to find an upper triangular matrix of coefficients, then back substitutes to find solutions
    - It requires a high number of operations, crashes on divisions of zero and accumulates inaccuracies due to round-off error
- Ill conditioned systems, where small changes in coefficients induce large changes in solution are not suited to elimination methods because of round-off error
    - Issues can be solved by using more sig figures to reduce round-off error and partial or full pivoting which is swapping rows with near zero coefficients with another row

Ordinary Differential Equations (week 6)

- The derivative of a function can be approximated linearly or by rearranging the Taylor series
    - The Taylor series is written with a truncation error that cannot be determined but can be controlled for different orders
- The Euler method computes a new value of y by extrapolating linearly over the step using a slope approximated with the derivative in the original point, where the solution and derivatives are known
    - The error can be decreased by using smaller steps
- Runge-Kutta methods achieve high accuracy without using higher order derivatives by choosing an order and working out coefficients in the Taylor series expansion
    - All orders will have one more unknown than an equation, with one of the coefficients needing to be specified and allowing an infinite number of Runge-Kutta methods for each order
    - The most popular Runge-Kutta method is the fourth order version

Systems of ODEs (week 7)

- A system of ODEs with initial conditions can be solved using the Euler method or python libraries

- Differential equations can be said to be stable if the product of the step and equation is within a region on the complex plane
    - When solved with a larger step, the numeric solution diverges from the exact solution and is unstable
- Stiff ODEs have fast (small steps) and slow components (solve equation over a large interval) and require a small step over the entire solution interval
    - Implicit methods use information at locations not computed yet and can be used to solve stiff ODEs for large steps without diverging
    - The implicit Euler method can be used, which uses the derivative of the next point to estimate the slope, with the next point appearing on both sides of the formula

Numerical Integration (week 9)

- Integration can be performed numerically with quadrature techniques (evaluating the area under the curve) or adaptive techniques, with quadrature techniques work well depending on the shape of the function
- The midpoint rule estimates the area under the curve as a rectangle from the middle point, while the trapezoidal rule estimates a trapezoid between two points
- Simpson's Third Rule estimates a quadratic with three points and can give exact answers for a third order integral
    - Simpson's Three Eight's Rule is a more sophisticated interpolates a cubic with arbitrary coefficients along four points on the function
- Adaptive Algorithms subdivide intervals during the numerical integration if sufficient accuracy is not achieved after a certain number of steps and can be applied dynamically to any of the quadrature techniques
    - Simpson's Rule can be adapted to allow an adjustment of step size when the error of the developing solution is greater than a pre-set value

Optimisation (week 10/11)

- The optimal point of a function is where the gradient is flat, usually occurring at a maximum or minimum point
    - If the number of inequality and equality constraints is greater than the degrees of dimensions for the x vector, the optimisation is over constrained
- One dimensional optimisation searches for the a point on a curve in a plane
- The golden search technique is a basic one dimensional unconstrained search
    - Two estimate points are taken around a maximum or minimum, and the search domain is narrowed with a new estimate point found using the golden ratio
    - Convergence is guaranteed though the rate of convergence is finite, and the approximation error can be estimated
- Parabolic interpolation
    - Any three points are joined on a plane, with one of the new estimate points chosen from the maximum or minimum estimated from the parabola
- Newton's method
    - A new root is calculated from the current root subtracted by the derivative over the second derivative of the function
- Two-dimensional optimisation requires the second derivative of the function with respect to both dimensions alongside the first and second derivatives to either dimension

    - Newton’s method can be applied again using the determinant of the hessian matrix as a test point for the maximum or minimum
- Unconstrained multivariant optimisation involves the solution of a surface function for a maximum or minimum value
- Gradient methods are the equivalent to finding the shortest route to a peak
    - The curve of travel in any direction on the surface point can be expressed by the optimisation path function, with the derivative of this function equal to 0 at the peak of travel
    - The next points on the surface can be expressed by general step functions
- The Lagrange multiplier incorporates the constraint function into the objective function to solve it more efficiently
    - The optimum point is found when the components of the main objective are differentiated and solved for zero

Formulas

$$\varepsilon_a = \left| \frac{x_r^{\text{new}} - x_r^{\text{old}}}{x_r^{\text{new}}} \right| 100\%$$