1 Numerical solutions of non-linear equations of one variable

1.1 Bisection Method

Theorem 1. *Intermediate Value Theorem*
Let $f : [a, b] \to \mathbb{R}$ be a continuous function. Let c be between $f(a)$ and $f(b)$. Then there exists $x \in (a, b)$ such that $f(x) = c$.

Algorithm 1. *Bisection Method*
1. Find a_0, b_0 such that $f(a_0)f(b_0) < 0$.
2. $k = 0$.
3. $x_k = \frac{a_k+b_k}{2}$
4. If $f(x_k) = 0$ then stop and return x_k
5. If $f(x_k)f(a_k) > 0$ then $a_{k+1} = x_k$ and $b_{k+1} = b_k$
else $b_{k+1} = x_k$ and $a_{k+1} = b_k$
6. If $|b_k - a_k| < \epsilon$ then stop and return x_k
else $k \leftarrow k + 1$ and goto 3

Theorem 2. *Convergence of the Bisection Method*
1. $f : [a, b] \to \mathbb{R}$
2. f is continuous (ie.$f \in \mathcal{C}$).
3. $a_0, b_0 \in [a, b]$ and we select a_k, b_k, x_k for $k \geq 0$ according to the above algorithm.
Then
1. $\lim_{k\to\infty} x_k = \lim_{k\to\infty} a_k = \lim_{k\to\infty} b_k = z \in [a, b]$ is a root of f.
2. $|x_k - z| \leq \frac{1}{2}|b_k - a_k| = \left(\frac{1}{2}\right)^{k+1} |b_0 - a_0|$

Example 1. *Consider real roots of $x^5 - x - 1 = 0$*
1.Find an interval that contains real roots.
2.Find the no of iterations needed to find a root to an accuracy of 0.001.
3.Do the iterations and find a root.

Casio 1. *Bisection Method*
ALPHA X ALPHA = (ALPHA A + ALPHA B) ÷ 2 ALPHA : ALPHA X ˆ 5 - ALPHA X - 1 CALC

Mathematica 1. *Bisection Method*

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In[3]:= f[x_] := x^5 - x - 1; a = 1; b = 2; k = 0;
        While[Abs[b - a] >= 0.0001, {x = (a + b) / 2, Print[{k, N[{a, b, x}, 15], N[f[x]]}], If[
           f[x] f[b] > 0, b = x, a = x], k++}]
```

1.2 Fixed Point(Iterative) Method

Definition 1. *Contraction*
Let $g : [a, b] \to \mathbb{R}$*. Iff for all* $\epsilon > 0$ *there exists* $0 < L < 1$ *for all* $x, y \in [a, b]$ *such that* $|g(x) - g(y)| \leq L|x - y|$*, then* g *is called a contraction.*

Note 1. *on continuity*
1. In general if there exixts any $0 < L$ *we say that* g *is Lipschitz continuous, L is called the Lipschitz constant*
2. Lipschitz continuous $\Rightarrow$ *Uniformly continuous* $\Rightarrow$ *Continuous*
3. Uniformly continuous means that δ *is independent of the point*
$\forall \epsilon > 0 \exists \delta > 0 \forall x, y; |x - y| < \delta \Rightarrow |f(x) - f(y)| < \epsilon$
4. If g *is differentiable (ie.*$g \in \mathcal{D}$*) and* $|g'(x)| \leq L$ *then* L *is a Lipschitz constant(by the Mean Value Theorem).*
5. Mean Value Theorem: Let f *be continous on* $[a, b]$ *and differentiable on* (a, b)*. Then there exists* $\zeta \in (a, b)$ *such that* $\frac{f(b)-f(a)}{b-a} = f'(\zeta)$*. Note that the requirements are achieved if we have* f *differentiable on a larger open inerval, ie on* $(a, d) \subset [a, b]$
6. If g' *is continuous (ie.*$g' \in \mathcal{C}$ *or* $g \in \mathcal{C}^1$*) on a closed interval, then* g *is Lipschitz continuous with* $L = \max\{|g'(x)|\}$*(by the Extremum Value Theorem)*
7. Extremum Value Theorem: Let f *be continuous on* $[a, b]$*. Then* f *attains its maximum and minimum on* $[a, b]$*, ie. there exists* $c, d \in [a, b]$ *such that* $f(c) = \max\{f(x)|x \in [a, b]\}$ *and* $f(d) = \min\{f(x)|x \in [a, b]\}$
8. Points x *such that* $x = g(x)$ *are called fixed points of* g*.*

Definition 2. *Cauchy Sequence*
Let u *be a sequence. Iff for all* $\epsilon > 0$ *there exists* $N > 0$ *for all* $n, m > 0$ *such that* $m, n > N$ *implies* $|u(m) - u(n)| < \epsilon$*, then* u *is called Cauchy.*

Note 2. *on sequences*
1. Spaces with a distance measuring function(metric) is called a matric space. Cauchy sequence u *must be defined on such spaces* A*, i.e* $u : \mathbb{N} \to A$*.*
2. Matric is a function $d : A \times A \to \mathbb{R}$ *satisfying the following properties for* $x, y, z \in A$
$d(x, y) \geq 0$
$d(x, y) = 0$ *iff* $x = y$
$d(x, y) = d(y, x)$
$d(x, y) \leq d(x, z) + d(z, y)$
3. In $A = \mathbb{R}$ *we can use the absolute value of* $x - y$ *as* $d(x, y)$*. In* $A = \mathbb{C}$ *we can use complex modulus as* $d(x, y)$*(see Note 3).*
4. In matric space we can define a ball $B(x, r) = \{y|d(x, y) < r\}$ *with center* x *and radius* r*.*
5. Limit points $\lim A$ *of a set* A *are those points such that balls with them as center will contain a point in* A *other than that point itself.*
ie. $x \in \lim A \Leftrightarrow \forall r > 0 \exists p \in A; p \in B(x, r)$ *and* $p \neq x$
6. A set is Closed iff it contains all its limit points(ie.$\lim A \subset A$*).*
7. A set is Open iff it's complement is closed.

8. A Neighbourhood of x is an open set containing x.
9. A Cover is a collection of open sets whose union is a superset of(ie. covers) the given set.
10. If every cover of a set has a finite sub cover(a subset of the cover with finite number of elements that is also a cover), such sets are called Compact.
11. In $\mathbb{R}^n$, a set is compact iff it is closed(Haine-Borel Theorem).
12. Therefore in $\mathbb{R}^n$, continuous functions on closed intervals are uniformly continuous.
13. If each Cauchy sequences on a set A is converging to a point in A, such sets are called Complete.
14. All converging sequences are Cauchy.
15. $\mathbb{R}^n$ is complete.
16. A closed subset of a complete space is complete.
17. A complete space is closed.

Theorem 3. *Global Convergence of the Fixed Point method(Banach Fixed Point Theorem)*
1.$g : [a, b] \to [a, b]$
2.g is a contraction with Lipschitz constant L
3.$x_0 \in [a, b]$ and $x_{k+1} = g(x_k), k \geq 0$
Then
1.$\lim_{k\to\infty} x_k = z \in [a, b]$ is a unique fixed point of g
2.$|x_k - z| \leq \frac{L^k}{1-L}|x_1 - x_0|$

Theorem 4. *Local convergence of the Fixed Point method*
Let $z = g(z)$ be a fixed point. If $g \in \mathcal{C}^1$ with $|g'(z)| < 1$, then there exists a neighbourhood of z such that the fixed point method is converging.

Algorithm 2. *Fixed Point Method*
1. Select x_0
2. $k = 0$.
3. $x_{k+1} = g(x_k)$
5. If $|x_{k+1} - x_k| < \epsilon$ then stop and return x_k else goto 3

Example 2. *Consider real roots of $x^5 - x - 1 = 0$*
1.Write $x^5 - x - 1 = 0$ as $x = g(x)$ to be solved by the fixed point method, is the method converging?
2.Find the no of iterations needed to find that root to an accuracy of 0.001.
3.Do the iterations and find the root.

Casio 2. *Fixed Point Method*
ALPHA X ALPHA = (1 + ALPHA X)ˆ (1 ÷ 5) CALC =

Mathematica 2. *Fixed Point Method*

```
In[1]:= g[x_] := (1 + x) ^ (1 / 5); x = 10; k = 0;
        While[k < 20, {Print[{k, N[x, 20], N[x - g[x]]}], x = N[g[x], 100], k++}]
```

Note 3. *See the note AllRoots.pdf on finding the complex roots of* $x^5 - x - 1 = 0$ *using the Fixed Point method.*

1.3 Newton's Method

Definition 3. *Newton's method for finding roots of* $f(x) = 0$
$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$

Theorem 5. *Local convergence of the Newton's method(taking it as an Fixed Point method).*
Let z *be a root of* f*. If* $f \in \mathcal{C}^2, f'(z) \neq 0$ *and* $|f(z)f''(z)| < (f'(z))^2$ *then there exists a neighbourhood of* z *such that the Newton's method is converging.*

Theorem 6. *Let* $f, g \in \mathcal{C}$ *and* g *does not change sign. Then there exist* $\zeta \in (a, b)$ *such that* $\int_a^b f(x)g(x)dx = f(\zeta) \int_a^b g(x)dx$

Theorem 7. *Taylor series of* f *at* a
$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + R_n(x, a)$
Taylor Polynomial, $T_n(x, a) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k$
Remainder $R_n(x, a) = \frac{1}{n!}\int_a^x f^{(n+1)}(t)(x-t)^n dt$ *where* $f \in \mathcal{C}^{n+1}$
Remainder $R_n(x, a) = \frac{f^{(n+1)}(\zeta)}{(n+1)!}(x-a)^{n+1}$ *where* $f \in \mathcal{D}^{n+1}$ *and* ζ *between* x *and* a

Example 3. *Consider the function* $f(x) = x^{1/10}$
1. Write down the nth degree Taylor Polynomial near $c > 0$.
2. Show that the remainder satisfies $|R_n(x, c)| < \begin{cases} \frac{x^{1/10}}{10(n+1)}\left(\frac{x-c}{c}\right)^{n+1} & x > c > 0 \\ \frac{c^{1/10}}{10(n+1)}\left(\frac{c-x}{c}\right)^{n+1} & c > x > 0 \end{cases}$
3.Show that the value of $1000^{1/10}$ *accurate to 3 decimal places is 1.995.*
4.Find the value of $1025^{1/10}$ *accurate to 10 decimal places.*

Example 4. *Let* $T_n(x) = \sum_{k=1}^{n} \frac{(-x)^k}{k!}$ *be the n th degree Taylor polynomial of* e^{-x} *at* $x = 0$ *and* $\lim_{x\to\infty} T_n(x) = e^{-x}$*. Solve* $x = T_2(x)$ *and find an approximate solution to* $x = e^{-x}$*. Also find a n for which the difference in the solutions to* $x = T_n(x)$ *and* $x = e^{-x}$ *is less than 0.001. Assume that one real solution to* $x = T_n(x)$ *remain in* $[0.5, 0.6]$ *for all* $n \geq 2$.

Theorem 8. *Global convergence of the Newton's method(Newton-Kantorovich Theorem, see Proofs.pdf for the proof)*
1. $f : [a, b] \to \mathbb{R}$
2. $f' \neq 0$ *and there exists* $\beta > 0$ *such that* $\frac{1}{|f'(x)|} \leq \beta$
3. f' *is Lipschitz continuous with constant* γ
4. $x_0 \in [a, b]$ *and* $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}, k \geq 0$
5. $\left|\frac{f(x_0)}{f'(x_0)}\right| = \alpha$
6. $q = \alpha\beta\gamma < \frac{1}{2}$
7. $[x_0 - 2\alpha, x_0 + 2\alpha] \subset [a, b]$
Then
1. $\lim_{k\to\infty} x_k = z \in [x_0 - 2\alpha, x_0 + 2\alpha]$ *is a unique root of* f
2. $|x_k - z| \leq 2\alpha q^{2^k - 1}$

Theorem 9. *Local convergence of the Newton's Method*
Let z be a root of f. If $f \in \mathcal{C}^2$ and $f'(z) \neq 0$ then there exists a neighbourhood of z where the Newton's method is converging.

Note 4. *See that now we don't need $|f(z)f''(z)| < (f'(z))^2$ which was a requirement for local convergence when we analyzed the Newton's method as an Fixed Point method.*

Example 5. *Consider the Newton's method of finding the real roots of $x^5 - x - 1 = 0$*
1. Treat the method as an fixed point method and find the no of iterations needed to calculate the root to an accuracy of 0.001 and find the root.
2. Use the error formula above for the Newton's method and find the no of iterations needed to calculate the root to an accuracy of 0.001 and find the root.
3.Use more terms in the Taylor series(instead of 2 terms used in the Newton's method) and propose a possibly faster method to find the root.
4. If f was not differentiable, propose a method which uses the secant(instead of the tangent) joining two successive points.
5. Try to find complex roots using the Newton's method(see Note 3).

Example 6.
1. Do Example 5 for $\sin x = 2x$ and $x = e^{-x}$
2. Try to solve $x^m = 0$ for $m \in \mathbb{R}$. What is going wrong/right?.
3. Show that the sequence $x_{k+1} = \frac{x_k}{2} + \frac{a}{2x_k}$ converges to $\sqrt{a}$, provided we select x_0 on a suitable range. What is such a range?
4. Suppose we want to solve $tan^{-1}x = 0$ by the Newton's method. Find the value z such that the Newton's method is converging for $0 < x_0 < z$, diverging for $x_0 > z$ and enters into a cycle for $x_0 = z$.
5. Your CASIO calculator can integrate, $\int_a^b f(x)dx$ is evaluated as $\int(f(x), a, b)$. Find the z value for which $P(x < z) = 0.8$ when $X \sim N(0,1)$, ie when X is Normally distributed with mean 0 and standard deviation 1 which is having a PDF $p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$.
6. Find the height of the circular sector with arc length $2x$ and chord length x.
7. What is the height if the shape is a parabola?

Example 7. *An fixed point method of finding solutions to a non-linear equation $f(x) = 0$ is said to have a convergence of order p iff $|x_{k+1} - z| \leq r|x_k - z|^p$ where x_k is the kth iteration, z is the solution and r is a constant. Show that $p = 1$ for the fixed point method and $p = 2$ for the Newtons method.*

Casio 3. *Solving cubic $x^3 + 2x^2 + 3x + 4 = 0$ with roots x_1, x_2, x_3*
MODE 5:EQN 4:$ax^3 + bx^2 + cx + d$ $1 = 2 = 3 = 4 == x1 = x2 = x3$

Mathematica 3.
$NRoots[x^5 - x - 1 == 0, x]$
$NSolve[f[x] == 0, x]$
$FindRoot[f[x] == 0, \{x, x0\}]$

2 Numerical Integration

2.1 Trapezoidal Rule

Theorem 10. *Trapezoidal Rule*
$f \in \mathcal{C}^2[a,b], h = \frac{b-a}{n}, x_0 = a, x_n = b, x_k = x_0 + kh, 0 \le k \le n, \zeta \in (a,b)$
$\int_a^b f(x)dx = \frac{h}{2}\left[f(x_0) + 2\sum_{k=1}^{n-1} f(x_k) + f(x_n)\right] - \frac{(b-a)^3}{12n^2} f''(\zeta)$

Example 8. *For each of the following integrals, use the Trapezoidal rule to find the number of divisions needed to find its value accurate to 0.001 and find the integral to that accuracy.*
1. $\int_0^1 e^{-\frac{x^2}{2}}dx$ 2. $\int_0^1 \sin(x^2)dx$ 3. $\int_0^{\frac{\pi}{2}} \sqrt{2-\cos^2 x}dx$ 4. $\int_2^{10} \frac{x}{\log x}dx$

2.2 Simpson's Rule

Theorem 11. *Simpson's Rule(see Proofs.pdf for the proof for the error)*
$f \in \mathcal{C}^4[a,b], n$ *is even*, $h = \frac{b-a}{n}, x_0 = a, x_n = b, x_k = x_0 + kh, 0 \le k \le n, \zeta \in (a,b)$
$\int_a^b f(x)dx = \frac{h}{3}\left[f(x_0) + 4\sum_{\substack{k=1 \\ kodd}}^{n-1} f(x_k) + 2\sum_{\substack{k=2 \\ keven}}^{n-2} f(x_k) + f(x_n)\right] - \frac{(b-a)^5}{180n^4} f^{(4)}(\zeta)$

Example 9.
1. Do the same thing in Example 8 using the Simpson's rule.
2. Show directly that cubic polynomials are integrated exactly by the Simpson's rule.
3. Derive a numerical integration rule and its error that uses the function value at the mid point (Mid Point Rule), left end point, right end point of each interval.
4. Use Mid Point Rule rule to do the same question in Example 5.
5. Use integration by parts to prove the error formula for the Trapezoidal rule.
6. Use the remainder in the Lagrange Polynomial(see 3.1) to derive the error formula for the Trapezoidal rule.
7. Use Taylor series to derive approximate formulas for the remainder in both Trapezoidal and Simpson's rule.
8. Use a variant of the Lagrange Polynomial remainder(see Proofs.pdf) to derive the error formula for the Simpson's rule.

Example 10. *One method of doing numerical integration is Gaussian Quadrature. Note that both the Trapezoidal and the Simpsons rules looks like* $\int_a^b f(x)dx \approx \sum_k w_k f(x_k)$ *and we knew* x_k *and found* w_k*. In this method we find both* x_k *and* w_k *so that the integral and the sum are equal for a given n degree polynomial* $p(x)$ *, by forcing both sides equal for each power of* x^j *for* $j = 0, 1, 2, , n$*. What is the degree of the polynomial we need to use if we want 3 points? Find them for* $[a,b] = [-1,1]$ *and use it to approximate* $\int_{-1}^1 e^{-\frac{x^2}{2}}dx$*.*
Casio fx-991ES uses a variant of this method.

Casio 4. $\int(f(X), a, b, m)$ *and the default variable is X and* $n = 2^m$ *for the Simpson's method in model fx-991MS*

Mathematica 4. $NIntegrate[f(x), \{x, a, b\}, Method->TrapezoidalRule]$

3 Interpolation

3.1 Interpolating Polynomial

Theorem 12. *Lagrange Method of finding the Interpolating Polynomial* $p(x)$ *of* $f(x)$ *for the points* $x_k, 0 \le k \le n$
$w_j(x) = \prod_{\substack{i=0\\i\neq j}}^{n}(x - x_i)$
$w(x) = \prod_{i=0}^{n}(x - x_i)$
$\ell_j(x) = \frac{w_j(x)}{w_j(x_j)} = \prod_{\substack{i=0\\i\neq j}}^{n}\left(\frac{x-x_i}{x_j-x_i}\right) = \frac{w(x)}{(x-x_j)w'(x_j)}$ *and* $\ell_j(x_k) = 0$ *if* $j \neq k$ *and 1 if* $j = k$.
$p(x) = \sum_{k=0}^{n} f(x_k)\ell_k(x)$ *and* $p(x_j) = f(x_j), 0 \le j \le n$
$f(x) = p(x) + \frac{f^{(n+1)}(\zeta)}{(n+1)!}w(x)$ *with* $\zeta \in (x_0, x_n)$ *when* $f \in \mathcal{C}^{(n+1)}$

Example 11. *Consider the data set* $\{(2,1),(3,2),(4,3),(6,4)\}$
1. Find the Interpolating polynomial directly by matrix inversion
2. Use the Lagrange Method to find the Interpolating Polynomial
3. Assume that the data set is generated by the function $f(x) = 4\sin^2(\frac{\pi x}{12})$. *Find an upper bound for the error.*
4. Use a suitable numerical method to find the maximum of $w(x) = (x-2)(x-3)(x-4)(x-6)$ *on* $[2,6]$ *and redo the calculation in 3.*
6. For the same function on $[0,6]$, *find the number of points required to make the error* ≤ 0.001 *and find the Interpolating Polynomial.*

Example 12.
1. Consider the data set $\{(1,1),(2,1),(3,2),(4,3)\}$. *Find the Lagrange polynomial. Assume that the above data are obtained from the Fibonacci sequence with* $F(n) = \frac{1}{\sqrt{5}}(\phi^n - \psi^n)$ *where* $\phi > 0$ *and* $\psi < 0$ *are the roots of* $y^2 - y - 1 = 0$.
If the continuous version is $f(x) = \Re F(x) = \frac{1}{\sqrt{5}}(\phi^x - (-\psi)^x \cos\pi x)$, *find the maximum error.*
2. One method of finding the Interpolating polynomial is to use the Newtons divided differences. For x_0, x_1, x_2 *we define* $f[x_0,x_1] = \frac{f(x_1)-f(x_0)}{x_1-x_0}$ *and* $f[x_0,x_1,x_2] = \frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$ *and so on and the Lagrange polynomial is given by* $p(x) = f(x_0) + f[x_0,x_1](x-x_0) + f[x_0,x_1,x_2](x-x_0)(x-x_1)$. *See why the formula is working and use it to find the Lagrange polynomial for* $\{(1,1),(2,1),(3,2),(5,5)\}$.
3. Yet another way of finding the Lagrange polynomial is to define it as the iterative process $p(x) = A_1 + P_1(x)(x-x_0)$ *and* $P_1(x) = A_2 + P_2(x)(x-x_1)$ *and so on. Use this to find the find the Lagrange polynomial for* $\{(1,1),(2,1),(3,2),(5,5)\}$. *Mathematica seems to use this method.*
4. Consider the data set $\{(1,1),(2,1),(3,2)\}$. *Find a polynomial (Hermite polynomial) that goes though the above points and satisfying* $p'(1) = 0, p'(2) = 1, p'(3) = 0$.
5.For the data set $\{(x_k,y_k)\}, k = 0,1,,n$ *a natural cubic spline is a twice differentiable piecewise cubic polynomial* $p(x)$ *which satisfies* $p(x_k) = y_k$ *with* $p''(x_0) = p''(x_n) = 0$. *Let* $p(x) = \sum_{k=0}^{n-1} p_k(x)$ *where* $p_k(x)$ *is the part of* $p(x)$ *on* $[x_k, x_{k+1}]$ *which is 0 elsewhere. Assume that* $p_k(x) = a_k(x-x_k)^3 + b_k(x-x_k)^2 + c_k(x-x_k) + d_k$ *and that* $x_{k+1} - x_k = h$ *is a constant. With* $s_k = p''(x_k)$ *derive the formula* $s_{k+2} + 4s_{k+1} + s_k = \frac{6}{h^2}h^2(y_{k+2} - 2y_{k+1} + y_k), k = 0,1,,n-2$.

Also write the system of equations in matrix form that must be solved find s_k for $k = 1, , n-1$. Get the value of USD w.r.t. LKR for the 1st day of every month this year and predict the value for the 1st February next year using natural cubic splines (just show the data set, the calculated s_k values and the final answer).

Mathematica 5. $InterpolatingPolynomial[\{\{2,1\},\{3,2\},\{4,3\},\{6,4\}\},x]$

3.2 Least Square Polynomial

Theorem 13. *Least Square Line $y = ax + b$ for the points $(x_k, y_k), 1 \le k \le n$ That minimizes $E(a,b) = \sum_{k=1}^{n}(ax_k + b - y_k)^2$ is given by*

$$\begin{pmatrix} \sum_{k=1}^{n} x_k^2 & \sum_{k=1}^{n} x_k \\ \sum_{k=1}^{n} x_k & \sum 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^{n} x_k y_k \\ \sum_{k=1}^{n} y_k \end{pmatrix}$$

This can also be written as $X^T X \begin{pmatrix} a \\ b \end{pmatrix} = X^T Y$ where

$$X^T = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{pmatrix} \text{ and } Y^T = \begin{pmatrix} y_1 & y_2 & \cdots & y_n \end{pmatrix}$$

Theorem 14. *Properties of the Least Square Line*
With $\overline{x} = \frac{1}{n}\sum_{k=1}^{n} x_k$, $\overline{y} = \frac{1}{n}\sum_{k=1}^{n} y_k$, $s_{xx} = \frac{1}{n}\sum_{k=1}^{n}(x_k - \overline{x})^2 = \frac{1}{n}\sum_{k=1}^{n} x_k^2 - \overline{x}^2$, and $s_{xy} = \frac{1}{n}\sum_{k=1}^{n}(x_k - \overline{x})(y_k - \overline{y}) = \frac{1}{n}\sum_{k=1}^{n} x_k y_k - \overline{x}\,\overline{y}$
We have $a = \frac{s_{xy}}{s_{xx}}$
Also $(\overline{x}, \overline{y})$ is on the Least square line and therefore $\overline{y} = a\overline{x} + b$ or $b = a\overline{x} - \overline{y}$
If $HE = \begin{pmatrix} E_{aa} & E_{ab} \\ E_{ba} & E_{bb} \end{pmatrix}$ is the Hessian of $E(a,b)$ we have $HE = 2X^T X$ and
$\det HE = E_{aa}E_{bb} - (E_{ab})^2 = 4n^2 s_{xx} > 0$ *when x_k are different and*
$\mathrm{tr}HE = E_{aa} + E_{bb} = 2\sum x_k^2 + 2n > 0$ *so (a,b) is a global minimum.*

Example 13. *Let $A = \{(2,1),(3,2),(4,3),(6,4)\}$*
1. Find the Lest Square Line for A.
2. Show that the Correlation Coefficient given by $r = \frac{s_{xy}}{\sqrt{s_{xx}s_{yy}}}$ is a measure of the linearity of data.
3. Show that the least square parabola $y = ax^2 + bx + c$ for the data set $(x_k, y_k), k = 1, 2, \cdots, n$ is given by

$$\begin{pmatrix} \sum x_k^4 & \sum x_k^3 & \sum x_k^2 \\ \sum x_k^3 & \sum x_k^2 & \sum x_k \\ \sum x_k^2 & \sum x_k & \sum 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} \sum x_k^2 y_k \\ \sum x_k y_k \\ \sum y_k \end{pmatrix}$$

4. Find the Least Square Parabola for A
5. Fit a least square function of the form $y = ae^x + b\sin x + c\cos x$ for A.

Casio 5. *CASIO fx-991ES*
MODE 3:STAT 3:_ $+ cx^2$ 2 = 3 = 4 = 6 = REPLAY UP 1 = 2 = 3 = 4 = SHIFT STAT(1) 1:Type, 2: Data, 3:Edit, 4:Sum(1:$\sum x^2$, 2:$\sum x$, 4:$\sum y$, 5:$\sum xy$, 6:$\sum x^3$, 7:$\sum x^2 y$, 8:$\sum x^4$), 7:Reg(1:A, 2:B, 3:C)

Mathematica 6. $Fit[\{\{2,1\},\{3,2\},\{4,3\},\{6,4\}\},\{x^2,x,1\},x]$

Methods discussed in class

Solving non-linear equations: Bisection, Fixed Point, Newton's
Numerical Integration: Trapezoidal, Simpson's, Gaussian Quadrature(Quiz 3)
Interpolation: Lagrange, Least Square, Cubic Spline(Quiz 2)

Methods discussed at tutorials

Solving non-linear equations: Secant method
Numerical Integration: Mid point method, Romberg Integration
Interpolation: Newton's divided differences, Product method used by Mathematica, Richardson Interpolation
Optimization: Golden section search, Steepest descent method
Solving ODE: Euler's method
Solving systems of linear equations: Least Square, Jacobi method, Gauss-Seidel method

Methods tested for exam

Solving non-linear equations: Bisection, Fixed Point, Newton's
Numerical Integration: Trapezoidal, Simpson's
Interpolation: Lagrange, Least Square