# Important Numerical Programs

Ajit Rajwade

Refer: Sections 5.7, 7.7, 8.3, 8.4 of the book by Abhiram Ranade

# Numerical Programs Covered Here

1. Least squares line fitting
2. GCD computation given two positive integers
3. Bisection method for finding the roots of an equation
4. Newton-Raphson method for finding the roots of an equation

# Least Squares Line Fitting

Ajit Rajwade

# 1. Least squares line fitting

- Suppose you are given some `n` points, each having an x coordinate and a y coordinate.
- Let the points be `(x1,y1), (x2,y2),...,(xn,yn).`
- Let us assume that these points **approximately** (but not exactly) lie on a line.
- Such situations are quite common, for example in experiments in a physics lab from your 12th grade.
- You want to find the best fit line `y = mx + c` with slope `m` and x-intercept `c`.
- What is meant by best fit?
- The **squared vertical distance** from any point `(xi,yi)` to the line `y=mx+c` is given by $(yi-m\ xi-c)^2$.
- We will try to find a line for which the sum total squared vertical distance for all `n` given points is the least, i.e. we find `m`, `c` to minimize:

$$J(m,c) = \sum_{i=1}^{n} (y_i - mx_i - c)^2$$

# Least squares line fitting

- Taking derivatives of J w.r.t. slope `m` and intercept `c`, we get the following two linear simultaneous equations:

$$-2\sum_{i=1}^{n} x_i(y_i - mx_i - c) = 0 \implies m\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} x_i y_i$$

$$-2\sum_{i=1}^{n}(y_i - mx_i - c) = 0 \implies m\sum_{i=1}^{n} x_i + cn = \sum_{i=1}^{n} y_i$$

- Let us define a few quantities to reduce symbol clutter:

$$p \triangleq \sum_{i=1}^{n} x_i^2, q \triangleq \sum_{i=1}^{n} x_i, r \triangleq \sum_{i=1}^{n} x_i y_i, s \triangleq \sum_{i=1}^{n} y_i$$

- The solution for `m` and `c` is as follows:

$$m = \frac{nr - qs}{np - q^2}, c = \frac{ps - qr}{np - q^2}$$

# Least squares line fitting: towards a program

- We are going to write a computer program for this.
- How do we get the points? It is tedious for a user to enter point coordinates manually, and definitely not a few dozen or hundred points!
- We will use the simplecpp package and ask the user to **click** on points on a canvas, with a mouse.
- Once the user is done clicking on the points, we will compute the **slope** and **intercept** of the best fit line.
- Finally, we will **draw** the line.
- The full program is on the next slide.
- You will learn a lot of new commands/functions in this program.

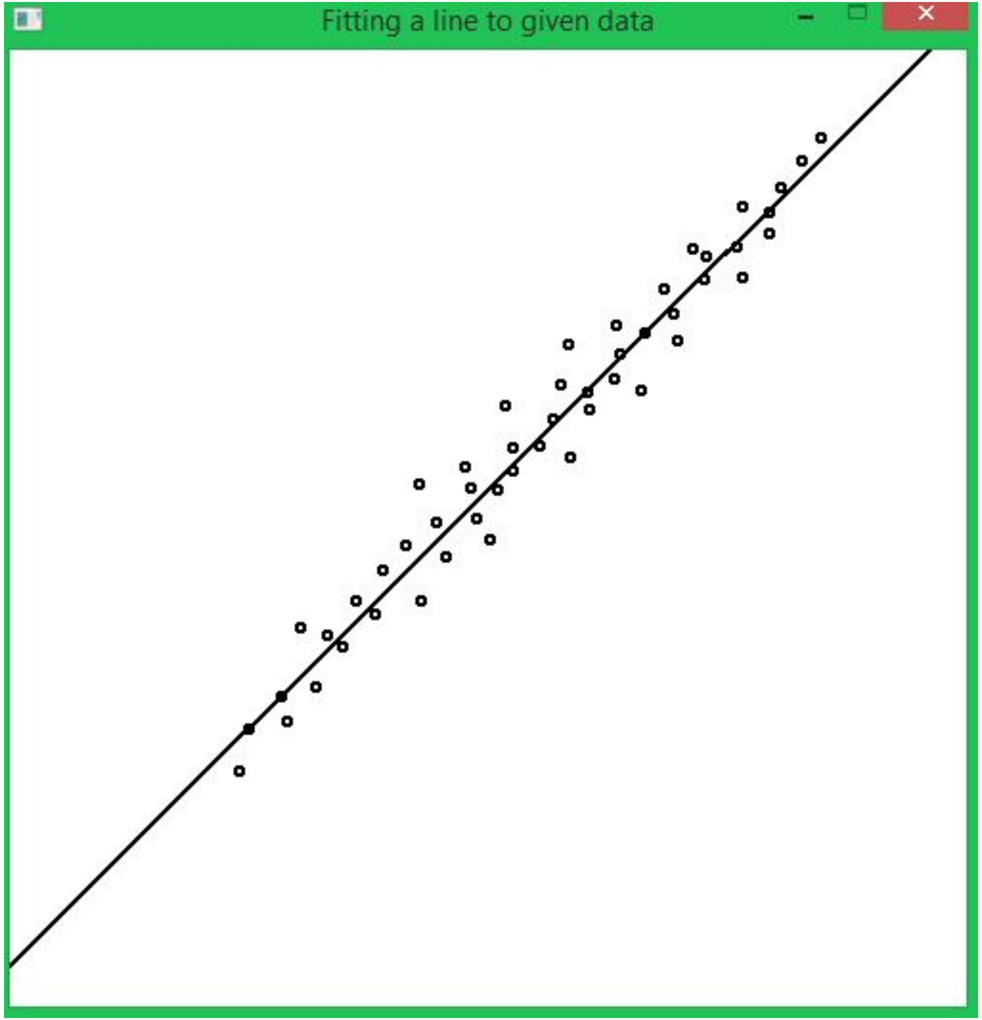
The position returned by `getClick();` is given by an integer value `v = 65536x + y`. The `x` and `y` coordinates of the point where the mouse was clicked are given by `x = floor(v/65536)` and `y = v % 65536`.

```
main_program{
int n;
double p,q,r,s;
p = q = r = s = 0.0;

cout << "Enter the number of points: "; cin >> n;
initCanvas ("Fitting a line to given data",500,500);  // inbuilt function to create a new
// window

Circle pt(0,0,0); // this will be used to draw a small circle around each clicked point
for (int i = 0; i < n; i++)
{
    int cPos = getClick(); // ask the user to click on a point
    double x = cPos/65536; // x coordinate of the point
    double y = cPos%65536; // the point's y coordinate
    pt.reset(x,y,3); // draw a small circle around that point
    pt.imprint(); //to retain that circle even when we move pt for getting other points

    p += x*x; q += x; r += x*y; s += y;
}
double m = (n*r-q*s)/(n*p-q*q);  // calculate slope
double c = (p*s - q*r)/(n*p - q*q);  // calculate intercept
Line l (0,c,500,500*m+c); // draw the line
wait (15);
}
```




Sample Output

# Least squares line fitting

- What we just did is called **least squares fitting**.
- In this case we fit a **line**. You could also fit a circle, parabola, etc.
- If instead of the squared vertical distance, we had minimized the **squared perpendicular distance**, it would be called **total least squares fitting**.
- Both least squares and total least squares are very important techniques in computer science and data science.

# Greatest Common Divisors

Ajit Rajwade

# Determining the greatest common divisor (GCD) of two numbers

- The GCD is the largest integer that divides both positive integers `m`, `n`.
- One strategy is to examine all numbers from 2 to `min (m,n)` and find the largest number that divides both.
- This method is correct, but slower than the method we will see later.
- Here is its code

```
main_program
{
    int m,n,i,min_mn;
    cout << "Enter the numbers "; cin >> m >> n;
    min_mn = min(m,n);
    for (i=min_mn; i >= 2; i--){
        if (m%i == 0 && n%i == 0) break;
    }
    cout << "Their GCD is: " << i;
}
```

# Euclid’s method for GCD

- Based on the following fact: If `d` is a common divisor of `m` and `n`, then `d` is also a divisor of `m-n`.
- Proof (assuming `m >= n`):
  - Since `d` divides `m`, then `m = ad`. Since `d` divides `n`, then `n = bd`. Here `a` and `b` are two integers.
  - Hence `m-n = (a-b)d.`
  - As `a` and `b` are integers, `a-b` is also an integer.
  - Thus we have proved that `d` divides `m-n.`
- Likewise, if `d` is a common divisor of `m-n` and `n`, then it is also a common divisor of `m` and `n`. The proof is similar.
- Thus `GCD(m,n) = GCD(m-n,n).`

# Euclid’s method for GCD

- Using the earlier fact, we have:
- `GCD(3977,943) = GCD(3977-943,943) = GCD(3034,943) = GCD(2091,943) = GCD(1148,943) = GCD(205,943)`
- You see that instead of running so many steps, we can also subtract all multiples in one shot leaving behind the remainder of dividing 3977 by 943.
- This can be formalized into the following fact: Let `m = nq + r` where `m,n,q,r` are integers and `q,r` are the quotient and remainder obtained when dividing `m` by `n`. Then `GCD(m,n) = GCD(n,r)`.
- **Proof:** If `d` divides `m` and `n`, then it divides `nq + r` and `n`. As `d` divides `n`, then it must divide `r` (otherwise it would not divide `m = nq+r`). Thus `GCD(m,n) = GCD(n,r)`. In other words `GCD(m,n) = GCD(n,m%n)`.
- **Note:** if `r = 0`, we can directly state `GCD(m,n) = n`.
- We will use these facts to design the algorithm for GCD computation.

# Euclid's method for GCD

- Using the aforementioned fact, we have `GCD(3977,943) = GCD(3977%943,943) = GCD(205,943).`
- Continuing further, `GCD(205,943) = GCD(205, 943%205) = GCD(205,123)`
- This is further equal to `GCD(123,205%123) = GCD(123,82) = GCD(82,123%82) = GCD(82,41) = 41.`
- We now write a piece of code for this.

# Euclid’s method for GCD

```
main_program
{
    int m,n,i;
    cout << "Enter the positive numbers (largest first): "; cin >> m >> n;
    while (m%n !=0)
    {
        int remainder = m%n;
        m = n;
        n = remainder; //if n does not divide m, GCD(m,n) = GCD(n,m%n)
    }
    cout << "Their GCD is: " << n; // if n divides m, GCD(m,n) = n
}
```

Let the original numbers be called `m0` and `n0`. Inside the while loop, after any iteration the GCD of `m` and `n` is equal to the GCD of `m0` and `n0` (as per our mathematical arguments in the previous slides). Also, at the end of each iteration, we always have `m > n > 0`.

The while loop is guaranteed to terminate in a finite number of iterations. Why? Because the value of `n` reduces to `m%n` which is clearly smaller than `n`. The value of `m` also reduces to `n`. Both `m` and `n` are guaranteed to remain positive (otherwise the while loop terminates)! The number of iterations cannot exceed `n0` ever (in fact it will terminate in **much fewer** iterations).

# Bisection Method for Finding Roots of an Equation

Ajit Rajwade

# Bisection Method for Root-finding

- The roots of a function `f(x)` are defined as those values for which `f(x) = 0`.
- It is easy to find roots of certain specific functions, like quadratic functions, because of readily available formulae.
- However for most functions, computational methods are required to determine (approximate) roots, i.e. values of `x` for which `f(x)` is close to zero (but maybe not exactly zero).
- The bisection method is one method to find the approximate root(s) of a continuous function `f(x)`.
- The method requires the user to specify an interval `[xL,xR]` such that `xL < xR` and `f(xL)` and `f(xR)` have opposite signs.
- By the intermediate value theorem, `f(x)` must then have a root inside `[xL,xR]`.

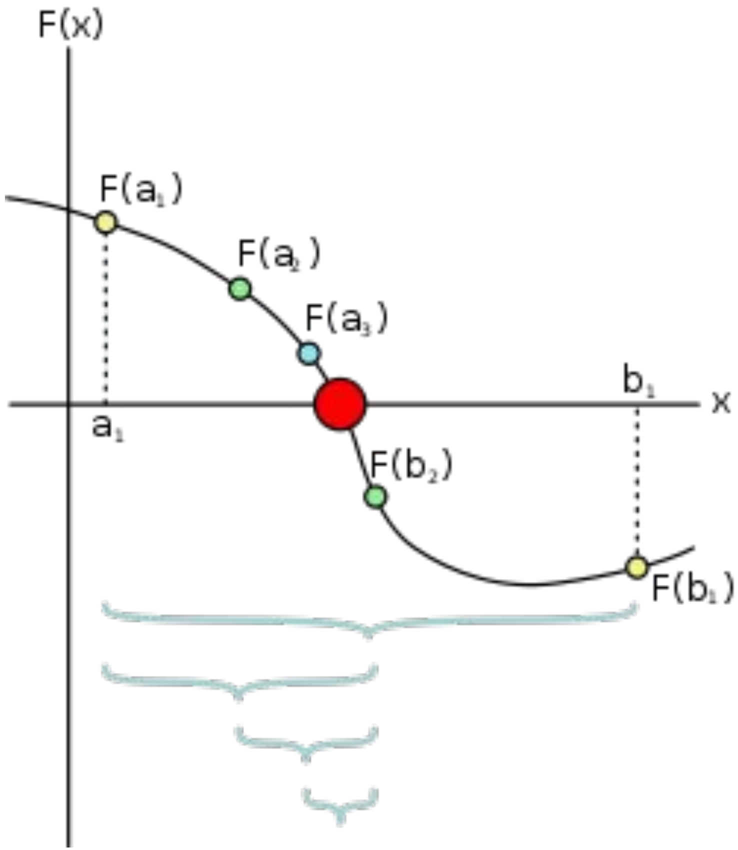
# Bisection Method for Root-finding

- By the intermediate value theorem, `f(x)` must then have a root inside `[xL,xR]`.
- **Intermediate value theorem:** If f(x) is a continuous function whose domain contains the interval [a,b], then f(x) must take on every value between f(a) and f(b) for some x in [a,b].
- Corollary: If a continuous function has values of opposite sign inside an interval, then it has a root in that interval (**Bolzano's theorem**).

# Bisection Method for Root-finding

- We can think of `xR-xL` as the maximum possible error in determining the root.
- A better approximation basically means obtaining a smaller interval.
- If the interval length is really small, either endpoint can be treated as an approximate root.
- How can we shrink the interval given initial values of `xL`, `xR`?
- Compute the midpoint `xM = (xL+xR)/2`.
- If `f(xM)` and `f(xL)` have different signs, then the root must lie in `[xL, xM]`, so you can set `xR` to `xM`.
- Instead if `f(xM)` and `f(xR)` have different signs, then the root must lie in `[xM,xR]`, so you can set `xL` to `xM`.
- Note that in either case, the new `xL`, `xR` satisfy the requirement that `f(xL)` and `f(xR)` have different signs.
- In both cases, the new interval has smaller width than the earlier one.
- This process needs to be continued in a loop until `xR-xL >=` some tolerance value ‘epsilon’, maybe something like 0.001 if you desire precision till the third decimal place.

# Bisection Method for Root-finding




https://en.wikipedia.org/wiki/Bisection_method

# Bisection method for roots of $f(x)=x^3-5$

```
main_program{
double xL = 1, xR = 2; // initial interval
double epsilon = 0.001; // precision of the root's value
bool flagL, flagR;
double xM;
bool flagM;
flagL = xL*xL*xL-5 > 0; flagR = xR*xR*xR-5 > 0;// signs of f(xL) and f(xR)
if (flagL != flagR)
{
      while (xR - xL > epsilon) // until the required precision is reached
      {
            xM = (xR+xL)/2; // interval midpoint
            flagM = xM*xM*xM-5 > 0;
            if (flagM != flagL) xR = xM; // signs of f(xM) and f(xL)
            else if (flagM != flagR) xL = xM;
      }
      cout << "the root is " << xL;
}
}
```

# Bisection Method for Root-finding

- We could have simply divided the interval `[xL, xR]` into a grid with 1/0.001 = 1000 points
- And evaluated `f(x)` at all those points, and chosen the value of `x` which produced the **smallest** value of `|f(x)|` as the approximate root.
- But this would require 1000 function evaluations.
- In contrast, the bisection method is much **faster**.
- How many evaluations of `f(x)` does it require? Equivalently, how many iterations does it require?
- To answer this, notice that the length of the interval is shrinking by a factor of 2 in each iteration.
- And we desire a precision of just about epsilon. In how many iterations (`N`) will the interval width fall below epsilon?
- `2^N = (xR-xL)/epsilon`, i.e. `N = log2((xR-xL)/epsilon)`.
- Note: we have assumed that the interval `[xL, xR]` contained only one root! If there are multiple roots in this interval, the method will output just one of the root and you will need to select a fresh interval for the others (why?)

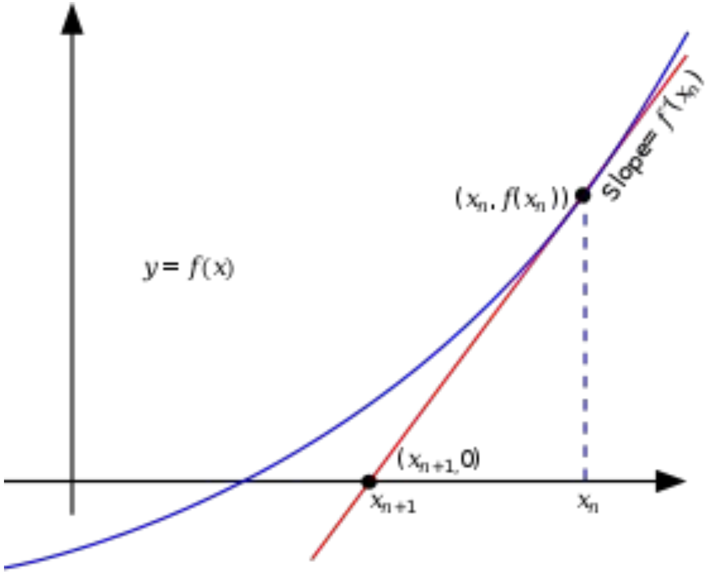
# Newton-Raphson Method for Finding Roots of an Equation

Ajit Rajwade

# Newton-Raphson Method for Root-finding

- This method starts from an initial guess for the root, call it `x0`, and keeps **evolving** the guess to make it better and better.
- It then **approximates** the function `f(x)` at `x0` by means of a tangent, i.e. `f(x) ≈ f(x0) + (x-x0)f'(x0)`.
- So what should the next guess `x1` be?
- Since we took the **tangent** approximation of `f(x)`, let `x1` be the root of that approximate function.
- This gives `f(x0) + (x-x0) f'(x0) = 0`, and `x1 = x = x0 - f(x0)/f'(x0)`.
- Of course the roots of `f(x)` and its tangent approximation are **different**, so `x1` only acts as a guess for the root.
- This process is iterated **several** times producing guesses `x0, x1, …, xi, …` until when `f(xi)` is close to 0, i.e. less than or equal to `epsilon = 0.001` (say).

# Newton-Raphson Method for Root-finding




https://en.wikipedia.org/wiki/Newton%27s_method

# Newton-Raphson Method for finding roots of roots of $f(x)=x^3-5$

```
main_program{
double x, epsilon = 0.001;
double dfx,fx;
cout << "enter initial guess of root: "; cin >> x;
while (fabs(x*x*x-5) > epsilon)
{
     fx = x*x*x-5;
     dfx = 3*x*x;
     x = x - fx/dfx;
}
cout << "The root is: " << x << "and the value of the function there is: " << fx;
}
```

# Newton-Raphson Method

- Unlike the bisection method, the Newton-Raphson method makes use of the first derivative of the function.
- It often works faster than the bisection method.
- But it is not always guaranteed to converge, i.e. end in a finite number of iterations.
- Also there is the problem of the derivative becoming zero.
- A full analysis of this method is beyond the scope of this course.