Over the last few decades, computers have become part of everyday life. Computational physics provides a means to solve complex numerical problems. An advantage of computational physics is that one can start with a simple problem which is easily solvable analytically. The analytical solution illustrates the underlying physics and allows one the possibility to compare the computer program with the analytical solution. Once a program has been written which can handle the case with the typical physicist's approximation, then you add more and more complex real-world factors.

An important part in a scientist's life is the interpretation of measured data or theoretical calculations. Usually when you do a measurement you will have a discrete set of points representing your experiment. For simplicity, we assume your experiment to be represented by pairs of values: an independent variable "*x*," which you vary and a quantity "*y*," which is the measured value at the point *x*. As an illustration, consider a radioactive source and a detector, which counts the number of decays. In order to determine the half-life of this source, you would count the number of decays N_0, N_1, N_2, …N_k at times t_0, t_1, t_2… t_k. In this case *t* would be your independent variable, which you hopefully would choose in such a way that it is suitable for your problem. However, what you measure is a discrete set of pairs of numbers (t_k, N_k) in the range of [t_0, t_k]. In order to extract information from such an experiment, we would like to be able to find an analytical function which would give us N for any arbitrary chosen point t. But, sometimes trying to find an analytical function is impossible, or even though the function might be known, it is too time consuming to calculate or we might be only interested in a small local region of the independent variable. To illustrate this point, assume your radioactive source is 241Am, an α-emmiter. Its half-life is $\tau_{1/2}$ = 430 years. Clearly you cannot determine the half-life by measuring it. Because it is very slowly decaying you probably will measure the activity over a longer time period, say every Monday for a couple of months. After five months you would stop and look at the data. One question you might want to answer is: what was the activity on Wednesday of the third week? Because this day is inside your range of [t_0, t_k] you would use interpolation techniques to determine this value. If, on the other hand, you want to know the activity eight months from the end of your measurement, you would extrapolate to this point from the previous series of measurements. The idea of interpolation is to select a function g(x) such that $g(x_i)= f_i$ for each data point i and that this function is a good approximation for any other x lying between the original data points.

Definitions:

1. **Interpolation**: Estimating the attribute values of locations that are *within* the range of available data using known data values.
2. **Extrapolation**: Estimating the attribute values of locations *outside* the range of available data using known data values.

Interpolation:

There are many methods for interpolation. Interpolation is done by generating a function which best fits the known points. Interpolation is carried out using approximating functions such as:

1. Polynomials

2. Trigonometric functions
3. Exponential functions
4. Fourier methods

Following interpolating methods are most polular:

1. Lagrange Interpolation (unevenly spaced data)
2. Newton's Divided Difference (evenly spaced data)
3. Central difference method

LANGRANGE'S INTERPOLATION:

Suppose that our data pairs are $(x_0,f(x_0))$, $(x_1,f(x_1))$,…, $(x_n,f(x_n))$. The Langrange's polynomial is given by:

$$P(x)=\frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f(x_0)+\frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f(x_1)$$
$$+\frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}f(x_2)+\frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}f(x_3)$$

In short, it can be written as:

$$P(x)=\sum_{j=1}^{n}P_j(x)$$

Where

$$P_j(x)=y_j\prod_{\substack{k=1\\k\neq j}}^{n}\frac{x-x_k}{x_j-x_k}$$

Hence, by putting the value of x_i and y_i we can calculate the value of x at any unknown point.

NEWTON'S FORMULAE:

Another popular method for interpolation is Newton's formula. There are three types of formulae:

1. Forward difference interpolation formula
2. Backward difference interpolation formula
3. Divided difference interpolation formula

Forward difference interpolation formula:

$$P(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \ldots..$$

Where $p = \frac{x-x_0}{h}$

Backward difference interpolation formula:

$$P(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \frac{p(p+1)(p+2)(p+3)}{4!}\nabla^4 y_n + \frac{p(p+1)(p+2)(p+3)(p+4)}{5!}\nabla^5 y_n + \ldots$$

Divided difference interpolation formula:

A divided difference is defined as the difference in the function values at two points, divided by the difference in the values of the corresponding independent variable.

Thus, the first divided difference at point is defined as

$$f[x_0, x_1] = \frac{f_0 - f_1}{x_0 - x_1}$$

$P(x) = y_0 + f[x_0, x_1](x - x_0) + f[x_0, x_2](x - x_0)(x - x_1) + f[x_0, x_3](x - x_0)(x - x_1)(x - x_2) + \ldots$

EXTRAPOLTION

There are many methods of extrapolation. The following methods will be briefly outlined:

1. Linear Extrapolation
2. Polynomial Extrapolation
3. Conic Extrapolation

Linear Extrapolation:

- Linear Extrapolation means creating a tangent line at the end of the known data and extending it beyond that limit.
- Linear extrapolation will provide good results only when used to extend the graph of an approximately linear function or not too far beyond the known data.
- If the two data points nearest to the point x_* to be extrapolated are (x_k, y_k) and (x_{k-1}, y_{k-1}), linear extrapolation gives the function

$$y(x_*) = y_{k-1} + \frac{x_* - x_{k-1}}{x_k - x_{k-1}}(y_k - y_{k-1}).$$

Polynomial Extrapolation:

A polynomial curve can be created through the entire known data or just near the end. The resulting curve can then be extended beyond the end of the known data. Polynomial extrapolation is typically done by means of Lagrange interpolation or using Newton's method of finite differences to create a Newton series that fits the data. The resulting polynomial may be used to extrapolate the data.

Conic Extrapolation:

A conic section can be created using five points near the end of the known data. If the conic section created is an ellipse or circle, it will loop back and rejoin itself. A parabolic or hyperbolic curve will not rejoin itself, but may curve back relative to the X-axis. This type of extrapolation could be done with a conic sections template (on paper) or with a computer.