# Inverse Interpolation: The Rate of Enzymatic Reaction based Finite differences, Formulas for obtaining intermediate values of Temperature, Substrate Concentration, Enzyme Concentration and their Estimation of Errors

# Nizam Uddin

M. B. Khalsa College, Indore, Madhya Pradesh, India

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**ABSTRACT:** Inverse interpolation is the process of finding the values of the argument corresponding to a given value of the function when the latter is intermediate between two tabulated values. The finite differences are differences between the values of the function or the difference between the past differences. Finite differences are forward difference, backward difference and divide difference. Temperature, concentration of substrate, concentration of enzyme and other factors are affected the rate of enzymatic reaction. The concentration of substrate is the limiting factor, as the substrate concentration increases, the Enzyme reaction rate increases. Assuming a sufficient concentration of substrate is available, increasing Enzyme concentration of enzyme are increased the rate of enzymatic reaction. Temperature, concentration of substrate and concentration of enzyme are increased the rate of enzymatic reaction at a limit which is called optimum limit. On the basis of this concept mathematical functions are defined. These mathematical functions are worked in "n" limit. Take the rate of enzymatic reaction is independent variable for finite differences, formulas and their estimation of errors. These formulas are used to obtaining intermediate values of Temperature, substrate concentration and enzyme concentration. If the point lies in the upper half then used forward difference interpolation. If the point lies in the lower half then used backward difference interpolation.

**KEYWORDS:** Inverse interpolation, Finite differences, Estimation of Errors, Rate of enzymatic reaction.

# **1** INTRODUCTION

The rate of enzymatic reaction is affected by Temperature, concentration of substrate, concentration of enzyme and other factors [1]. The rise in Temperature accelerates an Enzyme reaction but at the same time causes inactivation of the protein. At certain Temperature known as the optimum Temperature the activity is maximum [2]. The concentration of substrate is the limiting factor, as the substrate concentration increases, the Enzyme reaction rate increases. Assuming a sufficient concentration of substrate is available, increasing Enzyme concentration will increase the enzymatic reaction rate. Temperature, concentration of substrate and concentration of enzyme are increased the rate of enzymatic reaction at a limit which is called optimum limit [1]-[3]. The finite differences are differences between the values of the function or the difference between the past differences. Finite differences are forward difference, backward difference and divide difference [4]-[15]. Inverse interpolation is the process of finding the values of the argument corresponding to a given value of the function when the latter is intermediate between two tabulated values [16][17].

# 2 INVERSE INTERPOLATION

Let y = f(x) be a function where y is dependent variable and x is independent variable. The technique of determining the values of x corresponding to the value of y from the set of tabulated values, is known as inverse

interpolation [16][17]. In enzymatic reaction, Temperature, concentration of substrate and concentration of enzyme are worked in n limit which are defined three mathematical functions:

$$V^{T} = f(T)$$
$$V^{S} = f(S)$$
$$V^{E} = f(E)$$

Where T is the temperature, S is the concentration of substrate, E is the concentration of enzyme,  $V^{T}$  is the rate of enzymatic reaction with temperature,  $V^{S}$  is the rate of enzymatic reaction with concentration of enzyme. And other factors are be constant in each functions [1]-[3]. In above mathematical functions, we take the rate of enzymatic reaction is Independent variable. Temperature, concentration of substrate and concentration of enzyme are being dependent variable for inverse interpolation.

### **3** FORWARD DIFFERENCE OF TEMPERATURE

If  $(V_0^T, T_0), (V_1^T, T_1), (V_2^T, T_2), \dots, (V_n^T, T_n)$  denoted the values of the inverse function then  $T_1 - T_0$ ,  $T_2 - T_1$ ,  $T_3 - T_2$ ,  $T_4 - T_3$ , ...,  $T_n - T_{n-1}$  are called the forward differences of T [18]. These differences are denoted as  $\Delta T_0$ ,  $\Delta T_1$ ,  $\Delta T_2$ ,  $\Delta T_3$ , ...,  $\Delta T_{n-1}$  therefore

 $\Delta T \circ = T_{1} - T_{\circ},$   $\Delta T_{1} = T_{2} - T_{1},$   $\Delta T_{2} = T_{3} - T_{2},$   $\Delta T_{3} = T_{4} - T_{3},:$ :
:
:  $\Delta T_{n-1} = T_{n} - T_{n-1}$ 

Where  $\Delta$  is called the forward difference operator, and  $\Delta T_0$ ,  $\Delta T_1 \Delta T_2 \Delta T_3 \dots \Delta T_{n-1}$  are called first order forward differences. The differences of the first order difference are called second order forward differences and are denoted as  $\Delta^2 T_0$ ,  $\Delta^2 T_1$ ,  $\Delta^2 T_2$ ,  $\Delta^2 T_3$ , ... etc.

 $\Delta^2 T_0 = \Delta T_1 - \Delta T_0$  $\Delta^2 T_1 = \Delta T_2 - \Delta T_1$  $\Delta^2 T_2 = \Delta T_3 - \Delta T_2$  $\Delta^2 T_3 = \Delta T_4 - \Delta T_3$ 

In general, the first order forward difference at the  $i^{th}$  point is

$$\Delta T_i = T_{i+1} - T_i$$

And the order forward difference at the point is

 $\Delta^j T_i = \Delta^{j-1} T_{i+1} - \Delta^{j-1} T_i$ 

#### **3.1** FORMULA FOR FORWARD DIFFERENCE INTERPOLATION

If  $f(a), f(a+h), \dots, f(a+nh)$  are be values of inverse function then

$$V^T = a, a+h, \dots, a+nh$$

Let  $f(V^T)$  be a polynomial of degree n and let

$$f(V^{T}) = A_{0} + A_{1}(V^{T} - a) + A_{2}(V^{T} - a)(V^{T} - a - h) + A_{3}(V^{T} - a)(V^{T} - a - h)(V^{T} - a - 2h) + \dots + A_{n}[(V^{T} - a)(V^{T} - a - h)\dots \{V^{T} - a - (n - 1)h\}]$$
(1)

Where  $A_0, A_1, \dots, A_n$  all are constants [19].

Putting  $V^T = a$  in equation (1), we got:

$$f(a) = A_0 \tag{2}$$

Again putting  $V^{T} = a + h$  in equation (1), we got:

$$f(a+h) = A_0 + A_1 h$$
  

$$A_1 h = f(a+h) - A_0$$
  

$$= f(a+h) - f(a)$$
  

$$= \Delta f(a)$$
  

$$A_1 = \frac{\Delta f(a)}{\Delta f(a)}$$

$$A_1 = \frac{-25}{h}$$

Again putting  $V^T = a + 2h$  in equation (1), we got:

$$f(a+2h) = A_0 + A_1(2h) + A_2(2h)(h)$$
  
=  $A_0 + 2hA_1 + A_0 + 2h^2A_2$  [from equation (2) and (3)]

Or 
$$2h^2 A_2 = f(a+2h) - A_0 - 2hA_1$$
  
=  $f(a+2h) - f(a) - 2\Delta f(a)$   
=  $f(a+2h) - f(a) - 2\{f(a+h) - f(a)\}$   
=  $f(a+2h) - 2\{f(a+h) + f(a)\}$   
=  $\Delta^2 f(a)$ 

$$\therefore A_2 = \frac{1}{2h^2} \Delta^2 f(a)$$
or  $A_2 = \frac{1}{2!h^2} \Delta^2 f(a)$ 
(4)

Similarly

rly 
$$A_3 = \frac{1}{3!h^3} \Delta^3 f(a)$$
 (5)

Proceeding in similar way, we got:

: :

$$A_n = \frac{1}{n!h^n} \Delta^n f(a) \tag{6}$$

(3)

substituting the values of  $A_0, A_1, A_2, \dots, A_n$  in equation (1), we got:

$$f(V) = f(a) + \frac{\Delta f(a)}{h} (V^{T} - a) + \frac{\Delta^{2} f(a)}{2!h^{2}} (V^{T} - a) (V^{T} - a - h) + \dots + \frac{\Delta^{n} f(a)}{n!h^{n}} (V^{T} - a) (V^{T} - a - h) \dots \{V^{T} - a - (n-1)h\}$$
(7)

Now let:  $V^T = a + hu$ 

$$\therefore V^{T} - a = hu$$

$$V^{T} - a - h = (u - 1)h$$

$$V^{T} - a - 2h = (u - 2)h$$

$$\vdots$$

$$\vdots$$

$$V^{T} - a - (n - 1)h = \{u - (n - 1)\}h$$

Putting these values in equation (7), we got:

$$f(a+hu) = f(a) + \frac{\Delta f(a)}{h}(uh) + \frac{\Delta^2 f(a)}{2!h^2}(uh)(u-1)h + \dots + \frac{\Delta^n f(a)}{n!h^n}(uh)(u-1)h \dots \{u-(n-1)h\}$$

Simplifying, we got:

$$f(a+hu) = f(a) + u\Delta f(a) + \frac{\Delta^2 f(a)}{2!} \{u(u-1)\} + \dots + \frac{\Delta^n f(a)}{n!} (u)(u-1) \dots \{u-(n-1)\}$$
(8)

Also we know that

$$u^{(m)} = u(u-1)(u-2).....\{u-(m-1)\}$$
(9)

From equation (8) and (9), we have:

$$f(a+hu) = f(a) + \Delta f(a) \frac{u^{(1)}}{1!} + \Delta^2 f(a) \frac{u^{(2)}}{2!} + \Delta^3 f(a) \frac{u^{(3)}}{3!} + \dots + \Delta^n f(a) \frac{u^{(n)}}{n!}$$
(10)

### 3.1.1 ESTIMATION OF ERROR

If inverse function defined by (n+1) points  $(V_0^T, T_0), (V_1^T, T_1), \dots, (V_n^T, T_n)$ . When  $V_0^T, V_1^T, V_2^T, V_3^T, \dots, V_n^T$  are equally spaced with interval h and this function is continuous and differentiable (n+1) times.

The function be approximated by a polynomial  $P_n(V^T)$  of degree not exceeding a such that

$$P_n(V_i^T) = T_i$$
 [Where  $i = 0, 1, 2, 3, ..., n$ ] (11)

Since the expression  $f(V^T) - P_n(V^T)$  vanishes for  $V^T = V_0^T, V_1^T, V_2^T, V_3^T, \dots, V_n^T$ ,

We put

$$f(V^{T}) - P_{n}(V^{T}) = K\varphi(V^{T})$$
(12)

Where 
$$\varphi(V^T) = (V^T - V_0^T)(V^T - V_1^T)....(V^T - V_n^T)$$
 (13)

And K is to be determined in such a way that equation (12) holds for any intermediate values of  $V^{T}$ , say  $V^T - V^T$  [where  $V_0^T \leq V^T \leq V_n^T$ ].

Therefore from equation (12),

$$K = \frac{f(V'^{T}) - P(V'^{T})}{\varphi(V'^{T})}$$
(14)

Now we construct a function  $f(V^T)$  such that

$$f(V_0^T) = f(V_1^T) - P_n(V^T) - K\varphi(V^T)$$

Where K is given by equation (14).

It is clear that

$$f(V_0^T) = f(V_1^T) = f(V_2^T) = f(V_3^T) = \dots f(V_n^T) = f(V^T) = 0$$
(15)

Let  $f(V^T)$  vanishes (n+2) times in the interval  $V_0^T \le V^T \le V_n^T$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^T)$  must vanish (n+1) times,  $f''(V^T)$  must vanish n times etc in the interval  $V_0^T \le V_n^T \le V_n^T$ .

Particularly,  $f^{(n+1)}(V^T)$  must vanish once in the interval  $V_0^T \le V^T \le V_n^T$ . Let this point be  $V^T = W$ ,  $V_0^T < W < V_n^T.$ 

Now differentiating equation (15) (n+1) times with respect to  $V^T$  and putting  $V^T = W$ , we got:

$$f^{(n+1)}(W) - K(n+1)! = 0$$

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(16)

Or

Putting this value of K in equation (14), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V'^{T}) - P_{n}(V'^{T})}{\varphi(V'^{T})}$$
  
Or 
$$f(V'^{T}) - P_{n}(V'^{T}) = \frac{f^{(n+1)}(W)}{(n+1)!}\varphi(V'^{T}) \quad , \qquad V_{0}^{T} < W < V_{n}^{T}$$

С

Since  $V^{T}$  is arbitrary therefore on dropping the prime on  $V^{T}$  we got:

$$f(V^{T}) - P_{n}(V^{T}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi(V^{T}), \quad V_{0}^{T} < W < T_{n}^{T}$$
(17)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(18)

Neglecting the terms containing second and higher powers of h in equation (18), we got:

$$f(W+h) = f(W) + hf'(W)$$

$$f'(W) = \frac{f(W+h) - f(W)}{h}$$
(19)

Or

Or

$$f'(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore \Delta f(V^T + h) f(V^T)]$$
$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore D = \frac{d}{dW}]$$
$$D = \frac{1}{h} \Delta \qquad [\text{Because } f(W) \text{ is arbitrary}]$$
$$\therefore D^{n+1} = \frac{1}{h^{n+1}} \Delta^{n+1}$$

From equation (19), we got:

$$f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$$

Putting the values of  $f^{(n+1)}(W)$  in equation (17), we got:

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{\varphi(V^{T})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)\right]$$
$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})....(V^{T} - V_{0}^{T})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)\right]$$
(20)

Then

$$V^{T} - V_{0}^{T} = h\beta$$

$$V^{T} - V_{1}^{T} = V^{T} - (V_{0}^{T} - h) = (V^{T} - V_{0}^{T}) - h = (h\beta - h) = h(\beta - 1)$$
Similarly  $V^{T} - V_{2}^{T} = h(\beta - 2)$ 
:

Similarly  $V^T - V_n^T = h(\beta - n)$ 

:

Putting these values in equation (20), we got:

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{(h\beta)\{h(\beta-1)\}\{h(\beta-2)\}\{h(\beta-3)\}\dots\{(\beta-n)\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

### 4 BACKWARD DIFFERENCE OF TEMPERATURE

If  $(V_0^T, T_0), (V_1^T, T_1), (V_2^T, T_2), \dots, (V_n^T, T_n)$  denoted the values of the inverse function then  $T_1 - T_0$ ,  $T_2 - T_1$ ,  $T_3 - T_2$ ,  $T_4 - T_3$ , ...,  $T_n - T_{n-1}$  are called the backward differences of T [18]. These differences are denoted as  $\nabla T_1, \nabla T_2, \nabla T_3$ , ...,  $\nabla T_{n-1}$  therefore

 $\Delta T_n = T_n - T_{n-1}$ 

Where  $\nabla$  is called the backward difference operator, and  $\nabla T_1 \nabla T_2$ ,  $\nabla T_3$ ,....,  $\nabla T_{n-1}$  are called first order backward differences. The differences of the first order difference are called second order backward differences and are denoted as,  $\nabla^2 T_2$ ,  $\nabla^2 T_3$ ,  $\nabla^2 T_4$ ,  $\nabla^2 T_5$ .....etc.

$$\nabla^2 T_2 = \nabla T_2 - \nabla T_1$$
$$\nabla^2 T_3 = \nabla T_3 - \nabla T_2$$
$$\nabla^2 T_4 = \nabla T_4 - \nabla T_3$$
$$\nabla^2 T_5 = \nabla T_5 - \nabla T_4$$

In general, the first order forward difference at the  $i^{th}$  point is

$$\nabla T_i = T_i - T_{i-1}$$

And the order forward difference at the point is

$$\nabla^{j} T_{i} = \nabla^{j-1} T_{i} - \nabla^{j-1} T_{i-1}$$

# 4.1 FORMULA FOR BACKWARD DIFFERENCE INTERPOLATION

If  $f(k), f(k+h), \dots, f(k+nh)$  are be values of inverse function then

$$V^{T} = k, k + h, \dots, k + nh$$

Let  $f(V^T)$  be a polynomial of degree n and let

$$f(V^{T}) = K_{0} + K_{1}(V^{T} - k - nh) + K_{2}(V^{T} - k - nh) \{V^{T} - K(n - 1)h\} + K_{3}(V^{T} - k - nh) \{V^{T} - k - (n - 1)h\}$$

$$\{V^{T} - k - (n - 2)h\} + \dots + K_{n}[(V^{T} - k - nh) \{V^{T} - k - (n - 1)h\} \dots + (V^{T} - k - h)] \{V^{T} - k - (n - 1)h\} + \dots + K_{n}[(V^{T} - k - nh) \{V^{T} - k - (n - 1)h\} \dots + (V^{T} - k - h)] \{V^{T} - k - (n - 1)h\} + \dots + K_{n}[(V^{T} - k - nh)] \{V^{T} - k - (n - 1)h\} \dots + K_{n}[(V^{T} - k - nh)] \{V^{T} - k - (n - 1)h\} + \dots + K_{n}[(V^{T} - k - nh)] \{V^{T} - k - (n - 1)h\}$$

Where  $K_0, K_1, K_{2}, \dots, K_n$  all are constants [19].

Putting  $V^T = k + nh$  in equation (21), we got:

$$f(k+nh) = K_0 \tag{22}$$

Again putting V = k + (n-1)h in equation (21), we got:

$$f\{k + (n-1)h\} = K_0 + K_1h$$

$$K_1h = K_0 - f\{k + (n-1)h\}$$

$$= f(k+nh) - f\{k + (n-1)h\}$$

$$= \Delta f(k+nh)$$

$$K_1 = \frac{\Delta f(k+nh)}{h}$$
(23)

Again putting  $V^{T} = k + (n-2)h$  in equation (21), we got:

$$f \{k + (n-2)h\} = K_0 + K_1(-2h) + K_2(-2h)(-h)$$

$$2h^2 K_2 = f \{K + (n-2)h\} - K_0 - 2hK_1$$
Or  $2h^2 K_2 = f \{k + (n-2)h\} - f (k+nh) + 2\nabla f (k+nh) \text{ [from eq.(22) and(23)]}$ 

$$= f \{k + (n-2)h\} - f (k+nh) + 2[\{f (k+nh)\} - f \{k + (n-1)h\}]$$

$$= f \{k + (n-2)h\} - f (k+nh) - 2f \{k + (n-1)h\}$$

$$= f (k+nh) - 2[f \{k + (n-1)h\} + f (k)]$$

$$= \Delta^2 f (k+nh)$$

$$\therefore K_2 = \frac{1}{2h^2} \Delta^2 f (k)$$
Or  $K_3 = -\frac{1}{2h^2} \Delta^2 f (k-nh)$ 
(24)

Or

$$K_{2} = \frac{1}{2!h^{2}} \Delta^{2} f(k = nh)$$
<sup>(24)</sup>

Similarly

:

 $K_3 = \frac{1}{3!h^3} \Delta^3 f(k+nh)$ (25) :

Proceeding in similar way, we got:  $K_n = \frac{1}{n!h^n} \Delta^n f(k+nh)$ (26)

substituting the values of  $K_0, K_1, K_2, \dots, K_n$  in equation (21), we got:

$$f(V^{T}) = f(k+nh) + \frac{\Delta f(k)}{h} (V^{T} - k - nh)$$
  
+  $\frac{\Delta^{2} f(k+nh)}{2!h^{2}} (V^{T} - k - nh) \{V^{T} - k - (n-1)h\} + \dots$   
+  $\frac{\Delta^{n} f(k+nh)}{n!h^{n}} (V^{T} - k - nh) \{V^{T} - k - (n-1)h\} \dots (V^{T} - k - n)$  (27)

Now let:  $V^T = k + nh + hu$  $\therefore V^T - k = nh + hu$  $V^{T} - k - (n-1)h = (u+1)h$  $V^{T} - k - (n-2)h = (u+2)h$  $V^{T} - k - h = \{u + (n-1)\}h$ 

Putting these values in equation (27), we got:

$$f(k+nh+hu) = f(k+nh) + \frac{\Delta f(k+nh)}{h}(uh) + \frac{\Delta^2 f(k+nh)}{2!h^2}(uh)(u+1)h + \dots + \frac{\Delta^n f(k+nh)}{n!h^n}(uh)(u+1)h\dots \{u+(n-1)h\}$$

Simplifying, we got:

$$f(k+nh+hu) = f(k+nh) + u\Delta f(k+nh) + \frac{\Delta^2 f(k+nh)}{2!} \{u(u+1)\} + \dots + \frac{\Delta^n f(k+nh)}{n!} \{u\}(u+1) \dots \{u+(n-1)\}$$
(28)

#### 4.1.1 **ESTIMATION OF ERROR**

If inverse function defined by (n + 1) points  $(V_0^T, T_0), (V_1^T, T_1), \dots, (V_n^S, T_n)$ . When  $V_0^T, V_1^T, V_2^T, V_3^T, \dots, V_n^T$  are equally spaced with interval h and this function is continuous and differentiable (n + 1) times.

The function be approximated by a polynomial  $P_n(V^T)$  of degree not exceeding a such that

$$P_n(V_i^T) = E_i$$
 [Where  $i = 1, 2, 3, ..., n$ ] (29)

Since the expression  $f(V^T) - P_n(V^T)$  vanishes for  $V^T = V_0^T, V_1^T, V_2^T, V_3^T, \dots, V_n^T$ 

We put 
$$f(V^T) - P_n(V^T) = K\varphi(V^T)$$
 (30)

Where 
$$\varphi_1(V^T) = (V^T - V_n^T)(V^T - V_{n-1}^T)....(V^T - V_0^T)$$
 (31)

And K is to be determined in such a way that equation (30) holds for any intermediate values of  $V^T$ , say  $V^T - V^T$ [where  $V_0^T \leq V^T \leq V_n^T$ ].

Therefore from equation (30),

$$K = \frac{f(V'^{T}) - P_{n}(V'^{T})}{\varphi_{1}(V'^{T})}$$
(32)

Now we construct a function  $f(V^T)$  such that:  $f(V_0^T) = f(V_1^T) - P_n(V^T) - K\varphi_1(V^T)$ 

Where K is given by equation (32).

It is clear that

$$f(V_0^T) = f(V_1^T) = f(V_2^T) = f(V_3^T) = \dots f(V_n^T) = f(V^T) = 0$$
(33)

Let  $f(V^T)$  vanishes (n+2) times in the interval  $V_0^T \le V^T \le V_n^T$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^T)$  must vanish (n+1) times,  $f''(V^T)$  must vanish n times etc in the interval  $V_0^T \le V_n^T \le V_n^T$ .

Particularly,  $f^{(n+1)}(V^T)$  must vanish once in the interval  $V_0^T \le V^T \le V_n^T$ . Let this point be  $V^T = W$ ,  $V_0^T < W < V_n^T$ .

Now differentiating equation (15) (n+1) times with respect to  $V^T$  and putting  $V^T = W$ , we got:

$$f^{(n+1)}(W) - K(n+1)! = 0$$

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(34)

Or

Or

Putting this value of K in equation (32), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V^{T}) - P_n(V^{T})}{\varphi_1(V^{T})}$$
$$f(V^{T}) - P_n(V^{T}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi_1(V^{T}), \qquad V_0^T < W < V_n^T$$

Since  $V^{T}$  is arbitrary therefore on dropping the prime on  $V^{T}$  we got:

$$f(V^{T}) - P_{n}(V^{T}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi_{1}(V^{T}), \quad V_{0}^{T} < W < V_{n}^{T}$$
(35)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(36)

Neglecting the terms containing second and higher powers of h in equation (18), we got:

$$f(W + h) = f(W) + hf'(W)$$

$$f'(W) = \frac{f(W + h) - f(W)}{h}$$
(37)

Or

Or

$$f'(W) = \frac{1}{h}\Delta f(W) \qquad [\therefore \Delta f(W) = f(W+h) - f(W)]$$

$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore D = \frac{u}{dW}]$$
$$D = \frac{1}{h} \Delta \qquad [Because \ f(W) \text{ is arbitrary}]$$
$$\therefore D^{n+1} = \frac{1}{h^{n+1}} \Delta^{n+1}$$

From equation (37), we got:  $f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$ 

Putting the values of  $f^{(n+1)}(Y)$  in equation (35), we got:

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{\varphi_{1}(V^{T})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)\right]$$

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{0}^{T})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)\right]$$
(38)
$$\text{If } \frac{V^{T} - V_{n}^{T}}{h} = \beta$$

Then

$$V^{T} - V_{n}^{T} = h\beta$$
  

$$V^{T} - V_{n-1}^{T} = V^{T} - (V_{n}^{T} - h) = (V^{T} - V_{n}^{T}) + h = (h\beta + h) = h(\beta + 1)$$

Similarly 
$$V^T - V_{n-2}^T = h(\beta + 2)$$

	•	
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	•	
	•	

Similarly  $V^T - V_0^T = h(\beta + n)$ 

Putting these values in equation (38), we got:

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{(h\beta)\{h(\beta+1)\}\{h(\beta+2)\}\{h(\beta+3)\}\dots\{(\beta+n)\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

OR

$$f(V^{T}) - P_{n}(V^{T}) = \left[\frac{\beta(\beta+1)(\beta+2)(\beta+3)...(\beta+n)}{(n+1)!}\right] \left[\Delta^{(n+1)}f(W)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

# 5 DIVIDE DIFFERENCE OF TEMPERATURE

If  $(V_0^T, T_0), (V_1^T, T_1), \dots, (V_n^T, T_n)$  denoted the values of the inverse function where  $V^T$  is the rate of enzymatic reaction with Temperature then  $\frac{T_1 - T_0}{V_1^T - V_0^T} \frac{T_2 - T_1}{V_2^T - V_1^T}$ ,  $\frac{T_3 - T_2}{V_3^T - V_2^T}$ ,  $\frac{T_4 - T_3}{V_4^T - V_3^T}$ ,  $\dots, \frac{T_n - T_{n-1}}{V_n^T - V_{n-1}^T}$ , are called the divide differences of T. These differences are denoted as  $\Delta_d T_0 \Delta_d T_1$ ,  $\Delta_d T_2$ ,  $\Delta_d T_3$ ,  $\dots, \Delta_d T_{n-1}$  therefore

$$\Delta_{d}T_{0} = \frac{T_{1} - T_{0}}{V_{1}^{T} - V_{0}^{T}}$$

$$\Delta_{d}T_{1} = \frac{T_{2} - T_{1}}{V_{2}^{T} - V_{1}^{T}},$$

$$\Delta_{d}T_{2} = \frac{T_{3} - T_{2}}{V_{3}^{T} - V_{2}^{T}},$$

$$\Delta_{d}T_{3} = \frac{T_{4} - T_{3}}{V_{4}^{T} - V_{3}^{T}},$$
:
:
:
$$\Delta_{d}T_{n-1} = \frac{T_{n} - T_{n-1}}{V_{n}^{T} - V_{n-1}^{T}}$$

Where  $\Delta_d$  is called the divide difference operator, and  $\Delta_d T_0 = \Delta_d T_1 = \Delta_d T_2 = \Delta_d T_3 \dots \Delta_d T_{n-1}$  are called first order divide differences. The differences of the first order difference are called second order divide differences and are denoted as  $\Delta^2_d T_0 = \Delta^2_d T_1$ ,  $\Delta^2_d T_2$ ,  $\Delta^2_d T_3$ ,... etc.

$$\Delta_{d}^{2}T_{0} = \frac{\Delta_{d}T_{1} - \Delta_{d}T_{0}}{V_{2}^{T} - V_{0}^{T}}$$
$$\Delta_{d}^{2}T_{1} = \frac{\Delta_{d}T_{2} - \Delta_{d}T_{1}}{V_{3}^{T} - V_{1}^{T}}$$
$$\Delta_{d}^{2}T_{2} = \frac{\Delta_{d}T_{3} - \Delta_{d}T_{2}}{V_{4}^{T} - V_{2}^{T}}$$
$$\Delta_{d}^{2}T_{3} = \frac{\Delta_{d}T_{4} - \Delta_{d}T_{3}}{V_{5}^{T} - V_{3}^{T}}$$

In general, the first order divide difference at the  $i^{th}$  point is

$$\Delta_d T_i = \frac{T_{i+1} - T_i}{V_{i+1}^T - V_i^T}$$

And the order divide difference at the point is

$$\Delta^{j}T_{i} = \frac{\Delta^{j-1}T_{i+1} - \Delta^{j-1}T_{i}}{V_{i+j}^{T} - V_{i}^{T}}$$
$$\Delta^{j}T_{i} = \frac{\Delta^{j-1}T_{i+1} - \Delta^{j-1}T_{i}}{V_{i+j}^{T} - V_{i}^{T}}$$

### 5.1 FORMULA FOR DIVIDE DIFFERENCE INTERPOLATION

By the definition of divide difference

$$f(V^{T}, V_{0}^{T}) = \frac{f(V^{T})f(V_{0}^{T})}{V^{T} - V_{0}^{T}}$$
(39)

Or 
$$f(V^T) = f(V_0^T) + (V^T - V_0^T)f(V^T, V_0^T)$$

Again by the definition of second divided difference

$$f(V^{T}, V_{0}^{T}, V_{1}^{T}) = \frac{f(V^{T}, V_{0}^{T}) - f(V_{0}^{T}, V_{1}^{T})}{V^{T} - V_{1}^{T}}$$
$$f(V^{T}, V_{0}^{T}) = f(V_{0}^{T}, V_{1}^{T}) + (V^{T} - V_{1}^{T})f(V^{T}, V_{0}^{T}, V_{1}^{T})$$
(40)

Or

Similarly

$$f(V^{T}, V_{0}^{T}, V_{1}^{T}) = f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}) + (V^{T} - V_{2}^{T})f(V^{T}, V_{0}^{T}, V_{1}^{T}, V_{2}^{T})$$
(41)

:

Proceeding in similar way, we got:

$$f(V^{T}, V_{0}^{T}, V_{1}^{T}, \dots, V_{n-1}^{T}) = f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}, \dots, V_{n}^{T}) + (V^{T} - V_{n}^{T})f(V^{T}, V_{0}^{T}, V_{n}^{T})$$
(42)  
Multiplying equation (40) by  $(V^{T} - V_{0}^{T})$ ,

Multiplying equation (41) by  $(V^T - V_0^T) (V^T - V_1^T)$ ,

Multiplying equation (42) by  $(V^T - V_0^T)$   $(V^T - V_1^T)$  ..... $(V^T - V_{n-1}^T)$ 

And adding to equation (39), we got:

$$f(V^{T}) = f(V_{0}^{T}) + (V^{T} - V_{0}^{T})f(V_{0}^{T}, V_{1}^{T}) + (V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}) + \dots$$
  
$$\dots + (V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})\dots + (V^{T} - V_{n-1}^{T})f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}\dots + V_{n}^{T}) + R_{n}$$

Where  $R_n$  is the reminder and is given by

$$R_{n} = (V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})....(V^{T} - V_{n}^{T})f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}....V_{n}^{T})$$
  
If the function  $f(V^{T})$  is polynomial of degree  $n$ , then  $f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}, ....V_{n}^{T})$  vanishes so that

$$f(V^{T}) = f(V_{0}^{T}) + (V^{T} - V_{0}^{T})f(V_{0}^{T}, V_{1}^{T}) + (V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}) + \dots$$
  
$$\dots + (V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})\dots + (V^{T} - V_{n-1}^{T})f(V_{0}^{T}, V_{1}^{T}, V_{2}^{T}) \dots + V_{n}^{T})$$

# 5.1.1 ESTIMATION OF ERROR

Let  $f(V^T)$  be a real-valued function define n interval and (n+1) times differentiable on (a,b). If  $P_n(V^T)$  is the polynomial. Which interpolates  $f(V^T)$  at the (n+1) distinct points  $V_0^T, V_1^T \dots V_n^T \in (a,b)$ , then for all  $\overline{V^T} \in [a,b]$ , there exists  $\xi = \xi (\overline{V^T}) \in (a,b)$ 

$$e_n\left(\overline{V^T}\right) = f\left(\overline{V^T}\right) - P_n\left(\overline{V^T}\right)$$
$$= \frac{f^{(n+1)}\left(\xi\right)}{(n+1)} \prod_{j=0}^n \left(\overline{V^T} - V_j^T\right)$$

This is mathematical expression for estimation of error, if intervals are not being equally spaced.

# 6 WHEN THE TABULATED VALUES OF $V^{T} = f(T)$ ARE NOT EQUIDISTANT

If  $f(V_0^T), f(V_1^T), f(V_2^T)$ ..... $f(V_n^T)$  is to be vales of the inverse function corresponding to arguments  $V_0^T, V_1^T, V_2^T$ .... $V_n^T$  not necessarily equally spaced.

Let  $f(V^T)$  be a polynomial of degree n in  $V^T$  and since (n+1) values of  $f(V^T)$  are given so  $(n+1)^{th}$  difference are zero.

Consider,

Where  $A_0, A_1, A_2, \dots, A_n$  all are constants[19].

Now put  $V^T = V_0^T$  in equation (43), we got:

$$f(V_0^T) = A_0(V_0^T - V_1^T)(V_0^T - V_2^T).....(V_0^T - V_n^T)$$
  
$$\therefore A_0 = \frac{f(V_0^T)}{(V_0^T - V_1^T)(V_0^T - V_2^T)....(V_0^T - V_n^T)}$$
(44)

Again put  $V^{T} = V_{1}^{T}$  in equation (43), we got:

$$f(V_1^T) = A_1(V_1^T - V_1^T)(V_1^T - V_2^T)....(V_1^T - V_n^T)$$
  
$$\therefore A_1 = \frac{f(V_1^T)}{(V_1^T - V_1^T)(V_1^T - V_2^T)...(V_1^T - V_n^T)}$$
(45)

Similarly 
$$\therefore A_2 = \frac{f(V_2^T)}{(V_2^T - V_1^T)(V_2^T - V_2^T)....(V_2^T - V_n^T)}$$
 (46)

Proceeding in similar way, we got:

$$\therefore A_n = \frac{f(V_n^T)}{(V_n^T - V_1^T)(V_n^T - V_2^T)....(V_n^T - V_n^T)}$$
(47)

Substituting the values of  $A_0, A_1, A_2, \dots, A_n$  from equation (44), (45), (46), (47) in equation (43) we got:

$$f(V^{T}) = \frac{(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{n}^{T})}{(V_{0}^{T} - V_{1}^{T})(V_{0}^{T} - V_{2}^{T})...(V_{0}^{T} - V_{n}^{T})} f(V_{0}^{T}) + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{n}^{T})}{(V_{1}^{T} - V_{1}^{T})(V_{1}^{T} - V_{2}^{T})...(V_{1}^{T} - V_{n}^{T})} f(V_{1}^{T}) + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})...(V^{T} - V_{n}^{T})}{(V_{2}^{T} - V_{1}^{T})(V_{2}^{T} - V_{2}^{T})...(V_{2}^{T} - V_{n}^{T})} f(V_{2}^{T}) + .... + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{n}^{T})}{(V_{n}^{T} - V_{1}^{T})(V_{n}^{T} - V_{2}^{T})...(V_{n}^{T} - V_{n}^{T})} f(V_{n}^{T})$$

#### 6.1 ESTIMATION OF ERROR

Since the approximating polynomial  $f(V^T)$  given by Lagrangian formula has the same values  $f(V_0^T) f(V_1^T) f(V_2^T) f(V_3^T) f(V_4^T) \dots f(V_n^T)$  as does  $T = f(V^T)$  for the arguments  $V_0^T$ ,  $V_1^T$ ,  $V_2^T$ ,  $V_3^T$ ,  $V_4^T$  .....,  $V_0^T$  the error term must have zeros at these (n+1) points.

There for  $(V^T - V_0^T) (V^T - V_1^T) (V^T - V_2^T) (V^T - V_3^T)$  .....  $(V^T - V_n^T)$  must be factors of the error and we can write:

$$F(V^{T}) = f(V^{T}) + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})(V^{T} - V_{3}^{T})\dots(V^{T} - V_{n}^{T})}{(n+1)!}K(V^{T})$$
(48)

Let x to be fixed in value and consider the function

$$W(x) = F(x) - f(x) \frac{(x - V_0^T)(x - V_1^T)(x - V_2^T)(x - V_3^T)\dots(x - V_n^T)}{(n+1)!} K(V^T)$$
(49)

Then W(x) has zero  $x = V_0^T, V_1^T, V_2^T, V_3^T, \dots, V_n^T$  and  $V^T$ .

Since the  $(n+1)^{th}$  derivative of the  $n^{th}$  degree polynomial  $f(V^T)$  is zero.

$$W^{(n+1)}(x) = F^{(n+1)}(x) - K(V^{T})$$
(50)

As a consequence of Rolle's Theorem [20] [21], the  $(n+1)^{th}$  derivative of W(x) has at least one real zero  $x = \xi$  in the range  $V_0^T < \xi < V_n^T$ 

Therefore substituting  $x = \xi$  in equation (50)

$$W^{(n+1)}(\xi) = F^{(n+1)}(\xi) - K(V^{T})$$
$$K(V^{T}) = F^{(n+1)}(\xi) - W^{(n+1)}(\xi)$$
$$= F^{(n+1)}(\xi)$$

Or

Using this expression for  $K(V^T)$  and writing out  $f(V^T)$ 

$$f(V^{T}) = \frac{(V^{T} - V_{1}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{n}^{T})}{(V_{0}^{T} - V_{1}^{T})(V_{0}^{T} - V_{2}^{T})...(V_{0}^{T} - V_{n}^{T})}f(V_{0}^{T}) + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{2}^{T})...(V^{T} - V_{n}^{T})}{(V_{1}^{T} - V_{0}^{T})(V_{1}^{T} - V_{2}^{T})...(V_{1}^{T} - V_{n}^{T})}f(V_{1}^{T}) + .... + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})...(V^{T} - V_{n}^{T})}{(V_{n}^{T} - V_{0}^{T})(V_{n}^{T} - V_{1}^{T})...(V_{n}^{T} - V_{n-1}^{T})}f(V_{n}^{T}) + \frac{(V^{T} - V_{0}^{T})(V^{T} - V_{1}^{T})...(V^{T} - V_{n}^{T})}{(n+1)!}f^{(n+1)}(\xi)$$

Where  $V_0^T < \xi < V_n^T$ 

This is mathematical expression for estimation of error, if the tabulated values of the function are not equidistant.

#### 7 FORWARD DIFFERENCE FOR CONCENTRATION OF SUBSTRATE

If  $(V_0^S, S_0), (V_1^S, S_1), (V_2^S, S_2), \dots, (V_n^S, S_n)$  denoted the values of the inverse function then  $S_1 - S_0, S_2 - S_1, S_3 - S_2, S_4 - S_3, \dots, S_n - S_{n-1}, S$  are called the forward differences of S. These differences are denoted as  $\Delta S_0, \Delta S_1, \Delta S_2, \Delta S_3, \dots, \Delta S_{n-1}$  therefore

Where  $\Delta$  is called the forward difference operator, and  $\Delta S_0$ ,  $\Delta S_1 \Delta S_2 \Delta S_3 \dots \Delta S_{n-1}$  are called first order forward differences. The differences of the first order difference are called second order forward differences and are denoted as  $\Delta^2 S_0$ ,  $\Delta^2 S_1$ ,  $\Delta^2 S_2$ ,  $\Delta^2 S_3$ ,... etc.

 $\Delta^2 S_0 = \Delta S_1 - \Delta S_0$  $\Delta^2 S_1 = \Delta S_2 - \Delta S_1$  $\Delta^2 S_2 = \Delta S_3 - \Delta S_2$  $\Delta^2 S_3 = \Delta S_4 - \Delta S_3$ 

In general, the first order forward difference at the  $i^{th}$  point is

$$\Delta S_i = S_{i+1} - S_i$$

And the order forward difference at the point is

$$\Delta^j S_i = \Delta^{j-1} S_{i+1} - \Delta^{j-1} S_i$$

#### 7.1 FORMULA FOR FORWARD DIFFERENCE INTERPOLATION

If 
$$f(b), f(b+h), \ldots, f(b+nh)$$
 are be values of inverse function then

$$V^{S} = b, b + h, \dots, b + nh$$

Let  $f(V^S)$  be a polynomial of degree  $\mathcal{N}$  and let

$$f(V^{S}) = B_{0} + B_{1}(V^{S} - b) + B_{2}(V^{S} - b)(V^{S} - b - h) + B_{3}(V^{S} - b)(V^{S} - b - h)(V^{S} - b - 2h) + \dots + B_{n}[(V^{S} - b)(V^{S} - b - h).\dots, \{V^{S} - b - (n - 1)h\}]$$
(51)

Where  $B_0, B_1, \dots, B_n$  all are constants [19].

Putting  $V^{S} = a$  in equation (51), we got:

$$f(a) = B_0 \tag{52}$$

Again putting  $V^S = a + h$  in equation (51), we got:

$$f(b+h) = B_0 + B_1 h$$
  

$$A_1 h = f(b+h) - B_0$$
  

$$= f(b+h) - f(b)$$
  

$$= \Delta f(b)$$

$$A_1 = \frac{\Delta f(b)}{h}$$
(53)

Again putting  $V^{S} = b + 2h$  in equation (51), we got:

 $2h^2B_2 = f(b+2h) - B_0 - 2hB_1$ 

$$f(b+2h) = B_0 + B_1(2h) + B_2(2h)(h)$$
  
= B\_0 + 2hB\_1 + B\_0 + 2h^2B\_2 [from equation (52) and (53)]

Or

$$= f(b+2h) - f(b) - 2\Delta f(b)$$
  
=  $f(b+2h) - f(b) - 2\{f(b+h) - f(b)\}$   
=  $f(b+2h) - 2\{f(b+h) + f(b)\}$   
=  $\Delta^2 f(b)$ 

$$\therefore B_2 = \frac{1}{2h^2} \Delta^2 f(b)$$
Or  $B_2 = \frac{1}{2!h^2} \Delta^2 f(b)$ 
(54)

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(56)

Similarly 
$$B_3 = \frac{1}{3!h^3} \Delta^3 f(b)$$
 (55)

Proceeding in similar way, we got:  $B_n = \frac{1}{n!h^n} \Delta^n f(b)$ 

substituting the values of  $B_0, B_1, B_2, \dots, B_n$  in equation (51), we got:

$$f(V^{S}) = f(b) + \frac{\Delta f(b)}{h} (V^{S} - b) + \frac{\Delta^{2} f(b)}{2!h^{2}} (V^{S} - b) (V^{S} - b - h) + \dots + \frac{\Delta^{n} f(b)}{n!h^{n}} (V^{S} - b) (V^{S} - b - h) \dots \{V^{S} - b - (n-1)h\}$$
(57)

Now let  $V^S = b + hu$ 

:

$$\therefore V - b = hu$$

$$V^{s} - b - h = (u - 1)h$$

$$V^{s} - b - 2h = (u - 2)h$$

$$\vdots$$

$$\vdots$$

$$V^{s} - b - (n - 1)h = \{u - (n - 1)\}h$$

Putting these values in equation (57), we got:

$$f(b+hu) = f(b) + \frac{\Delta f(b)}{h}(uh) + \frac{\Delta^2 f(b)}{2!h^2}(uh)(u-1)h + \dots + \frac{\Delta^n f(b)}{n!h^n}(uh)(u-1)h \dots \{u-(n-1)h\}$$

Simplifying, we got:

$$f(b+hu) = f(b) + u\Delta f(b) + \frac{\Delta^2 f(b)}{2!} \{u(u-1)\} + \dots + \frac{\Delta^n f(b)}{n!} (u)(u-1)\dots \{u-(n-1)\}$$
(58)

Also we know that: 
$$u^{(m)} = u(u-1)(u-2)......\{u-(m-1)\}$$
 (59)

From equation (58) and (59), we have:

$$f(b+hu) = f(b) + \Delta f(b) \frac{u^{(1)}}{1!} + \Delta^2 f(b) \frac{u^{(2)}}{2!} + \Delta^3 f(b) \frac{u^{(3)}}{3!} + \dots + \Delta^n f(b) \frac{u^{(n)}}{n!}$$
(60)

### 7.1.1 ESTIMATION OF ERROR

Let V = f(T) be a function defined by (n+1) points  $(V_0^S, T_0), (V_1^S, T_1), \dots, (V_n^S, T_n)$ . When  $V_0^S, V_1^S, V_2^S, V_3^S, \dots, V_n^S$  are equally spaced with interval h and this function is continuous and differentiable (n+1) times.

The function be approximated by a polynomial  $P_n(V^S)$  of degree not exceeding a such that

$$P_n(V_i^S) = S_i$$
 [Where  $i = 0, 1, 2, 3, \dots, n$ ] (61)

Since the expression  $f(V^S) - P_n(V^S)$  vanishes for  $V^S = V_0^S, V_1^S, V_2^S, V_3^S, \dots, V_n^S$ ,

We put 
$$f(V^S) - P_n(V^S) = K\phi(V^S)$$
(62)

Where 
$$\phi(V^S) = (V^S - V_0^S)(V^S - V_1^S)....(V^S - V_n^S)$$
 (63)

And K is to be determined in such a way that equation (62) holds for any intermediate values of  $V^S$ , say  $V^S - V^{S}$ [where  $V_0^S \le V^S \le V_n^S$ ].

Therefore from equation (62),

$$K = \frac{f(V'^{s}) - P(V'^{s})}{\varphi(V'^{s})}$$
(64)

Now we construct a function  $f(V^S)$  such that

$$f(V_0^S) = f(V_1^S) - P_n(V^S) - K\varphi(V^S)$$

Where K is given by equation (64).

It is clear that

$$f(V_0^S) = f(V_1^S) = f(V_2^S) = f(V_3^S) = \dots f(V_n^S) = f(V^S) = 0$$
(65)

Let  $f(V^S)$  vanishes (n+2) times in the interval  $V_0^S \le V^S \le V_n^S$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^S)$  must vanish (n+1) times,  $f''(V^S)$  must vanish n times etc in the interval  $V_0^S \le V^S \le V_n^S$ .

Particularly,  $f^{(n+1)}(V^S)$  must vanish once in the interval  $V_0^S \le V^S \le V_n^S$ . Let this point be  $V^S = W$ ,  $V_0^S < W < V_n^S$ .

Now differentiating equation (65) (n+1) times with respect to  $V^{S}$  and putting  $V^{S} = W$ , we got:

$$f^{(n+1)}(W) - K(n+1)! = 0$$

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(66)

Or

Putting this value of K in equation (64), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V^{S}) - P_n(V^{S})}{\varphi(V^{S})}$$

Or 
$$f(V^{S}) - P_n(V^{S}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi(V^{S})$$
,  $V_0^S < W < V_n^S$ 

Since  $V^{S}$  is arbitrary therefore on dropping the prime on  $V^{S}$  we got:

$$f(V^{S}) - P_{n}(V^{S}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi(V^{S}), \quad V_{0}^{S} < W < V_{n}^{T}$$
(67)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(68)

Neglecting the terms containing second and higher powers of h in equation (68), we got:

$$f(W+h) = f(W) + hf'(W)$$

$$f'(W) = \frac{f(W+h) - f(W)}{h}$$
(69)

Or

Or

$$f'(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore \Delta f(V^S + h) f(V^S)]$$
$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore D = \frac{d}{h}]$$

$$Df(W) = \frac{-}{h}\Delta f(W) \qquad [\therefore D = \frac{w}{dW}]$$
$$D = \frac{1}{\Delta} \qquad [Because \ f(W) \text{ is arbitrary}]$$

$$D = \frac{1}{h}\Delta$$
 [Because  $f(W)$  is arbitrary]  
$$\therefore D^{n+1} = \frac{1}{h^{n+1}}\Delta^{n+1}$$

From equation (69), we got:

$$f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$$

Putting the values of  $f^{(n+1)}(W)$  in equation (67), we got:

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{\varphi(V^{S})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})(V^{S} - V_{2}^{S})...(V^{S} - V_{0}^{S})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$
(70)
$$\text{If } \frac{V^{S} - V_{n}^{S}}{h} = \beta$$

Then:

$$V^{S} - V_{0}^{S} = h\beta$$
  
$$V^{S} - V_{1}^{S} = V^{S} - (V_{0}^{S} - h) = (V^{S} - V_{0}^{S}) - h = (h\beta - h) = h(\beta - 1)$$

Similarly 
$$V^S - V_2^S = h(\beta - 2)$$

:

Similarly  $V^S - V_n^S = h(\beta - n)$ 

Putting these values in equation (70), we got:

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{(h\beta)\{h(\beta-1)\}\{h(\beta-2)\}\{h(\beta-3)\},\dots,\{(\beta-n)\}\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

# 8 BACKWARD DIFFERENCE OF SUBSTRATE CONCENTRATION

If  $(V_0^S, S_0), (V_1^S, S_1), (V_2^S, S_2), \dots, (V_n^S, S_n)$  denoted the values of the inverse then  $S_1 - S_0 S_2 - S_1$ ,  $S_3 - S_2, S_4 - S_3, \dots, S_n - S_{n-1}$  are called the backward differences of S. These differences are denoted as  $\nabla S_1, \nabla S_2, \nabla S_3, \dots, \nabla S_{n-1}$  therefore

Where  $\nabla$  is called the backward difference operator, and  $\nabla S_1 \nabla S_2 \nabla S_3$ ,....,  $\nabla S_{n-1}$  are called first order backward differences. The differences of the first order difference are called second order backward differences and are denoted as,  $\nabla^2 S_2$ ,  $\nabla^2 S_3$ ,  $\nabla^2 S_4$ ,  $\nabla^2 S_5$ .....etc.

$$\nabla^2 S_2 = \nabla S_2 - \nabla S_1$$
$$\nabla^2 S_3 = \nabla S_3 - \nabla S_2$$
$$\nabla^2 S_4 = \nabla S_4 - \nabla S_3$$
$$\nabla^2 S_5 = \nabla S_5 - \nabla S_4$$

In general, the first order forward difference at the  $i^{th}$  point is

$$\nabla S_i = S_i - S_{i-1}$$

And the order forward difference at the point is

$$\nabla^j S_i = \nabla^{j-1} S_i - \nabla^{j-1} S_{i-1}$$

#### 8.1 FORMULA FOR BACKWARD DIFFERENCE INTERPOLATION

If 
$$f(b), f(b+h), \dots, f(b+nh)$$
 are be values of inverse function then  
 $V^{s} = b, b+h, \dots, b+nh$ 

Let  $f(V^S)$  be a polynomial of degree n and let

$$f(V^{S}) = B_{0} + B_{1}(V^{S} - b - nh) + B_{2}(V^{S} - b - nh) \{V^{S} - b(n-1)h\} + B_{3}(V^{S} - b - nh) \{V^{S} - b - (n-1)h\} \{V^{S} - b - (n-2)h\} + \dots + B_{n}[(V^{S} - b - nh) \{V^{S} - b - (n-1)h\} \dots (V^{S} - b - h)$$
(71)

Where  $B_0, B_1, B_2, \dots, B_n$  all are constants [19].

Putting 
$$V^S = b + nh$$
 in equation (71), we got:  $f(b + nh) = B_0$  (72)

Again putting  $V^{S} = b + (n-1)h$  in equation (71), we got:

$$f \{b + (n-1)h\} = B_0 + B_1h$$
  

$$B_1h = B_0 - f \{b + (n-1)h\}$$
  

$$= f(b+nh) - f \{b + (n-1)h\}$$
  

$$= \Delta f (b+nh)$$
  

$$B_1 = \frac{\Delta f (b+nh)}{h}$$
(73)

Again putting  $V^{S} = b + (n-2)h$  in equation (71), we got:

$$f \{b + (n-2)h\} = B_0 + B_1(-2h) + B_2(-2h)(-h)$$

$$2h^2 B_2 = f \{b + (n-2)h\} - B_0 - 2hB_1$$
Or  $2h^2 B_2 = f \{b + (n-2)h\} - f (a + nh) + 2\nabla f (a + nh)$  [from equation(72) and (73)]
$$= f \{a + (n-2)h\} - f (a + nh) + 2[\{f (a + nh)\} - f \{a + (n-1)h\}]$$

$$= f \{a + (n-2)h\} - f (a + nh) - 2f \{a + (n-1)h\}$$

$$= f (a + nh) - 2[f \{a + (n-1)h\} + f (a)]$$

$$= \Delta^2 f (a + nh)$$

$$\therefore B_2 = \frac{1}{2h^2} \Delta^2 f (b)$$
Or  $A_2 = \frac{1}{2!h^2} \Delta^2 f (a = nh)$ 
Similarly  $A_3 = \frac{1}{3!h^3} \Delta^3 f (a + nh)$ 
(75)
$$\vdots$$

Proceeding in similar way, we got:  $A_n = \frac{1}{n!h^n} \Delta^n f(a+nh)$  (76)

substituting the values of  $A_0, A_1, A_2, \dots, A_n$  in equation (71), we got:

$$f(V^{S}) = f(a+nh) + \frac{\Delta f(a)}{h} (V^{S} - a - nh) + \frac{\Delta^{2} f(a+nh)}{2!h^{2}} (V^{S} - a - nh) \{V^{S} - a - (n-1)h\} + \dots$$

$$\dots + \frac{\Delta^{n} f(a+nh)}{n!h^{n}} (V^{S} - a - nh) \{V^{S} - a - (n-1)h\} \dots (V^{S} - a - n)$$
(77)

Now let:  $V^S = a + nh + hu$ 

$$\therefore V^{S} - a = nh + hu$$

$$V^{S} - a - (n-1)h = (u+1)h$$

$$V^{S} - a - (n-2)h = (u+2)h$$

$$\vdots$$

$$\vdots$$

$$V^{S} - a - h = \{u + (n-1)\}h$$

Putting these values in equation (77), we got:

$$f(a+nh+hu) = f(a+nh) + \frac{\Delta f(a+nh)}{h}(uh) + \frac{\Delta^2 f(a+nh)}{2!h^2}(uh)(u+1)h + \dots + \frac{\Delta^n f(a+nh)}{n!h^n}(uh)(u+1)h \dots \{u+(n-1)h\}$$

Simplifying, we got:

$$f(a+nh+hu) = f(a+nh) + u\Delta f(a+nh) + \frac{\Delta^2 f(a+nh)}{2!} \{u(u+1)\} + \dots + \frac{\Delta^n f(a+nh)}{n!} \{u(u+1), \dots, \{u+(n-1)\}\}$$
(78)

#### 8.1.1 ESTIMATION OF ERROR

Let V = f(T) be a function defined by (n+1) points  $(V_0^S, E_0), (V_1^S, E_1), \dots, (V_n^S, E_n)$ . When  $V_0^S, V_1^S, V_2^S, V_3^S, \dots, V_n^S$  are equally spaced with interval h and this function is continuous and differentiable (n+1) times.

The function be approximated by a polynomial  $P_n(V^S)$  of degree not exceeding a such that

$$P_n(V_i^S) = E_i$$
 [Where  $i = 1, 2, 3, ..., n$ ] (79)

Since the expression  $f(V^S) - P_n(V^S)$  vanishes for  $V^S = V_0^S$ ,  $V_1^S$ ,  $V_2^S$ ,  $V_3^S$ ...... $V_n^S$ ,

We put 
$$f(V^{S}) - P_{n}(V^{S}) = K\phi(V^{S})$$
(80)

Where 
$$\phi_1(V^S) = (V^S - V_n^S)(V^S - V_{n-1}^S)....(V^S - V_0^S)$$
 (81)

And K is to be determined in such a way that equation (81) holds for any intermediate values of  $V^S$ , say  $V^S - V^{S'}$  [where  $V_0^S \le V_0^S \le V_n^S$ ].

Therefore from equation (81),

$$K = \frac{f(V^{S}) - P_n(V^{S})}{\varphi_1(V^{S})}$$
(82)

Now we construct a function  $f(V^s)$  such that

$$f(V_0^S) = f(V_1^S) - P_n(V^S) - K\varphi_1(V^S)$$

Where K is given by equation (82).

It is clear that

Or

$$f(V_0^S) = f(V_1^S) = f(V_2^S) = f(V_3^S) = \dots f(V_n^S) = f(V'^S) = 0$$
(83)

Let  $f(V^S)$  vanishes (n+2) times in the interval  $V_0^S \le V^S \le V_n^S$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^S)$  must vanish (n+1) times,  $f''(V^S)$  must vanish n times etc in the interval  $V_0^S \le V_n^S \le V_n^S$ .

Particularly,  $f^{(n+1)}(V^S)$  must vanish once in the interval  $V_0^S \le V^S \le V_n^S$ . Let this point be  $V^S = W$ ,  $V_0^S < W < V_n^S$ . Now differentiating equation (83) (n+1) times with respect to  $V^S$  and putting  $V^S = W$ , we got:

$$f^{(n+1)}(W) - K(n+1)! = 0$$

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(84)

Putting this value of K in equation (82), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V^{1S}) - P_n(V^{1S})}{\varphi_1(V^{1S})}$$
  
Or  $f(V^{1S}) - P_n(V^{1S}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi_1(V^{1S}), \qquad V_0^S < W < V_n^S$ 

Since  $V^{S}$  is arbitrary therefore on dropping the prime on  $V^{S}$  we got:

$$f(V^{S}) - P_{n}(V^{S}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi_{1}(V^{S}), \quad V_{0}^{S} < W < V_{n}^{S}$$
(85)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(86)

Neglecting the terms containing second and higher powers of h in equation (86), we got:

$$f(W+h) = f(W) + hf'(W)$$

Or

$$f'(W) = \frac{f(W+h) - f(W)}{h}$$
(87)

Or

$$f'(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore \Delta f(W) = f(W+h) - f(W)]$$
$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore D = \frac{d}{dW}]$$

$$D = \frac{1}{h}\Delta$$
 [Because  $f(W)$  is arbitrary]  
$$\therefore D^{n+1} = \frac{1}{h^{n+1}}\Delta^{n+1}$$

From equation (87), we got:

$$f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$$

Putting the values of  $f^{(n+1)}(Y)$  in equation (85), we got:

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{\varphi_{1}(V^{S})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})(V^{S} - V_{2}^{S})....(V^{S} - V_{0}^{S})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$
(88)
$$\text{If } \frac{V^{S} - V_{n}^{S}}{h} = \beta$$

Then

$$V^{S} - V_{n}^{S} = h\beta$$
  
$$V^{S} - V_{n-1}^{S} = V^{S} - (V_{n}^{S} - h) = (V^{S} - V_{n}^{S}) + h = (h\beta + h) = h(\beta + 1)$$

Similarly  $V^S - V^S_{n-2} = h(\beta + 2)$ 

:

Similarly  $V^S - V_0^S = h(\beta + n)$ 

Putting these values in equation (20), we got:

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{(h\beta)\{h(\beta+1)\}\{h(\beta+2)\}\{h(\beta+3)\}\dots\{(\beta+n)\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

OR

$$f(V^{S}) - P_{n}(V^{S}) = \left[\frac{\beta(\beta+1)(\beta+2)(\beta+3)...(\beta+n)}{(n+1)!}\right] [\Delta^{(n+1)}f(W)]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

#### 9 DIVIDE DIFFERENCE OF SUBSRATE CONCENTRATION

If 
$$(V_1^S, S_1), (V_2^S, S_2), \dots, (V_n^S, S_n)$$
 denoted the values of the inverse function then  $\frac{S_2 - S_1}{V_2^S - V_1^S}$ ,  $\frac{S_3 - S_2}{V_3^S - V_2^S}$ ,

 $\frac{S_4 - S_3}{V_4^S - V_3^S}, \dots, \frac{S_n - S_{n-1}}{V_n^S - V_{n-1}^S} \text{ are called the divide differences of } S. \text{ These differences are denoted as } \Delta_d S_1, \Delta_d S_2, \Delta_d S_3, \dots, \Delta_d S_{n-1} \text{ therefore } S_n - 1 \text{ therefor$ 

:  

$$\Delta_d S_{n-1} = \frac{S_n - S_{n-1}}{V_n^S - V_{n-1}^S}$$

Where  $\Delta_d$  is called the divide difference operator, and  $\Delta_d S_1 \Delta_d S_2 \Delta_d S_3 \dots \Delta_d S_{n-1}$  are called first order divide differences. The differences of the first order difference are called second order divide differences and are denoted as  $\Delta_d^2 S_1$ ,  $\Delta_d^2 S_2$ ,  $\Delta_d^2 S_3$ , ... .etc.

$$\Delta_d^2 S_1 = \frac{\Delta_d S_2 - \Delta_d S_1}{V_3^S - V_1^S}$$
$$\Delta_d^2 S_2 = \frac{\Delta_d S_3 - \Delta_d S_2}{V_4^S - V_2^S}$$
$$\Delta_d^2 S_3 = \frac{\Delta_d S_4 - \Delta_d S_3}{V_5^S - V_3^S}$$

In general, the first order divide difference at the  $i^{th}$  point is

$$\Delta_{d} S_{i} = \frac{S_{i+1} - S_{i}}{V_{i+1}^{S} - V_{i}^{S}}$$

And the order divide difference at the point is

$$\Delta^{j} S_{i} = \frac{\Delta^{j-1} S_{i+1} - \Delta^{j-1} S_{i}}{V_{i+j}^{S} - V_{i}^{S}}$$

# 9.1 FORMULA FOR DIVIDE DIFFERENCE INTERPOLATION

By the definition of divide difference

$$f(V^{S}, V_{0}^{S}) = \frac{f(V^{S})f(V_{0}^{S})}{V^{S} - V_{0}^{S}}$$
(89)

Or 
$$f(V^S) = f(V_0^S) + (V^S - V_0^S)f(V^S, V_0^S)$$

Again by the definition of second divided difference

$$f(V^{S}, V_{0}^{S}, V_{1}^{S}) = \frac{f(V^{S}, V_{0}^{S}) - f(V_{0}^{S}, V_{1}^{S})}{V^{S} - V_{1}^{S}}$$

Or 
$$f(V^{S}, V_{0}^{S}) = f(V_{0}^{S}, V_{1}^{S}) + (V^{S} - V_{1}^{S})f(V^{S}, V_{0}^{S}, V_{1}^{S})$$
 (90)

Similarly 
$$f(V^{s}, V_{0}^{s}, V_{1}^{s}) = f(V_{0}^{s}, V_{1}^{s}, V_{2}^{s}) + (V^{s} - V_{2}^{s})f(V^{s}, V_{0}^{s}, V_{1}^{s}, V_{2}^{s})$$
 (91)

Proceeding in similar way, we got:

::

$$f(V^{S}, V_{0}^{S}, V_{1}^{S}, \dots, V_{n-1}^{S}) = f(V_{0}^{S}, V_{1}^{S}, V_{2}^{S}, \dots, V_{n}^{S}) + (V^{S} - V_{n}^{S})f(V^{S}, V_{0}^{S}, V_{n}^{S})$$
(92)

Multiplying equation (90) by  $\left(V^{\scriptscriptstyle S}-V^{\scriptscriptstyle S}_{\scriptscriptstyle 0}\right)$  ,

Multiplying equation (91) by  $(V^S - V^S_0) (V^S - V^S_0)$ ,

Multiplying equation (92) by 
$$(V^S - V_0^S)$$
  $(V^S - V_1^S)$  ......  $(V^S - V_{n-1}^S)$ 

And adding to equation (89), we got:

$$f(V^{s}) = f(V_{0}^{s}) + (V^{s} - V_{0}^{s})f(V_{0}^{s}, V_{1}^{s}) + (V^{s} - V_{1}^{s})(V^{s} - V_{2}^{s})f(V_{0}^{s}, V_{1}^{s}, V_{2}^{s}) + \dots + (V^{s} - V_{0}^{s})(V^{s} - V_{1}^{s})(V^{s} - V_{2}^{s})\dots + (V^{s} - V_{n-1}^{s})f(V_{0}^{s}, V_{1}^{s}, V_{2}^{s}\dots + V_{n}^{s}) + R_{n}$$

Where  $R_n$  is the reminder and is given by

$$R_n = (V^S - V_0^S)(V^S - V_1^S)(V^S - V_2^S)....(V^S - V_n^S)f(V_0^S, V_1^S, V_2^S..., V_n^S)$$

If the function  $f(V^S)$  is polynomial of degree n, then  $f(V_0^S, V_1^S, V_2^S, ..., V_n^S)$  vanishes so that

$$f(V^{s}) = f(V_{0}^{s}) + (V^{s} - V_{0}^{s})f(V_{0}^{s}, V_{1}^{s}) + (V^{s} - V_{1}^{s})(V^{s} - V_{2}^{s})f(V_{0}^{s}, V_{1}^{s}, V_{2}^{s}) + \dots$$
  
$$\dots + (V^{s} - V_{0}^{s})(V^{s} - V_{1}^{s})(V^{s} - V_{2}^{s})\dots + (V^{s} - V_{n-1}^{s})f(V_{0}^{s}, V_{1}^{s}, V_{2}^{s}) + \dots$$

#### 9.1.1 ESTIMATION OF ERROR

Let  $f(V^S)$  be a real-valued function define n interval and (n+1) times differentiable on (a,b). If  $P_n(V^S)$  is the polynomial. Which interpolates  $f(V^S)$  at the (n+1) distinct points  $V_0^S, V_1^S \dots V_n^S \in (a,b)$ , then for all  $\overline{V^S} \in [a,b]$ , there exists  $\xi = \xi (\overline{V^S}) \in (a,b)$ 

$$e_n\left(\overline{V^S}\right) = f\left(\overline{V^S}\right) - P_n\left(\overline{V^S}\right)$$
$$= \frac{f^{(n+1)}\left(\xi\right)}{(n+1)} \prod_{j=0}^n \left(\overline{V^S} - V_j^S\right)$$

This is mathematical expression for estimation of error, if intervals are not be equally spaced.

# 10 WHEN THE TABULATED VALUES OF $V^{s} = f(S)$ are not Equidistant

If  $f(V_0^S), f(V_1^S), f(V_2^S), \dots, f(V_n^S)$  is to be vales of the inverse function corresponding to arguments  $V_0^S, V_1^S, V_2^S, \dots, V_n^S$  not necessarily equally spaced.

Let  $f(V^S)$  be a polynomial of degree n in  $V^S$  and since (n+1) values of  $f(V^S)$  are given so  $(n+1)^{th}$  difference are zero.

Consider:

$$f(V^{T}) = A_{0}(V^{S} - V_{1}^{S})(V^{S} - V_{2}^{S})....(V^{S} - V_{n}^{S}) + A_{1}(V^{S} - V_{0}^{S})(V^{S} - V_{2}^{S})....(V^{S} - V_{n}^{S}) + A_{2}(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})....(V^{S} - V_{n}^{S}) + .....(V^{S} - V_{n}^{S}) + ......(V^{S} - V_{n}^{S}) ..... + A_{n}(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})....(V^{S} - V_{n-1}^{S})$$
(93)

Where  $A_0, A_1, A_2$ ..... $A_n$  all are constants.

Now put  $V^{S} = V_{0}^{S}$  in equation (93), we got:

$$f(V_0^S) = A_0(V_0^S - V_1^S)(V_0^S - V_2^S)....(V_0^S - V_n^S)$$
  
$$\therefore A_0 = \frac{f(V_0^S)}{(V_0^S - V_1^S)(V_0^S - V_2^S)...(V_0^S - V_n^S)}$$
(94)

Again put  $V^{S} = V_{1}^{S}$  in equation (93), we got:

$$f(V_1^S) = A_1(V_1^S - V_1^S)(V_1^S - V_2^S)....(V_1^S - V_n^S)$$
  
$$\therefore A_1 = \frac{f(V_1^S)}{(V_1^S - V_1^S)(V_1^S - V_2^S)...(V_1^S - V_n^S)}$$
(95)

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Similarly 
$$\therefore A_2 = \frac{f(V_2^S)}{(V_2^S - V_1^S)(V_2^S - V_2^S)....(V_2^S - V_n^S)}$$
(96)
  
:
  
:
  
:

Proceeding in similar way, we got:

$$\therefore A_n = \frac{f(V_n^S)}{(V_n^S - V_1^S)(V_n^S - V_2^S)....(V_n^S - V_n^S)}$$
(97)

Substituting the values of  $A_0, A_1, A_2, \dots, A_n$  from equation (94),(95),(96),(97) in equation (93)we got:

$$f(V^{S}) = \frac{(V^{S} - V_{1})(V^{S} - V_{2}^{S})....(V^{S} - V_{n}^{S})}{(V_{0}^{S} - V_{1}^{S})(V_{0}^{S} - V_{2}^{S})....(V_{0}^{S} - V_{n}^{S})} f(V_{0}^{S}) + \frac{(V^{S} - V_{0}^{S})(V^{S} - V_{2}^{S})....(V^{S} - V_{n}^{S})}{(V_{1}^{S} - V_{1}^{S})(V_{1}^{S} - V_{2}^{S})....(V_{1}^{S} - V_{n}^{S})} f(V_{1}^{S}) + \frac{(VS - V_{0}^{S})(V^{S} - V_{1}^{S})....(V^{S} - V_{n}^{S})}{(V_{2}^{S} - V_{1}^{S})(V_{2}^{S} - V_{2}^{S})....(V_{2}^{S} - V_{n}^{S})} f(V_{2}^{S}) + ..... + \frac{(V^{S} - V_{0}^{S})(V^{S} - V_{2}^{S})....(V^{S} - V_{n}^{S})}{(V_{n}^{S} - V_{1}^{S})(V_{n}^{S} - V_{2}^{S})....(V_{n}^{S} - V_{n}^{S})} f(V_{n}^{S})$$

#### **10.1** ESTIMATION OF ERROR

Since the approximating polynomial  $f(V^S)$  given by Lagrangian formula has the same values  $f(V_0^S) f(V_1^S) f(V_2^S) f(V_3^S) f(V_4^S)$ ..... $f(V_n^S)$  as does  $T = f(V^S)$  for the arguments  $V_0^s$ ,  $V_1^s$ ,  $V_2^s$ ,  $V_3^s$ ,  $V_4^s$ ...., $V_4^s$  the error term must have zeros at these (n+1) points.

There for  $(V^S - V_0^S) (V^S - V_1^S) (V^S - V_2^S) (V^S - V_3^S)$  .....  $(V^S - V_n^S)$  must be factors of the error and we can write:

$$F(V^{s}) = f(V^{s}) + \frac{(V^{s} - V_{0}^{s})(V^{s} - V_{1}^{s})(V^{s} - V_{2}^{s})(V^{s} - V_{3}^{s})\dots(V^{s} - V_{n}^{s})}{(n+1)!}K(V^{s})$$
(98)

Let x to be fixed in value and consider the function

$$W(x) = F(x) - f(x) \frac{(x - V_0^S)(x - V_1^S)(x - V_2^S)(x - V_3^S)\dots(x - V_n^S)}{(n+1)!} K(V^S)$$
(99)

Then W(x) has zero  $x = V_0^S, V_1^S, V_2^S, V_3^S, \dots, V_n^S$  and  $V^S$ .

Since the  $(n+1)^{th}$  derivative of the  $n^{th}$  degree polynomial  $f(V^S)$  is zero.

$$W^{(n+1)}(x) = F^{(n+1)}(x) - K(V^{S})$$
(100)

As a consequence of Rolle's Theorem [15] [16], the  $(n+1)^{th}$  derivative of W(x) has at least one real zero  $x = \xi$  in the range  $V_0^s < \xi < V_n^s$ 

Therefore substituting  $x = \xi$  in equation (100)

Or

$$W^{(n+1)}(\xi) = F^{(n+1)}(\xi) - K(V^{S})$$
$$K(V^{S}) = F^{(n+1)}(\xi) - W^{(n+1)}(\xi)$$
$$= F^{(n+1)}(\xi)$$

Using this expression for  $K(V^S)$  and writing out  $f(V^S)$ 

$$f(V^{S}) = \frac{(V^{S} - V_{1}^{S})(V^{S} - V_{2}^{S})...(V^{S} - V_{n}^{S})}{(V_{0}^{S} - V_{1}^{S})(V_{0}^{S} - V_{2}^{S})...(V_{0}^{S} - V_{n}^{S})}f(V_{0}^{S}) + \frac{(V^{S} - V_{0}^{S})(V^{S} - V_{2}^{S})...(V^{S} - V_{n}^{S})}{(V_{1}^{S} - V_{0}^{S})(V_{1}^{S} - V_{2}^{S})...(V_{1}^{S} - V_{n}^{S})}f(V_{1}^{S}) + .... + \frac{(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})...(V^{S} - V_{n-1}^{S})}{(V_{n}^{S} - V_{0}^{S})(V_{n}^{S} - V_{1}^{S})...(V_{n}^{S} - V_{n-1}^{S})}f(V_{n}^{S}) + \frac{(V^{S} - V_{0}^{S})(V^{S} - V_{1}^{S})...(V^{S} - V_{n}^{S})}{(n+1)!}f^{(n+1)}(\xi)$$

Where  $V_0^S < \xi < V_n^S$ 

This is mathematical expression for estimation of error, if the tabulated values of the function are not equidistant.

#### 11 FORWARD DIFFERENCE OF ENZYME CONCENTRATION

If  $(V_0^E, E_0), (V_1^E, E_1), (V_2^E, E_2), \dots, (V_n^E, E_n)$  denoted the values of the inverse function then  $E_1 - E_0$ ,  $E_2 - E_1$ ,  $E_3 - E_2$ ,  $E_4 - E_3$ ,  $\dots, E_n - E_{n-1}$ , E are called the forward differences of E. These differences are denoted as  $\Delta E_0$ ,  $\Delta E_1$ ,  $\Delta E_2$ ,  $\Delta E_3$ ,  $\dots, \Delta E_{n-1}$  therefore

 $\Delta E_0 = E_1 - E_0$   $\Delta E_1 = E_2 - E_1,$   $\Delta E_2 = E_3 - E_2,$   $\Delta E_3 = E_4 - E_3,$ :
:
:  $\Delta E_{n-1} = E_n - E_{n-1}$ 

Where  $\Delta$  is called the forward difference operator, and  $\Delta E_0$ ,  $\Delta E_1 \Delta E_2 \Delta E_3 \dots \Delta E_{n-1}$  are called first order forward differences. The differences of the first order difference are called second order forward differences and are denoted as  $\Delta^2 E_0$ ,  $\Delta^2 E_1$ ,  $\Delta^2 E_2$ ,  $\Delta^2 E_3$ , ... .etc.

$$\Delta^{2} E_{0} = \Delta E_{1} - \Delta E_{0}$$
$$\Delta^{2} E_{1} = \Delta E_{2} - \Delta E_{1}$$
$$\Delta^{2} E_{2} = \Delta E_{3} - \Delta E_{2}$$
$$\Delta^{2} E_{3} = \Delta E_{4} - \Delta E_{3}$$

In general, the first order forward difference at the  $i^{th}$  point is

$$\Delta E_i = E_{i+1} - E_i$$

And the order forward difference at the point is :  $\Delta^{j}E_{i} = \Delta^{j-1}E_{i+1} - \Delta^{j-1}E_{i}$ 

#### 11.1 FORMULA FOR FORWARD DIFFERENCE INTERPOLATION

If 
$$f(g), f(g+h), \dots, f(g+nh)$$
 are be values of inverse function then

$$V^E = g, g + h, \dots, g + nh$$

Let  $f(V^{\scriptscriptstyle E})$  be a polynomial of degree  ${\it n}$  and let

$$f(V^{E}) = G_{0} + G_{1}(V^{E} - g) + G_{2}(V^{E} - g)(V^{E} - g - h) + A_{3}(V^{E} - g)(V^{E} - g - h)(V^{E} - g - 2h) + \dots + G_{n}[(V^{E} - g)(V^{E} - g - h) \dots \{V^{E} - g - (n - 1)h\}]$$
(101)

Where  $G_0, G_1, \ldots, G_n$  all are constants [19].

Putting  $V^E = g$  in equation (101), we got:

• •

$$f(g) = G_0 \tag{102}$$

Again putting  $V^E = g + h$  in equation (101), we got:

$$f(g+h) = G_0 + G_1 h$$

$$G_1 h = f(g+h) - G_0$$

$$= f(g+h) - f(g)$$

$$= \Delta f(g)$$

$$G_1 = \frac{\Delta f(g)}{h}$$
(103)

Again putting  $V^{E} = g + 2h$  in equation (101), we got:

$$f(g+2h) = G_0 + G_1(2h) + G_2(2h)(h)$$
  
= G\_0 + 2hG\_1 + G\_0 + 2h^2G\_2 [from equation (102) and (103)]

 $2h^2G_2 = f(g+2h) - G_0 - 2hG_1$ 

$$= f(g+2h) - f(g) - 2\Delta f(g)$$
  
=  $f(g+2h) - f(g) - 2\{f(g+h) - f(g)\}$   
=  $f(g+2h) - 2\{f(g+h) + f(g)\}$   
=  $\Delta^2 f(g)$ 

$$\therefore G_2 = \frac{1}{2h^2} \Delta^2 f(g)$$
Or  $G_2 = \frac{1}{2!h^2} \Delta^2 f(g)$ 
(104)

(106)

Similarly 
$$G_3 = \frac{1}{3!h^3} \Delta^3 f(g)$$
 (105)

Proceeding in similar way, we got:  $G_n = \frac{1}{n!h^n} \Delta^n f(g)$ 

substituting the values of  $G_0, G_1, G_2, \dots, G_n$  in equation (101), we got:

$$f(V^{E}) = f(g) + \frac{\Delta f(g)}{h} (V^{E} - g) + \frac{\Delta^{2} f(g)}{2!h^{2}} (V^{E} - g) (V^{E} - g - h) + \dots + \frac{\Delta^{n} f(g)}{n!h^{n}} (V^{E} - g) (V^{E} - g - h) \dots \{V^{E} - g - (n-1)h\}$$
(107)

Now let  $V^E = g + hu$ 

:

$$\therefore V^{E} - a = hu$$

$$V^{E} - g - h = (u - 1)h$$

$$V^{E} - g - 2h = (u - 2)h$$

$$\vdots$$

$$\vdots$$

$$V^{E} - g - (n - 1)h = \{u - (n - 1)\}h$$

Putting these values in equation (107), we got:

$$f(g+hu) = f(g) + \frac{\Delta f(g)}{h} (uh) + \frac{\Delta^2 f(g)}{2!h^2} (uh)(u-1)h + \dots + \frac{\Delta^n f(g)}{n!h^n} (uh)(u-1)h \dots \{u-(n-1)h\}$$

Simplifying, we got:

$$f(g+hu) = f(g) + u\Delta f(g) + \frac{\Delta^2 f(g)}{2!} \{u(u-1)\} + \dots + \frac{\Delta^n f(g)}{n!} \{u(u-1), \dots, \{u-(n-1)\}\}$$
(108)

Also we know that

$$u^{(m)} = u(u-1)(u-2).....\{u-(m-1)\}$$
(109)

From equation (108) and (109), we have:

$$f(g+hu) = f(g) + \Delta f(g)\frac{u^{(1)}}{1!} + \Delta^2 f(g)\frac{u^{(2)}}{2!} + \Delta^3 f(g)\frac{u^{(3)}}{3!} + \dots + \Delta^n f(g)\frac{u^{(n)}}{n!}$$
(110)

#### 11.1.1 ESTIMATION OF ERROR

Let V = f(T) be a function defined by (n+1) points  $(V_0^E, E_0), (V_1^E, E_1), \dots, (V_n^E, E_n)$ . When  $V_0^E, V_1^E, V_2^E, V_3^E, \dots, V_n^E$  are equally spaced with interval h and this function is continuous and differentiable (n+1) times.

The function be approximated by a polynomial  $P_n(V^E)$  of degree not exceeding a such that

$$P_n(V_i^E) = E_i$$
 [Where  $i = 0, 1, 2, 3, \dots, n$ ] (111)

Since the expression  $f(V^E) - P_n(V^E)$  vanishes for  $V^E = V_0^E$ ,  $V_1^E$ ,  $V_2^E$ ,  $V_3^E$ , ...... $V_n^E$ ,

We put 
$$f(V^E) - P_n(V^E) = K\varphi(V^E)$$
(112)

Where 
$$\varphi(V^E) = (V^E - V_0^E)(V^E - V_1^E)....(V^E - V_n^E)$$
 (113)

And K is to be determined in such a way that equation (112) holds for any intermediate values of  $V^E$ , say  $V^E - V^{*E}$  [where  $V_0^E \leq V^* \leq V_n^E$ ].

Therefore from equation (112),

$$K = \frac{f(V^{E}) - P(V^{E})}{\varphi(V^{E})}$$
(114)

Now we construct a function  $f(V^E)$  such that

$$f(V_0^E) = f(V_1^E) - P_n(V^E) - K\varphi(V^E)$$

Where K is given by equation (114).

It is clear that

$$f(V_0^E) = f(V_1^E) = f(V_2^E) = f(V_3^E) = \dots f(V_n^E) = f(V^E) = 0$$
(115)

Let  $f(V^E)$  vanishes (n+2) times in the interval  $V_0^E \le V^E \le V_n^E$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^E)$  must vanish (n + 1) times,  $f''(V^E)$  must vanish n times etc in the interval  $V_0^E \le V^E \le V_n^E$ . Particularly,  $f^{(n+1)}(V^E)$  must vanish once in the interval  $V_0^E \le V^E \le V_n^E$ . Let this point be  $V^E = W$ ,  $V_0^E < W < V_n^E$ . Now differentiating equation (15) (n + 1) times with respect to  $V^E$  and putting  $V^E = W$ , we got:

$$f^{(n+1)}(W) - K(n+1)! = 0$$

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(116)

Or

Putting this value of  $\ K$  in equation (114), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V^{*E}) - P_n(V^{*E})}{\varphi(V^{*E})}$$
$$f(V^{*E}) - P_n(V^{*E}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi(V^{*E}) , \qquad V_0^E < W < V_n^E$$

Or

Since  $V^{^{1E}}$  is arbitrary therefore on dropping the prime on  $V^{^{1E}}$  we got:

$$f(V^{E}) - P_{n}(V^{E}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi(V^{E}), \quad V_{0}^{E} < W < V_{n}^{E}$$
(117)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(118)

Neglecting the terms containing second and higher powers of h in equation (118), we got:

$$f(W+h) = f(W) + hf'(W)$$
  
$$f'(W) = \frac{f(W+h) - f(W)}{h}$$
 (119)

Or

Or

$$f'(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore \Delta f(V^E + h) f(V^E)]$$
$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [\therefore D = \frac{d}{dW}]$$
$$D = \frac{1}{h} \Delta \qquad [Because \ f(W) \text{ is arbitrary}]$$
$$\therefore D^{n+1} = \frac{1}{h^{n+1}} \Delta^{n+1}$$

From equation (119), we got:  $f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$ 

Putting the values of  $\,f^{\scriptscriptstyle(n+1)}(W)$  in equation (117), we got:

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{\varphi(V^{E})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E}).....(V^{E} - V_{0}^{E})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$
(120)
$$\text{If } \frac{V^{E} - V_{n}^{E}}{h} = \beta \quad \text{Then:}$$

$$V^{E} - V_{0}^{E} = h\beta$$

$$V^{E} - V_{1}^{E} = V^{E} - (V_{0}^{E} - h) = (V^{E} - V_{0}^{E}) - h = (h\beta - h) = h(\beta - 1)$$
Similarly  $V^{E} - V_{2}^{E} = h(\beta - 2)$ 

$$\vdots$$

$$\vdots$$

Similarly  $V^E - V_n^E = h(\beta - n)$ 

Putting these values in equation (20), we got:

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{(h\beta)\{h(\beta-1)\}\{h(\beta-2)\}\{h(\beta-3)\}\dots\{(\beta-n)\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

#### 12 BACKWARD DIFFERENCE OF ENZYME CONCENTRATION

If  $(V_0^E, E_0), (V_1^E, E_1), (V_2^E, E_2), \dots, (V_n^E, E_n)$  denoted the values of the inverse then  $E_2 - E_1$ ,  $E_3 - E_2$ ,  $E_4 - E_3, \dots, E_n - E_{n-1}$  are called the backward differences of E. These differences are denoted as  $\nabla E_1, \nabla E_2, \nabla E_3, \dots, \nabla E_{n-1}$  therefore:

 $\Delta E_n = E_n - E_{n-1}$ 

Where  $\nabla$  is called the backward difference operator, and  $\nabla E_1 \nabla E_2 \nabla E_3 \dots \nabla E_{n-1}$  are called first order backward differences. The differences of the first order difference are called second order backward differences and are denoted as,  $\nabla^2 E_2$ ,  $\nabla^2 E_3$ ,  $\nabla^2 E_4$ ,  $\nabla^2 E_5$  .....etc.

 $\nabla^{2} E_{2} = \nabla E_{2} - \nabla E_{1}$  $\nabla^{2} E_{3} = \nabla E_{3} - \nabla E_{2}$  $\nabla^{2} E_{4} = \nabla E_{4} - \nabla E_{3}$  $\nabla^{2} E_{5} = \nabla E_{5} - \nabla E_{4}$ 

In general, the first order forward difference at the  $i^{th}$  point is:  $\nabla E_i = E_i - E_{i-1}$ And the order forward difference at the point is:  $\nabla^j E_i = \nabla^{j-1} E_i - \nabla^{j-1} E_{i-1}$ 

#### 12.1 FORMULA FOR BACKWARD DIFFERENCE INTERPOLATION

If 
$$f(k)$$
,  $f(k+h)$ ,...,  $f(k+nh)$  are be values of inverse function then:  $V^E = k, k+h, \dots, k+nh$ 

Let  $f(V^E)$  be a polynomial of degree  $\mathcal{N}$  and let

$$f(V^{E}) = K_{0} + K_{1}(V^{E} - k - nh) + K_{2}(V^{E} - k - nh) \{V^{E} - K(n - 1)h\} + K_{3}(V^{E} - k - nh) \{V^{E} - k - (n - 1)h\}$$

$$\{V^{E} - k - (n - 2)h\} + \dots + K_{n}[(V^{E} - k - nh) \{V^{E} - k - (n - 1)h\} \dots (V^{E} - k - h)$$
(121)

Where  $K_0, K_1, K_2, \dots, K_n$  all are constants [19].

Putting  $V^E = k + nh$  in equation (121), we got:  $f(k + nh) = K_0$ (122)

Again putting V = k + (n-1)h in equation (121), we got:

$$f \{k + (n-1)h\} = K_0 + K_1h$$
  

$$K_1h = K_0 - f \{k + (n-1)h\}$$
  

$$= f(k+nh) - f \{k + (n-1)h\}$$
  

$$= \Delta f (k+nh)$$
  

$$K_1 = \frac{\Delta f (k+nh)}{h}$$
(123)

Again putting  $V^E = k + (n-2)h$  in equation (121), we got:

$$f \{k + (n-2)h\} = K_0 + K_1(-2h) + K_2(-2h)(-h)$$

$$2h^2 K_2 = f \{K + (n-2)h\} - K_0 - 2hK_1$$
Or  $2h^2 K_2 = f \{k + (n-2)h\} - f(k+nh) + 2\nabla f(k+nh) \text{ [from equation(122) and (123)]}$ 

$$= f \{k + (n-2)h\} - f(k+nh) + 2[\{f(k+nh)\} - f\{k + (n-1)h\}]$$

$$= f \{k + (n-2)h\} - f(k+nh) - 2f\{k + (n-1)h\}$$

$$= f(k+nh) - 2[f\{k + (n-1)h\} + f(k)]$$

$$= \Delta^2 f(k+nh)$$

$$\therefore K_2 = \frac{1}{2h^2} \Delta^2 f(k)$$
Or
$$K_3 = -\frac{1}{2h^2} \Delta^2 f(k-nh)$$
(124)

Or

: :

$$K_{2} = \frac{1}{2!h^{2}} \Delta^{2} f(k = nh)$$
(124)

Similarly 
$$K_3 = \frac{1}{3!h^3} \Delta^3 f(k+nh)$$
 (125)

Proceeding in similar way, we got:  $K_n = \frac{1}{n!h^n} \Delta^n f(k+nh)$ (126)

substituting the values of  $K_0, K_1, K_2, \dots, K_n$  in equation (121), we got:

$$f(V^{E}) = f(k+nh) + \frac{\Delta f(k)}{h} (V^{E} - k - nh)$$
  
+  $\frac{\Delta^{2} f(k+nh)}{2!h^{2}} (V^{E} - k - nh) \{V^{E} - k - (n-1)h\} + \dots$   
+  $\frac{\Delta^{n} f(k+nh)}{n!h^{n}} (V^{E} - k - nh) \{V^{E} - k - (n-1)h\} \dots (V^{E} - k - n)$  (127)

Now let:  $V^E = k + nh + hu$  $\therefore V^E - k = nh + hu$  $V^{E} - k - (n-1)h = (u+1)h$  $V^{E} - k - (n-2)h = (u+2)h$  $V^{E} - k - h = \{u + (n-1)\}h$ 

Putting these values in equation (127), we got:

$$f(k+nh+hu) = f(k+nh) + \frac{\Delta f(k+nh)}{h}(uh) + \frac{\Delta^2 f(k+nh)}{2!h^2}(uh)(u+1)h + \dots + \frac{\Delta^n f(k+nh)}{n!h^n}(uh)(u+1)h \dots \{u+(n-1)h\}$$

Simplifying, we got:

$$f(k+nh+hu) = f(k+nh) + u\Delta f(k+nh) + \frac{\Delta^2 f(k+nh)}{2!} \{u(u+1)\} + \dots$$

$$+ \frac{\Delta^n f(k+nh)}{n!} \{u(u+1), \dots, \{u+(n-1)\}\}$$
(128)

### 12.1.1 ESTIMATION OF ERROR

Let V = f(T) be a function defined by (n+1) points  $(V_0^E, E_0), (V_1^E, E_1), \dots, (V_n^E, E_n)$ . When  $V_0^E$ ,  $V_1^E$ ,  $V_2^E$ ,  $V_3^E$ ,  $\dots$  are equally spaced with interval h and this function is continuous and differentiable (n+1)times.

The function be approximated by a polynomial  $P_n(V^E)$  of degree not exceeding a such that

$$P_n(V_i^E) = E_i$$
 [Where  $i = 1, 2, 3, ..., n$ ] (129)

Since the expression  $f(V^E) - P_n(V^E)$  vanishes for  $V^E = V_0^E, V_1^E, V_2^E, V_3^E, \dots, V_n^E$ 

 $f(V^{E}) - P_{n}(V^{E}) = K \varphi(V^{E})$ We put (130)

Wh

here 
$$\phi_1(V^E) = (V^E - V_n^E)(V^E - V_{n-1}^E)....(V^E - V_0^E)$$
 (131)

And K is to be determined in such a way that equation (12) holds for any intermediate values of  $V^E$ , say  $V^E - V^E$ [where  $V_0^E \leq V^{*E} \leq V_n^E$ ].

Therefore from equation (130),

$$K = \frac{f(V'^{E}) - P_{n}(V'^{E})}{\varphi_{1}(V'^{E})}$$
(132)

Now we construct a function  $f(V^E)$  such that

$$f(V_0^E) = f(V_1^E) - P_n(V^E) - K\varphi_1(V^E)$$

Where K is given by equation (132).

It is clear that

$$f(V_0^E) = f(V_1^E) = f(V_2^E) = f(V_3^E) = \dots f(V_n^E) = f(V^E) = 0$$
(133)

Let  $f(V^E)$  vanishes (n+2) times in the interval  $V_0^E \le V^E \le V_n^E$ ; consequently, by the repeated application of Rolle's Theorem [20] [21],  $f'(V^E)$  must vanish (n + 1) times,  $f''(V^E)$  must vanish n times etc in the interval  $V_0^E \le V^E \le V_n^E$ . Particularly,  $f^{(n+1)}(V^E)$  must vanish once in the interval  $V_0^E \le V^E \le V_n^E$ . Let this point be  $V^E = W$ ,  $V_0^E < W < V_n^E$ . Now differentiating equation (133) (n + 1) times with respect to  $V^E$  and putting  $V^E = W$ , we got:

 $f^{(n+1)}(W) = K(n+1)! = 0$ 

$$K = \frac{f^{(n+1)}(W)}{(n+1)!}$$
(134)

Or

Putting this value of K in equation (132), we got:

$$\frac{f^{(n+1)}(W)}{(n+1)!} = \frac{f(V^{*E}) - P_n(V^{*E})}{\varphi_1(V^{*E})}$$
  
Or  $f(V^{*E}) - P_n(V^{*E}) = \frac{f^{(n+1)}(W)}{(n+1)!}\varphi_1(V^{*E}), \quad V_0^E < W < V_n^E$ 

Since  $V^{*E}$  is arbitrary therefore on dropping the prime on  $V^{*E}$  we got:

$$f(V^{E}) - P_{n}(V^{E}) = \frac{f^{(n+1)}(W)}{(n+1)!} \varphi_{1}(V^{E}), \quad V_{0}^{E} < W < V_{n}^{E}$$
(135)

Now we use Taylor's theorem [22] [23]:

$$f(W+h) = f(W) + hf'(W) + \frac{h^2}{2!}f''(W) + \dots + \frac{h^n}{n!}f^n(W) + \dots$$
(136)

Neglecting the terms containing second and higher powers of h in equation (136), we got:

$$f(W+h) = f(W) + hf'(W)$$

$$f'(W) = \frac{f(W+h) - f(W)}{h}$$
(137)

Or

Or

$$f'(W) = \frac{1}{h} \Delta f(W) \quad [:: \Delta f(W) = f(W + h) - f(W)]$$
$$Df(W) = \frac{1}{h} \Delta f(W) \qquad [:: D = \frac{d}{dW}]$$
$$D = \frac{1}{h} \Delta \qquad [\text{Because } f(W) \text{ is arbitrary}]$$

$$\therefore D^{n+1} = \frac{1}{h^{n+1}} \Delta^{n+1}$$

From equation (137), we got:  $f^{(n+1)}(W) = \frac{1}{h^{(n+1)}} \Delta^{(n+1)} f(W)$ 

Putting the values of  $f^{(n+1)}(Y)$  in equation (135), we got:

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{\varphi_{1}(V^{E})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})...(V^{E} - V_{0}^{E})}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$
(138)
$$\text{If } \frac{V^{E} - V_{n}^{E}}{h} = \beta \quad \text{Then:}$$

$$V^{E} - V_{n}^{E} = h\beta$$
  

$$V^{E} - V_{n-1}^{E} = V^{E} - (V_{n}^{E} - h) = (V^{E} - V_{n}^{E}) + h = (h\beta + h) = h(\beta + 1)$$

Similarly  $V^E - V^E_{n-2} = h(\beta+2)$ 

::

Similarly 
$$V^E - V_0^E = h(eta + n)$$

Putting these values in equation (138), we got:

$$f(V^{E}) - P_{n}(V^{E}) = \left[\frac{(h\beta)\{h(\beta+1)\}\{h(\beta+2)\}\{h(\beta+3)\}\dots\{(\beta+n)\}}{(n+1)!}\right] \left[\frac{1}{h^{(n+1)}}\Delta^{(n+1)}f(W)\right]$$

OR

$$f(V^E) - P_n(V^E) = \left[\frac{\beta(\beta+1)(\beta+2)(\beta+3)\dots(\beta+n)}{(n+1)!}\right] \left[\Delta^{(n+1)}f(W)\right]$$

This is mathematical expression for estimation of error, if the point lies in the lower half.

# 13 DIVIDE DIFFERENCE OF ENZYME CONCENTRATION

If 
$$(V_1^E, E_1), (V_2^E, E_2), \dots, (V_n^E, E_n)$$
 denoted the values of the inverse function then  $\frac{E_2 - E_1}{V_2^E - V_1^E}$ ,  
 $\frac{E_3 - E_2}{E_1 - E_2}$ 

$$\frac{V_{3}^{E} - V_{2}^{E}}{V_{4}^{E} - V_{3}^{E}}$$

 $\frac{E_n - E_{n-1}}{V_n^E - V_{n-1}^E}$ , are called the divide differences of E. These differences are denoted as  $\Delta_d E_1$ ,  $\Delta_d E_2$ ,  $\Delta_d E_3$ ,...... $\Delta_d E_{n-1}$  therefore

::

Where  $\Delta_d$  is called the divide difference operator, and  $\Delta_d E_1 \Delta_d E_2 \Delta_d E_3 \dots \Delta_d E_{n-1}$  are called first order divide differences. The differences of the first order difference are called second order divide differences and are denoted as  $\Delta_d^2 E_1$ ,  $\Delta_d^2 E_2$ ,  $\Delta_d^2 E_3$ ,.....etc.

$$\Delta_d^2 E_1 = \frac{\Delta_d E_2 - \Delta_d E_1}{V_3^E - V_1^E}$$
$$\Delta_d^2 E_2 = \frac{\Delta_d E_3 - \Delta_d E_2}{V_4^E - V_2^E}$$
$$\Delta_d^2 E_3 = \frac{\Delta_d E_4 - \Delta_d E_3}{V_5^E - V_3^E}$$

In general, the first order divide difference at the  $i^{th}$  point is:

$$\Delta_d E_i = \frac{E_{i+1} - E_i}{V_{i+1}^E - V_i^E}$$

$$\Delta^{j} E_{i} = \frac{\Delta^{j-1} E_{i+1} - \Delta^{j-1} E_{i}}{V_{i+j}^{E} - V_{i}^{E}}$$

#### **13.1** FORMULA FOR DIVIDE DIFFERENCE

By the definition of divide difference:  $f(V^E, V_0^E) = \frac{f(V^E)f(V_0^E)}{V^E - V_0^E}$  (139)

Or  $f(V^E) = f(V_0^E) + (V^E - V_0^E)f(V^E, V_0^E)$ 

Again by the definition of second divided difference:  $f(V^E, V_0^E, V_1^E) = \frac{f(V^E, V_0^E) - f(V_0^E, V_1^E)}{V^E - V_1^E}$ 

Or 
$$f(V^E, V_0^E) = f(V_0^E, V_1^E) + (V^E - V_1^E)f(V^E, V_0^E, V_1^E)$$
 (140)

Similarly 
$$f(V^{E}, V_{0}^{E}, V_{1}^{E}) = f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}) + (V^{E} - V_{2}^{E})f(V^{E}, V_{0}^{E}, V_{1}^{E}, V_{2}^{E})$$
 (141)

Proceeding in similar way, we got:

:

$$f(V^{E}, V_{0}^{E}, V_{1}^{E}, \dots, V_{n-1}^{E}) = f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}, \dots, V_{n}^{E}) + (V^{E} - V_{n}^{E})f(V^{E}, V_{0}^{E}, V_{n}^{E})$$
(142)

Multiplying equation (140) by  $(V^E - V_0^E)$  ,

Multiplying equation (141) by  $\left(V^{E}-V^{E}_{0}
ight)~\left(V^{E}-V^{E}_{1}
ight)$  ,

Multiplying equation (142) by 
$$(V^E - V_0^E) (V^E - V_1^E)$$
 ......  $(V^E - V_{n-1}^E)$ 

And adding to equation (139), we got:

$$f(V^{E}) = f(V_{0}^{E}) + (V^{E} - V_{0}^{E})f(V_{0}^{E}, V_{1}^{E}) + (V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}) + \dots + (V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})\dots(V^{E} - V_{n-1}^{E})f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}\dots V_{n}^{E}) + R_{n}$$

Where  $R_n$  is the reminder and is given by

$$R_n = (V^E - V_0^E)(V^E - V_1^E)(V^E - V_2^E)...(V^E - V_n^E)f(V_0^E, V_1^E, V_2^E...V_n^E)$$

If the function  $f(V^E)$  is polynomial of degree n, then  $f(V_0^E, V_1^E, V_2^E, \dots, V_n^E)$  vanishes so that:

$$f(V^{E}) = f(V_{0}^{E}) + (V^{E} - V_{0}^{E})f(V_{0}^{E}, V_{1}^{E}) + (V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}) + \dots$$
  
$$\dots + (V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})\dots + (V^{E} - V_{n-1}^{E})f(V_{0}^{E}, V_{1}^{E}, V_{2}^{E}) + \dots$$

# 13.1.1 ESTIMATION OF ERROR

Let  $f(V^E)$  be a real-valued function define n interval and (n+1) times differentiable on (a,b). If  $P_n(V^E)$  is the polynomial. Which interpolates  $f(V^E)$  at the (n+1) distinct points  $V_0^E, V_1^E \dots V_n^E \in (a,b)$ , then for all  $\overline{V^E} \in [a,b]$ , there exists  $\xi = \xi \left( \overline{V^E} \right) \in (a,b)$ 

$$e_{n}\left(\overline{V^{E}}\right) = f\left(\overline{V^{E}}\right) - P_{n}\left(\overline{V^{E}}\right)$$
$$= \frac{f^{(n+1)}\left(\xi\right)}{\left(n+1\right)} \prod_{j=0}^{n} \left(\overline{V^{E}} - V_{j}^{E}\right)$$
(143)

This is mathematical expression for estimation of error, if intervals are not be equally spaced.

# 14 WHEN THE TABULATED VALUES OF $V^{E} = f(E)$ are not Equidistant

If  $f(V_0^E), f(V_1^E), f(V_2^E)$ ..... $f(V_n^E)$  is to be vales of the inverse function corresponding to arguments  $V_0^E, V_1^E, V_2^E$ .... $V_n^E$  not necessarily equally spaced.

Let  $f(V^T)$  be a polynomial of degree n in  $V^E$  and since (n+1) values of  $f(V^E)$  are given so  $(n+1)^{th}$  difference are zero.

Consider,

$$f(V^{E}) = A_{0}(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})....(V^{E} - V_{n}^{E}) + A_{1}(V^{E} - V_{0}^{E})(V^{E} - V_{2}^{E})....(V^{E} - V_{n}^{E}) + A_{2}(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})....(V^{E} - V_{n}^{E}) + .... ....+ A_{n}(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})....(V^{E} - V_{n-1}^{E})$$
(144)

Where  $A_0, A_1, A_2$  ...... $A_n$  all are constants.

Now put  $V^E = V_0^E$  in equation (144), we got:

$$f(V_0^E) = A_0(V_0^E - V_1^E)(V_0^E - V_2^E)....(V_0^E - V_n^E)$$
  
$$\therefore A_0 = \frac{f(V_0^E)}{(V_0^E - V_1^E)(V_0^E - V_2^E)....(V_0^E - V_n^E)}$$
(145)

Again put  $V^E = V_1^E$  in equation (144), we got:

$$f(V_1^E) = A_1(V_1^E - V_1^E)(V_1^E - V_2^E)....(V_1^E - V_n^E)$$
  
$$\therefore A_1 = \frac{f(V_1^E)}{(V_1^E - V_1^E)(V_1^E - V_2^E)...(V_1^E - V_n^E)}$$
(146)

Similarly  $\therefore A_2 = \frac{f(V_2^E)}{(V_2^E - V_1^E)(V_2^E - V_2^E)....(V_2^E - V_n^E)}$  (147)

Proceeding in similar way, we got:

$$\therefore A_n = \frac{f(V_n^E)}{(V_n^E - V_1^E)(V_n^E - V_2^E)\dots(V_n^E - V_n^E)}$$
(148)

Substituting the values of  $A_0, A_1, A_2, \dots, A_n$  from equation (145), (146), (147), (148) in equation (144) we got:

$$f(V^{E}) = \frac{(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E}).....(V^{E} - V_{n}^{E})}{(V_{0}^{E} - V_{1}^{E})(V_{0}^{E} - V_{2}^{E}).....(V_{0}^{E} - V_{n}^{E})} f(V_{0}^{E}) + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{2}^{E}).....(V^{E} - V_{n}^{E})}{(V_{1}^{E} - V_{1}^{E})(V_{0}^{E} - V_{2}^{E}).....(V_{1}^{E} - V_{n}^{E})} f(V_{1}^{E}) + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})....(V_{1}^{E} - V_{n}^{E})}{(V_{2}^{E} - V_{1}^{E})(V_{2}^{E} - V_{2}^{E}).....(V_{2}^{E} - V_{n}^{E})} f(V_{2}^{E}) + ..... + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{2}^{E}).....(V_{2}^{E} - V_{n}^{E})}{(V_{n}^{E} - V_{1}^{E})(V_{n}^{E} - V_{2}^{E}).....(V_{n}^{E} - V_{n}^{E})} f(V_{n}^{E})$$

#### 14.1 ESTIMATION OF ERROR

Since the approximating polynomial  $f(V^E)$  given by Lagrangian formula has the same values  $f(V_0^E) f(V_1^E) f(V_2^E) f(V_3^E) f(V_4^E)$ ..... $f(V_n^E)$  as does  $T = f(V^E)$  for the arguments  $V_0^E, V_1^E, V_2^E$ .... $V_n^E$  the error term must have zeros at these (n+1) points.

There for  $(V^E - V_0^E) (V^E - V_1^E) (V^E - V_2^E) (V^E - V_3^E)$  ..... $(V^E - V_n^E)$  must be factors of the error and we can write:

$$F(V^{E}) = f(V^{E}) + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})(V^{E} - V_{3}^{E})....(V^{E} - V_{n}^{E})}{(n+1)!}K(V^{E})$$
(149)

Let x to be fixed in value and consider the function

$$W(x) = F(x) - f(x) \frac{(x - V_0^E)(x - V_1^E)(x - V_2^E)(x - V_3^E)...(x - V_n^E)}{(n+1)!} K(V^E)$$
(150)

Then W(x) has zero  $x = V_0^E, V_1^E, V_2^E, V_3^E, \dots, V_n^E$  and  $V^E$ .

Since the  $(n+1)^{th}$  derivative of the  $n^{th}$  degree polynomial  $f(V^E)$  is zero.

$$W^{(n+1)}(x) = F^{(n+1)}(x) - K(V^{E})$$
(151)

As a consequence of Rolle's Theorem [15] [16], the  $(n+1)^{th}$  derivative of W(x) has at least one real zero  $x = \xi$  in the range  $V_0^T < \xi < V_n^E$ 

Therefore substituting  $x = \xi$  in equation (151)

Or

$$K(V^{E}) = F^{(n+1)}(\xi) - W^{(n+1)}(\xi)$$
$$= F^{(n+1)}(\xi)$$

 $W^{(n+1)}(\xi) = F^{(n+1)}(\xi) - K(V^{E})$ 

Using this expression for  $K(V^E)$  and writing out  $f(V^E)$ 

$$\begin{split} f(V^{E}) &= \frac{(V^{E} - V_{1}^{E})(V^{E} - V_{2}^{E})....(V^{E} - V_{n}^{E})}{(V_{0}^{E} - V_{1}^{E})(V_{0}^{E} - V_{2}^{E})...(V_{0}^{E} - V_{n}^{E})}f(V_{0}^{E}) + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{2}^{E})...(V^{E} - V_{n}^{E})}{(V_{1}^{E} - V_{0}^{E})(V_{1}^{E} - V_{2}^{E})....(V_{1}^{E} - V_{n}^{E})}f(V_{1}^{E}) + .....\\ & \dots + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})...(V^{E} - V_{n-1}^{E})}{(V_{n}^{E} - V_{0}^{E})(V_{n}^{E} - V_{1}^{E})...(V_{n}^{E} - V_{n-1}^{E})}f(V_{n}^{E}) + \frac{(V^{E} - V_{0}^{E})(V^{E} - V_{1}^{E})....(V^{E} - V_{n}^{E})}{(n+1)!}f^{(n+1)}(\xi) \end{split}$$

Where  $V_0^E < \xi < V_n^E$ 

This is mathematical expression for estimation of error, if the tabulated values of the function are not equidistant.

## 15 CONCLUSION

The higher order differences become smaller in size. Further, in the forward and backward interpolation, the  $n^{th}$  order difference is divided by n!, thereby further reducing its contribution to the value of the interpolation function. If the function happens to be a polynomial of degree n, then the  $n^{th}$  order difference would be constant and the (n + 1) and higher differences would be zero. Derived formulas are useful to obtaining intermediate values of the Temperature, substrate concentration and enzyme concentration. Mathematical expressions are useful to estimation of the errors in the formulas for obtaining intermediate values of the Temperature, substrate concentration and enzyme concentration. All formulas and expressions are worked in n limit which is the optimum limit.

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