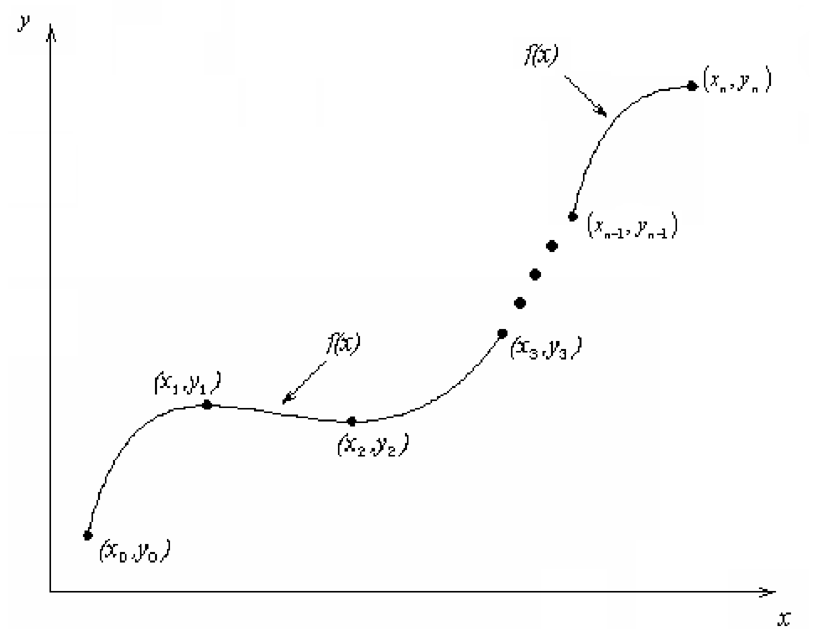
Interpolation

WHAT IS INTERPOLATION?

Given (x_0,y_0), (x_1,y_1), …, (x_n,y_n), finding the value of 'y' at a value of 'x' in (x_0, x_n) is called **interpolation.**



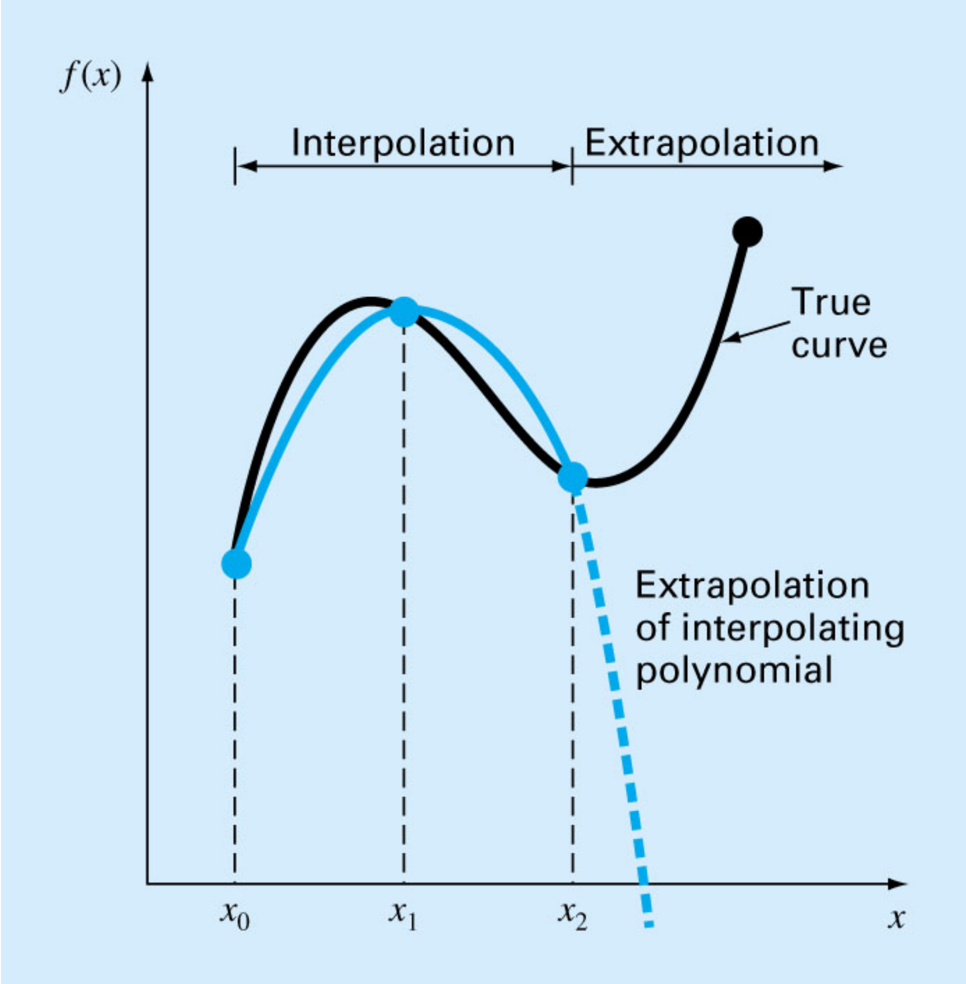
Interpolation produces **a function** that matches the given data exactly. The function then can be utilized to approximate the data values at intermediate points.

Extrapolation

- **Extrapolation** is the process of estimating a value of $f(x)$ that lies outside the range of the known base points,

  $x_0, x_1, \ldots, x_n$.

- Extreme care should be exercised where one must extrapolate.



Interpolation

Unequal Interval

- Lagrange Interpolation
- Newton’s Divided Difference Interpolation

Equal interval

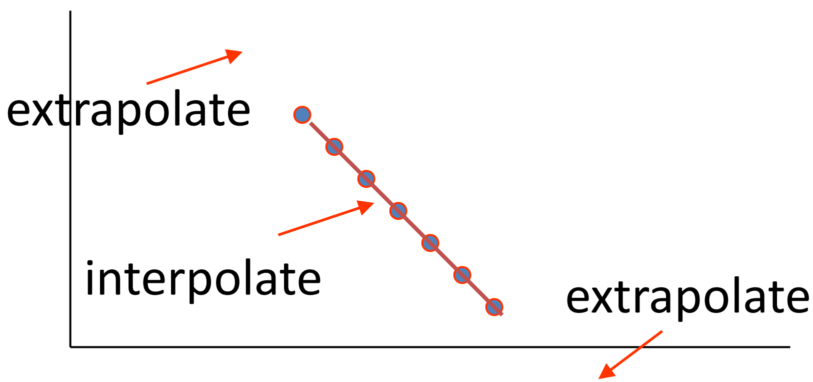
- Newton’s Forward/Backward Interpolation
- Gauss Forward/Backward Interpolation
- Stirling’s / Bessel’s Formula

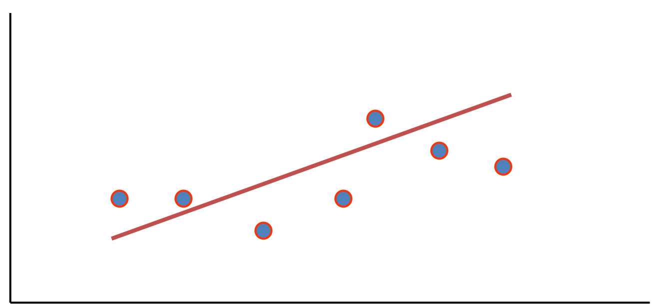
Regression

- Least Squares Regression

Interpolation Vs Regression

- Distinctly different approaches depending on the quality of the data
- Consider the pictures below:





Pretty confident:
there is a polynomial relationship
Little/no scatter
Want to find an expression
that passes **exactly** through all the points

Unsure what the relationship is
Clear scatter
Want to find an expression
that captures the trend:
minimize some measure of the error
Of all the points…

Polynomial Interpolation

- Concentrate first on the case where we believe there is no error in the data (and round-off is assumed to be negligible).
- So we have $y_i = f(x_i)$ at $n+1$ points $x_0, x_1 \ldots x_i, \ldots x_n$: $x_j > x_{j-1}$
- In general, we do not know the underlying function $f(x)$
- Polynomial interpolation consists of determining the unique **n^th^-order** polynomial that fits $n+1$ data points.
- This polynomial can be used to compute intermediate values.
- Conceptually, interpolation consists of two stages:
  - Develop a simple function $f(x)$ that
    - Approximates $f(x)$
    - Passes through all the points x_i
  - Evaluate $f(x_t)$ where $x_0 < x_t < x_n$

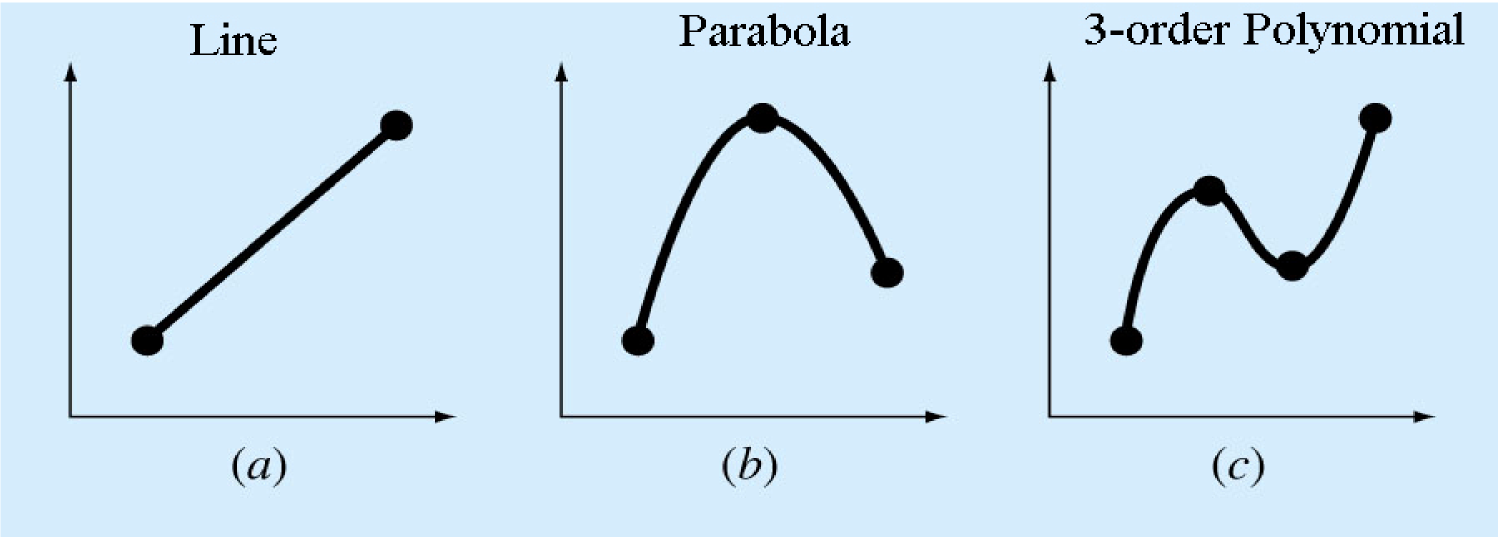
Polynomial Interpolation

Objective:

Given n+1 points, we want to find the polynomial of order n

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

that passes through all the points.



Lagrange Polynomials

- A straightforward approach is the use of Lagrange polynomials.
- The polynomial of order *n* used to interpolate in between all data pairs $(x_0, f(x_0)), (x_1, f(x_1)), \ldots, (x_n, f(x_n))$ is given by

$$P_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

where

$$L_i(x) = \prod_{k=0, k \neq i}^{n} \frac{(x - x_k)}{(x_i - x_k)} \quad \Rightarrow \quad \sum_i L_i(x) = 1$$

Lagrange Polynomials

- The linear interpolating polynomial

$$P_1(x) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

- The second-order interpolating polynomial

$$P_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

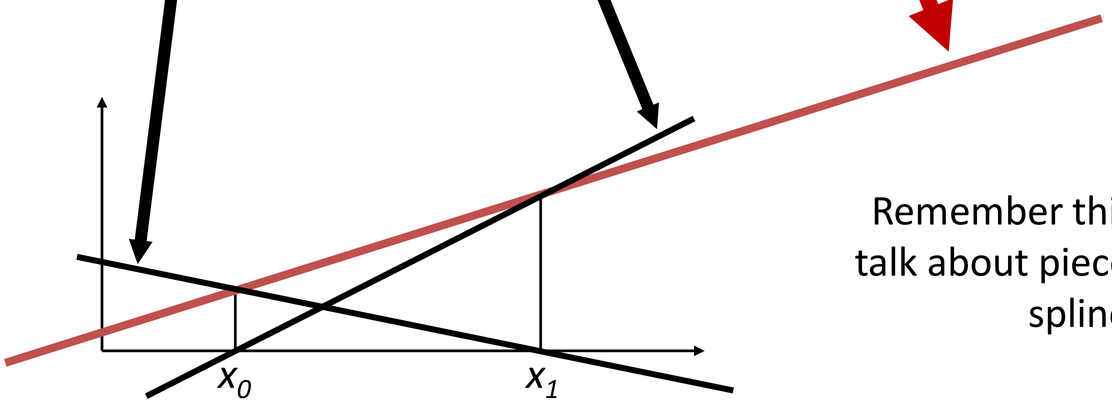
- The general form

$$P_n(x) = \frac{(x - x_1)(x - x_2)\ldots(x - x_n)}{(x_0 - x_1)(x_0 - x_2)\ldots(x_0 - x_n)} f(x_0) + \frac{(x - x_0)(x - x_2)\ldots(x - x_n)}{(x_1 - x_0)(x_1 - x_2)\ldots(x_1 - x_n)} f(x_1) + \ldots + \frac{(x - x_0)(x - x_1)\ldots(x - x_n)}{(x_{n-1} - x_0)(x_{n-1} - x_1)\ldots(x_{n-1} - x_n)} f(x_n)$$

Linear Interpolation

- Summation of two lines:

$$P_1(x) = \sum_{i=0}^{1} L_i(x) f(x_i)$$
$$= \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$



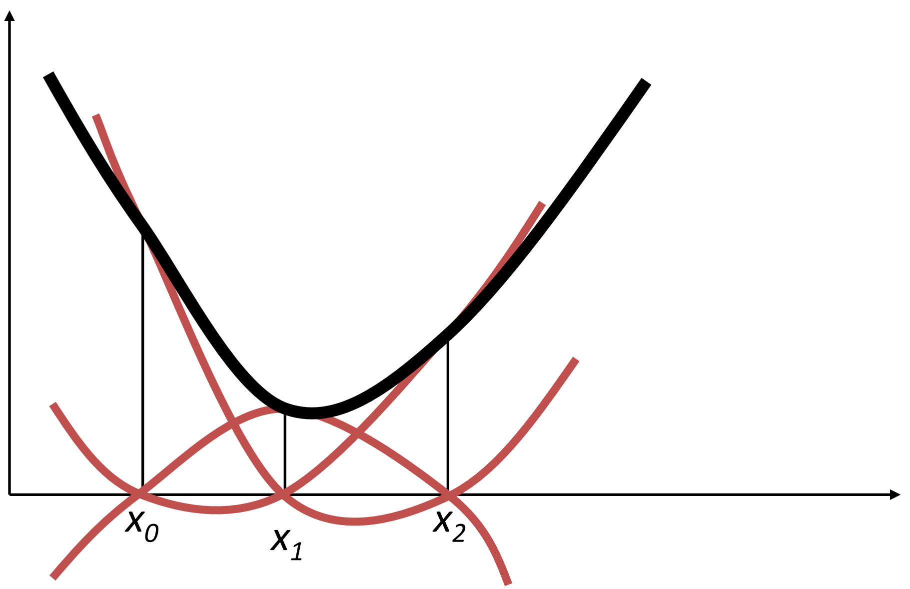
Remember this when we talk about piecewise-linear splines

Quadratic Polynomials

- 2^{nd} Order Case => quadratic polynomials

Adding them all together, we get the interpolating quadratic polynomial, such that:

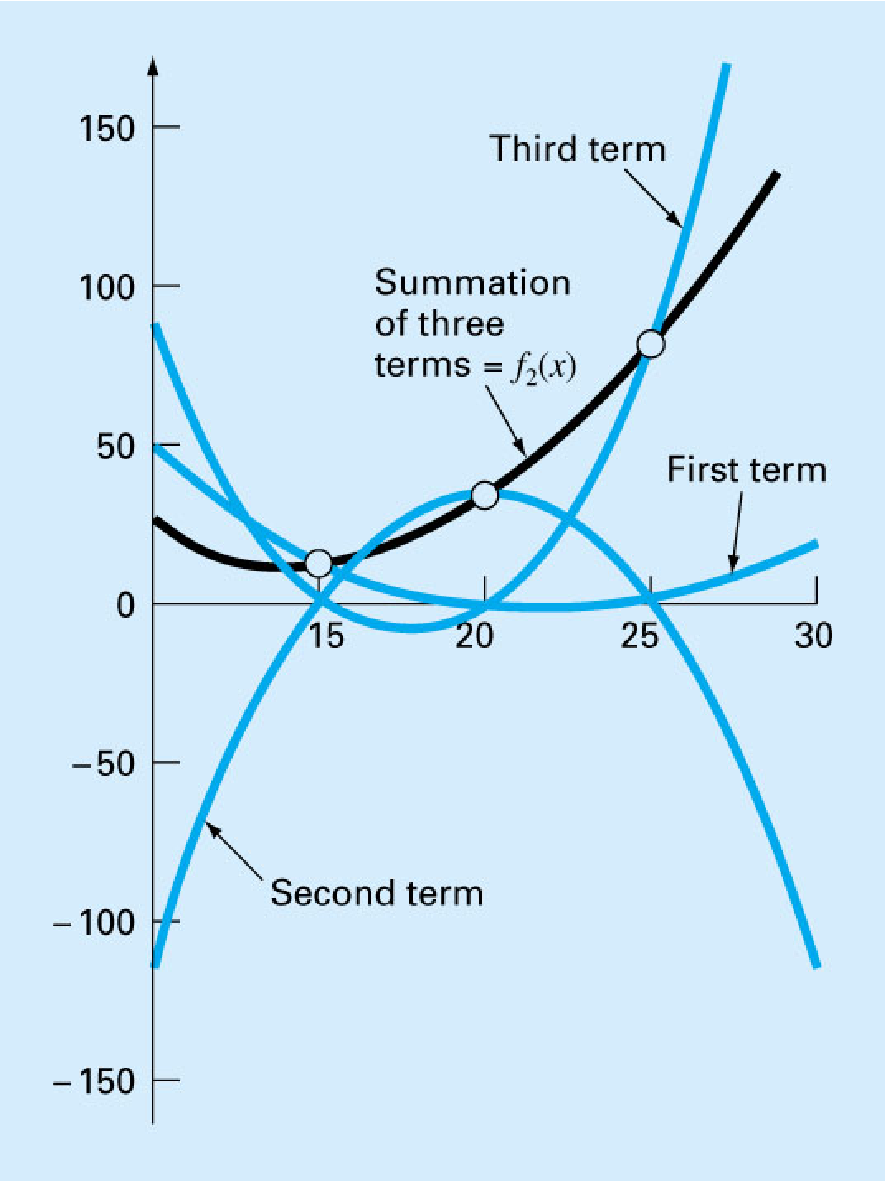
- $P(x_0) = f_0$
- $P(x_1) = f_1$
- $P(x_2) = f_2$



Second order case of Lagrange polynomial.

Each of the three terms is a 2nd-order polynomial that passes through one of the data points and is zero at the other two(Notice that each term $L_i(x)$ will be 1 at $x = x_i$ and 0 at all other sample points).

The summation of three terms must, therefore, be the unique 2nd-order polynomial that passes exactly through three points.



Lagrange Polynomials

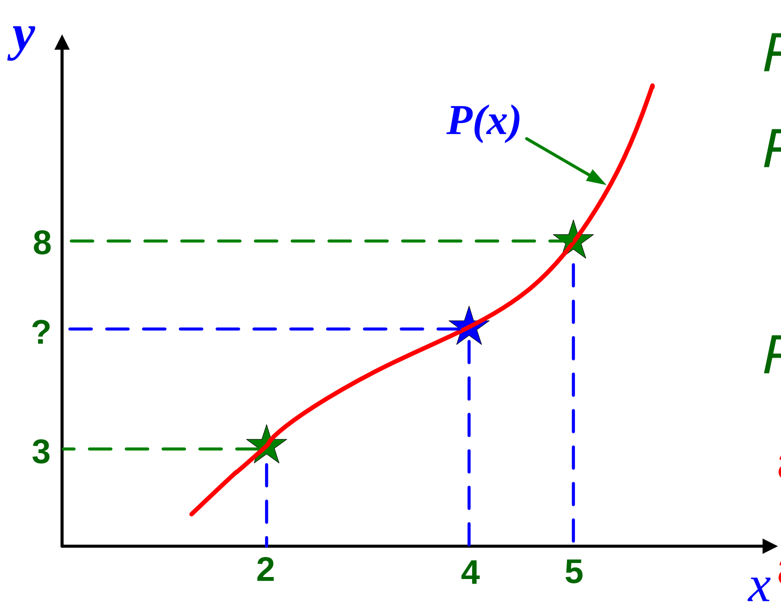
1. Given data points obtaining a function, P(x)

2. P(x) goes through the data points

3. Use P(x) to estimate values at intermediate points

Given data points: At $x_0 = 2$, $y_0 = 3$ and at $x_1 = 5$, $y_1 = 8$

Find the following: At $x = 4$, $y = ?$



$P(x)$ should satisfy the following conditions:

$P(x = 2) = 3$ and $P(x = 5) = 8$

$$P_1(x) = 3L_0(x) + 8L_1(x)$$

$P(x)$ can satisfy the above conditions if

at $x = x_0 = 2$, $L_0(x) = 1$ and $L_1(x) = 0$ and

at $x = x_1 = 5$, $L_0(x) = 0$ and $L_1(x) = 1$

The conditions can be satisfied if $L_0(x)$ and $L_1(x)$ are defined in the following way.

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \quad \text{and} \quad L_1(x) = \frac{x - x_0}{x_1 - x_0}$$

$$L_0(x) = \frac{x - 5}{2 - 5} \quad \text{and} \quad L_1(x) = \frac{x - 2}{5 - 2}$$

$$P_1(x) = L_0(x) y_0 + L_1(x) y_1 \quad \Rightarrow \quad P_1(x) = 3L_0(x) + 8L_1(x)$$

Lagrange Interpolating Polynomial

$$P_1(x) = L_0(x) f(x_0) + L_1(x) f(x_1)$$

$$P_1(x) = \left(\frac{x-5}{2-5}\right)(3) + \left(\frac{x-2}{5-2}\right)(8) \quad \Rightarrow \quad P_1(x) = \frac{5x-1}{3}$$

At $x = 4$

$$y = f(4) = \frac{5 \times 4 - 1}{3} = 6.333$$

The Lagrange interpolating polynomial passing through **three** given points; (x_0, y_0), (x_1, y_1) and (x_2, y_2) is:

$$P_2(x) = L_0(x)y_0 + L_1(x)y_1 + L_2(x)y_2$$

or $$P_2(x) = L_0(x)f(x_0) + L_1(x)f(x_1) + L_2(x)f(x_2)$$

where $$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}$$

At x_0, $L_0(x)$ becomes 1. At all other given data points $L_0(x)$ is 0.

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}$$

At x_1, $L_1(x)$ becomes 1. At all other given data points $L_1(x)$ is 0.

$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

At x_2, $L_2(x)$ becomes 1. At all other given data points $L_2(x)$ is 0.

General form of the Lagrange Interpolating Polynomial

$$P_n(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2) + \ldots + L_n(x) f(x_n)$$

$$L_k(x) = \frac{(x - x_0)(x - x_1)\ldots(x - x_{k-1})(x - x_{k+1})\ldots(x - x_n)}{(x_k - x_0)(x_k - x_1)\ldots(x_k - x_{k-1})(x_k - x_{k+1})\ldots(x_k - x_n)}$$

$$L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^{n} \frac{(x - x_i)}{(x_k - x_i)}$$

Numerator of $L_k(x)$

$$(x - x_0)(x - x_1)(x - x_2) \times \cdots \times (x - x_{k-1})(x - x_{k+1}) \times \cdots \times (x - x_{n-1})(x - x_n)$$

Denominator of $L_k(x)$

$$(x_k - x_0)(x_k - x_1)(x_k - x_2)\times\cdots\times(x_k - x_{k-1})(x_k - x_{k+1})\times\cdots\times(x_k - x_{n-1})(x_k - x_n)$$

Example: Find the Lagrange Interpolating Polynomial using the three given points.

$$(x_0, y_0) = (2,\ 0.5),\ (x_1, y_1) = (2.5,\ 0.4),\ (x_2, y_2) = (4,\ 0.25)$$

$$L_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \frac{(x - 2.5)(x - 4)}{(2 - 2.5)(2 - 4)} = x^2 - 6.5x + 10$$

$$L_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} = \frac{(x - 2)(x - 4)}{(2.5 - 2)(2.5 - 4)} = \frac{-x^2 + 6x - 8}{0.75}$$

$$L_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} = \frac{(x - 2)(x - 2.5)}{(4 - 2)(4 - 2.5)} = \frac{x^2 - 4.5x + 5}{3}$$

$$P_2(x) = L_0(x) f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$$

$$P_2(x) = \left(\frac{x^2 - 6.5x + 10}{1}\right)(0.5) + \left(\frac{-x^2 + 6x - 8}{0.75}\right)(0.4) + \left(\frac{x^2 - 4.5x + 5}{3}\right)(0.25)$$

$$P_2(x) = 0.05x^2 - 0.425x + 1.15$$

The three given points were taken from the function

$$f(x) = \frac{\mathbf{1}}{x} \quad \Rightarrow \quad f(3) = \frac{1}{3} = 0.333$$

An approximation can be obtained from the Lagrange Interpolating Polynomial as:

$$P_2(3) = 0.05(3)^2 - 0.425(3) + 1.15 = 0.325$$

Example: Find the first and second order interpolating polynomials of ln x for $x_0 = 1$, $x_1 = 4$, $x_2 = 6$, and use the polynomials to estimate ln 2.

Solution:

$$x_0 = 1, \; f(x_0) = 0$$
$$x_1 = 4, \; f(x_1) = 1.386294$$
$$x_2 = 6, \; f(x_2) = 1.791759$$

First order polynomial:

$$P_1(x) = \frac{x-4}{1-4} f(1) + \frac{x-1}{4-1} f(4) = \frac{x-4}{1-4}(0) + \frac{x-1}{4-1}(1.386294)$$

$$f(2) = 0.4620981$$

Second order polynomial:

$$P_2(x) = \frac{(x-4)(x-6)}{(1-4)(1-6)} f(1) + \frac{(x-1)(x-6)}{(4-1)(4-6)} f(4) + \frac{(x-1)(x-4)}{(6-1)(6-4)} f(6)$$

$$= \frac{(x-4)(x-6)}{(1-4)(1-6)}(0) + \frac{(x-1)(x-6)}{(4-1)(4-6)}(1.386294) + \frac{(x-1)(x-4)}{(6-1)(6-4)}(1.791760)$$

$$f(2) = 0.5658444$$

Example: Let the data set {(-1,-4),(0,-5),(1,-2)} be the data set we want to interpolate.

$$P_2(x) = (-4)\frac{(x-0)(x-1)}{(-1-0)(-1-1)} + (-5)\frac{(x+1)(x-1)}{(0+1)(0-1)} + (-2)\frac{(x+1)(x-0)}{(1+1)(1-0)}$$

$$= \frac{-4}{2}\left(x^2 - x\right) + \frac{-5}{-1}\left(x^2 - 1\right) + \frac{-2}{2}\left(x^2 + x\right)$$

$$= -2x^2 + 2x + 5x^2 - 5 - x^2 - x \qquad = 2x^2 + x - 5$$

Plugging in the values of *x* we get:

$f(-1) = 2(-1)^2 + (-1) - 5 = 2 - 1 - 5 = -4$

$f(0) = 2(0)^2 + 0 - 5 = 0 + 0 - 5 = -5$

$f(1) = 2(1)^2 + 1 - 5 = 2 + 1 - 5 = -2$

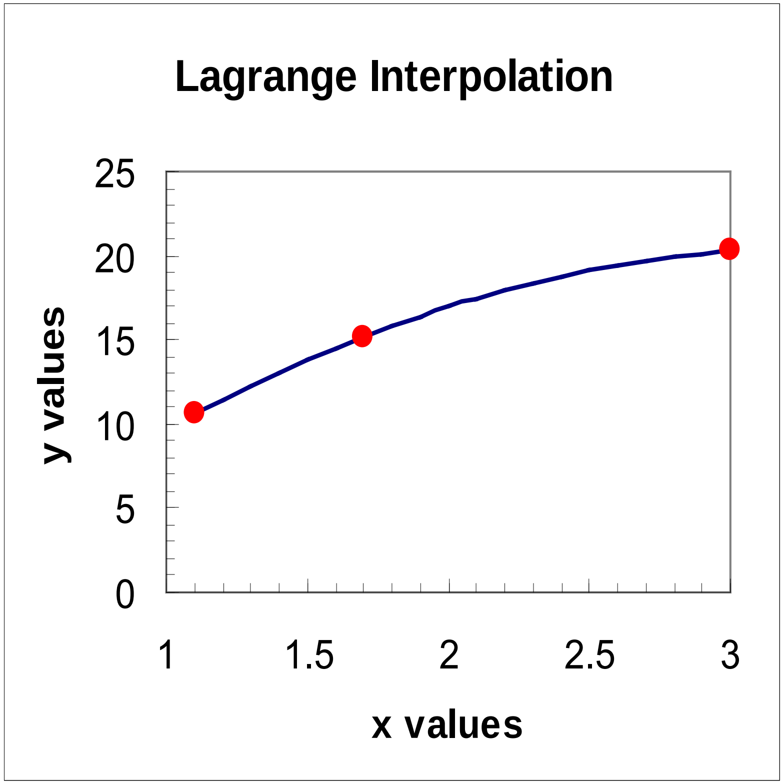
Example: What is the value of $P_2(2.3)$?

x	y	C_i
1.1	10.6	9.2983
1.7	15.2	-19.4872
3	20.3	8.2186

$$C_1 = \frac{y_1}{(x_1 - x_2)(x_1 - x_3)} = \frac{10.6}{(1.1-1.7)(1.1-3.0)} = 9.2983$$

$$C_2 = \frac{15.2}{(1.7-1.1)(1.7-3.0)} = -19.4872$$

$$C_3 = \frac{20.3}{(3.0-1.1)(3.0-1.7)} = 8.2186$$



The values are evaluated

P_2(x) = 9.2983*(x-1.7)(x-3.0)
- 19.4872*(x-1.1)(x-3.0)
+ 8.2186*(x-1.1)(x-1.7)

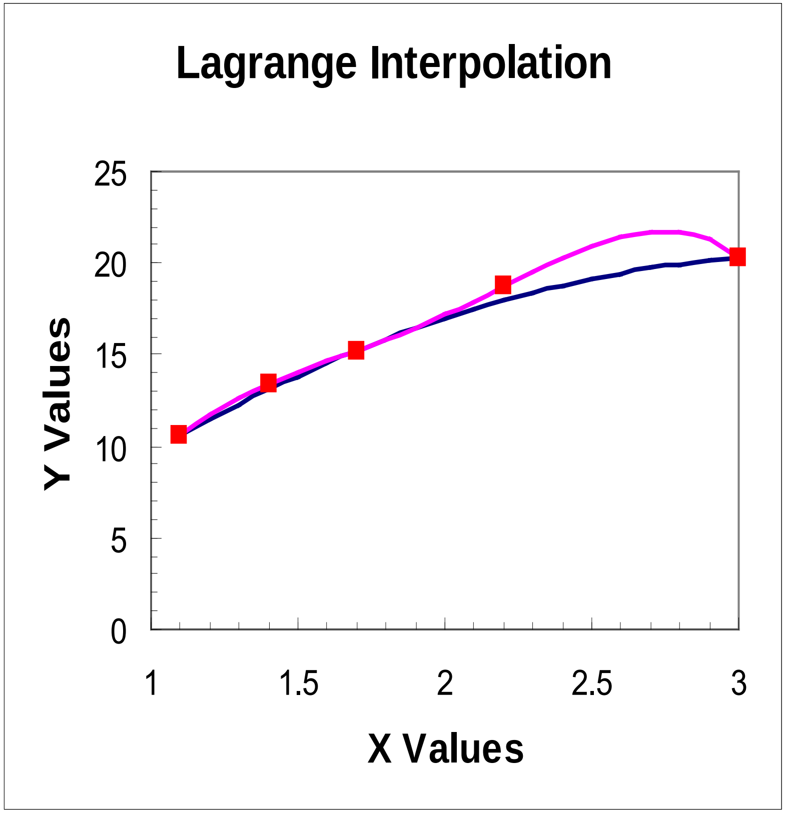
f(2.3) = 9.2983*(2.3-1.7)(2.3-3.0)
- 19.4872*(2.3-1.1)(2.3-3.0)
+ 8.2186*(2.3-1.1)(2.3-1.7)
= 18.3813

- Consider the table of 5 points we wish to fit. The interpolation polynomial is,

$$
\begin{aligned}
P_4(x) = {} & C_1(x-x_2)(x-x_3)(x-x_4)(x-x_5) + C_2(x-x_1)(x-x_3)(x-x_4)(x-x_5) \\
& + C_3(x-x_1)(x-x_2)(x-x_4)(x-x_5) + C_4(x-x_1)(x-x_2)(x-x_3)(x-x_5) \\
& + C_5(x-x_1)(x-x_2)(x-x_3)(x-x_4)
\end{aligned}
$$

- What happens if we increase the number of data points?

x	y	C_i
1.1	10.6	28.1765
1.7	15.2	129.9145
3	20.3	6.4208
1.4	13.4	-116.319
2.2	18.7	-53.125



Note: Comparison between the original $P_2(x)$ and $P_4(x)$ polynomial. The problem with adding additional points will create "bulges" in the graph.

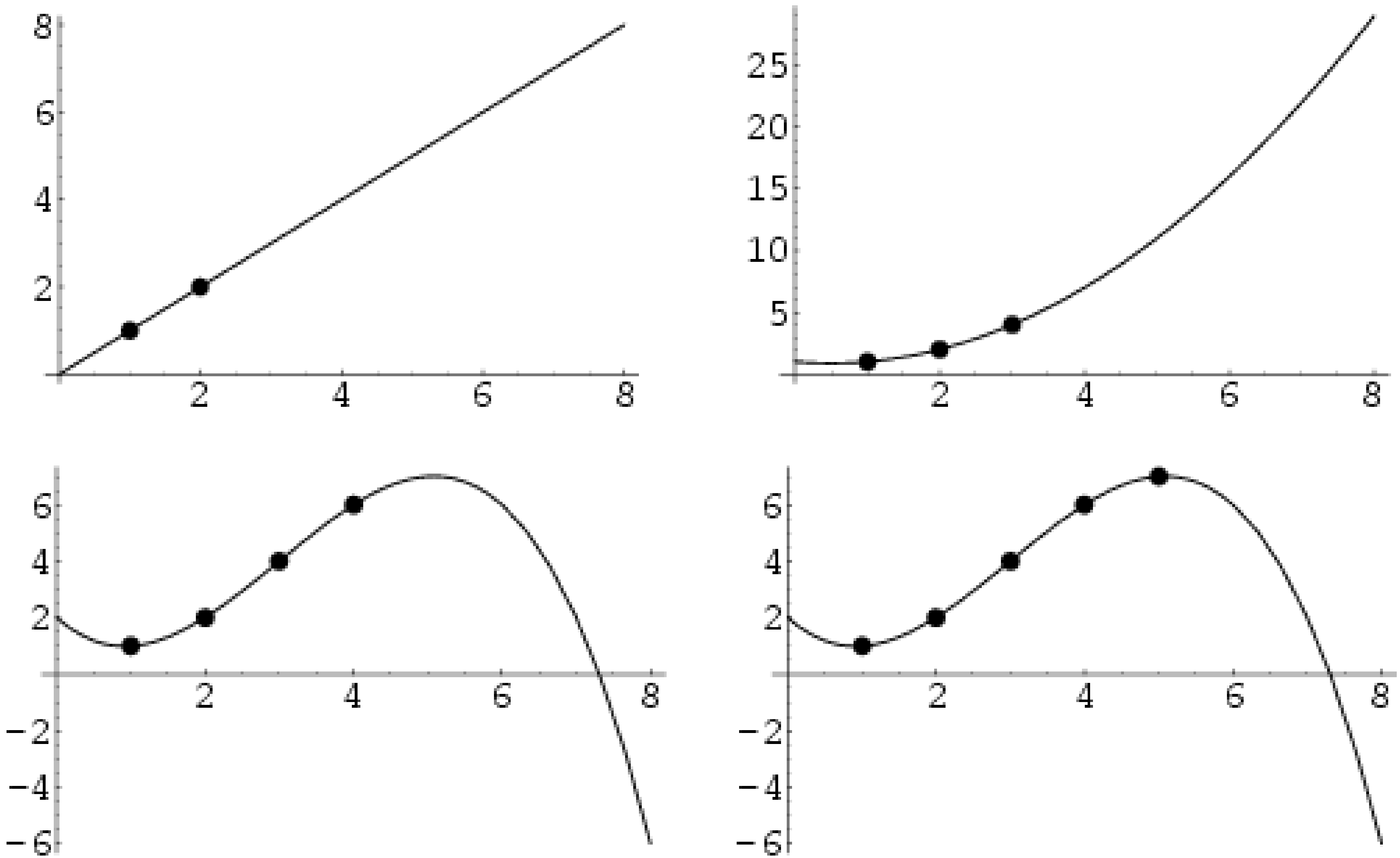
Advantages

- The Lagrange formula is popular because it is well known and is easy to code.
- Also, the data are not required to be specified with x in ascending or descending order.

Disadvantages

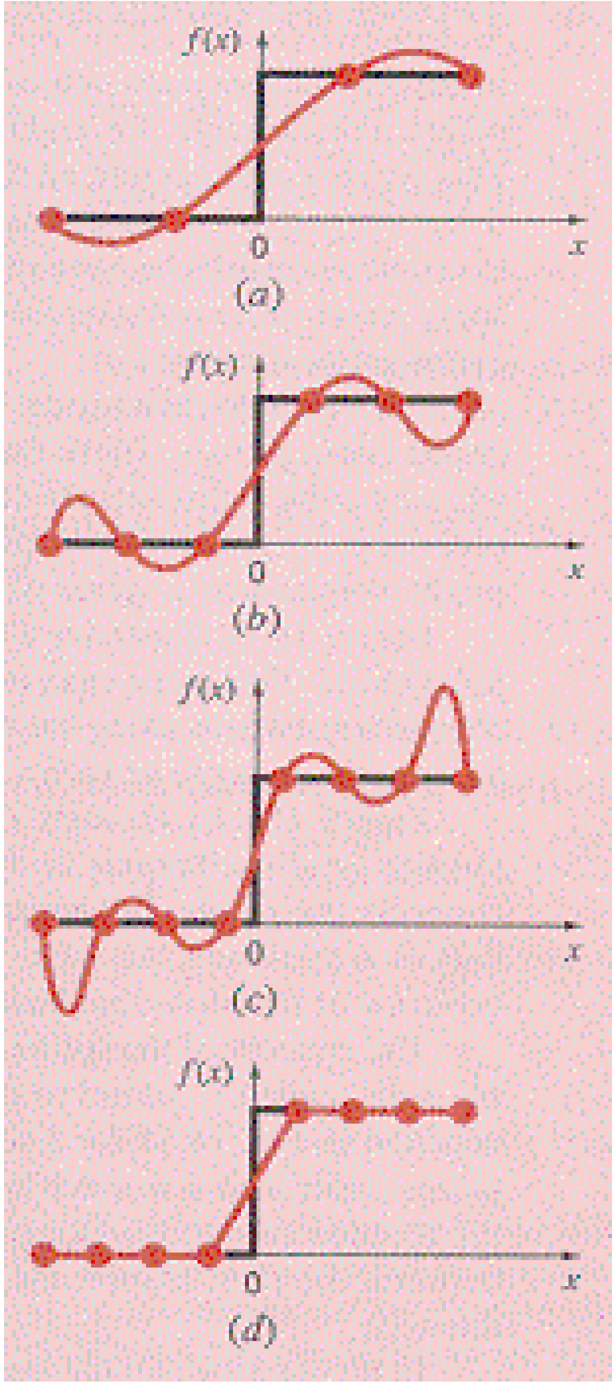
- Although the computation of $P_n(x)$ is simple, the method is still not particularly efficient for large values of n.
- When n is large and the data for x is ordered, some improvement in efficiency can be obtained by considering only the data pairs in the vicinity of the x value for which $P_n(x)$ is sought.
- The price of this improved efficiency is the possibility of a poorer approximation to $P_n(x)$.

Diagram showing Interpolation incrementally from one to 5 points with proper selection.



Problems with over fit of the Lagrange Interpolation

- Is it always a good idea to use higher and higher order polynomials?
- Normally: 3-4 points usually good: 5-6 is ok further than that not good.
- See tendency of polynomial to “wiggle”
- Particularly for sharp edges: check from figures



Lagrange Interpolating Polynomial Algorithm

To implement the Lagrange Polynomial in Programming the Algorithm, it is a matter of following the formula for the set of data:

$$\{(x_1,y_1),(x_2,y_2),(x_3,y_3)\ldots(x_m,y_m)\} \Longrightarrow p(x)=\sum_{i=1}^{m} y_i \prod_{\substack{j=1\\ i\neq j}}^{m} \frac{(x-x_j)}{(x_i-x_j)}$$

Lagrange Interpolation Program 1

```
alldiffx ← True
For[ i=1, i ≤ m , i++
        For[ j=1, j<i, j++,
                alldiffx=alldiffx and (x_i ≠ x_j)]]
If alldiffx
        psum=0
        For[i=1, i ≤ m , i++
                pprod=y_i
                For[ j=1, j<i, j++,
                        If i≠j then pprod=pprod*(x –x_j)/(x_i – x_j)]
                psum=psum+pprod]
(* else *)
        Print[“Data set can not be interpolated by a function”]
```

Lagrange Interpolation Program 2

```
FUNCTION Lagrng(x, y, n, xx)
  sum = 0
  DO i = 0, n
    product = y_i
    DO j = 0, n
      IF i ≠ j THEN
        product = product*(xx − x_j)/(x_i − x_j)
      ENDIF
    END DO
    sum = sum + product
  END DO
  Lagrng = sum
END Lagrng
```

- The variables *x* and *y* are vectors.
- *xx* is the value you want to evaluate the polynomial at.

Newton's Divided-Difference Polynomials

Linear Interpolation

- The simplest form of interpolation connecting two data points $(x_0, y_0),(x_1, y_1)$ is a straight line.

$$\frac{P_1(x) - f(x_0)}{x - x_0} = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$P_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

Slope is a finite divided difference approximation to 1st derivative

Linear-interpolation formula

- *$P_1(x)$* designates a first-order interpolating polynomial.
- 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.

Newton's Interpolating Polynomials

Newton's equation of a function that passes through two points (x_0, y_0) and (x_1, y_1) is written as

$$P_1(x) = b_0 + b_1(x - x_0) \quad \text{where slope} \quad b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

- The term $\dfrac{f(x_1) - f(x_0)}{x_1 - x_0}$ is a

finite–divided–difference approximation of the first derivative of $f(x)$.

- The smaller the interval between x_0 and x_1 is, the better the approximation.

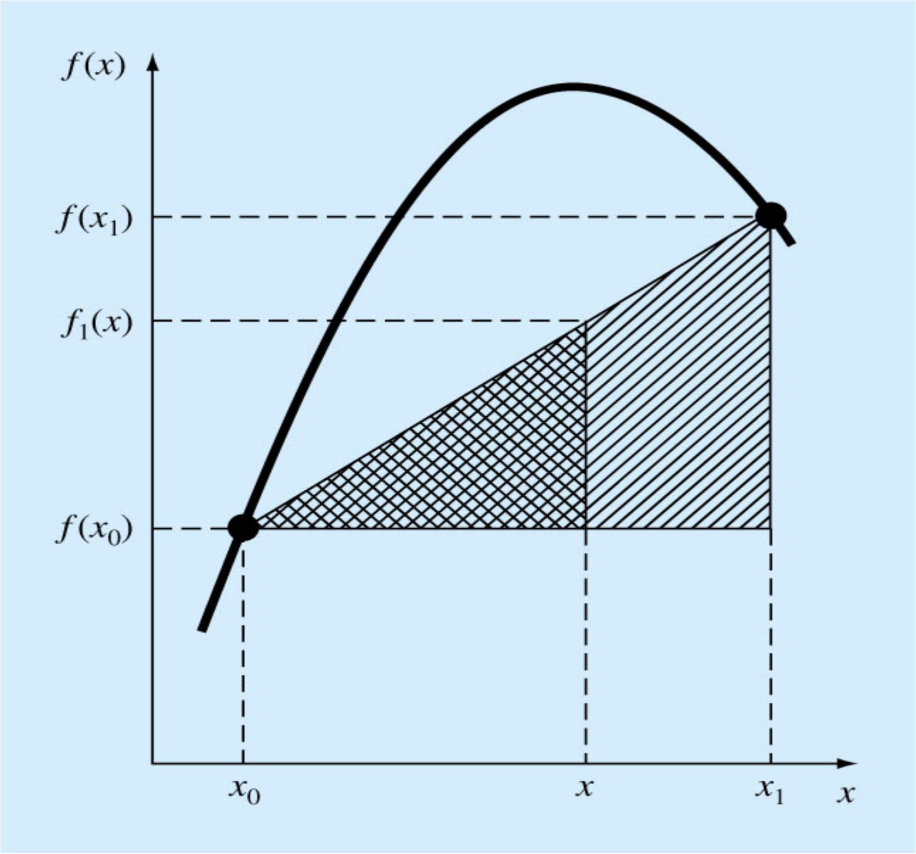
Set $x = x_0$

$$f(x_0) = y_0 = b_0$$

Set $x = x_1$

$$f(x_1) = y_1 = b_0 + b_1(x_1 - x_0)$$

$$b_1 = \frac{y_1 - y_0}{x_1 - x_0}$$



Quadratic Interpolation

- If three data points $(x_0, y_0), (x_1, y_1), (x_2, y_2)$ are available, the estimation is improved by introducing some curvature into the line connecting the points.
- A second-order polynomial can be used to determine the values of the coefficients.

$$P_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

Where b_0, b_1, b_2 can be found from substitution of three points in the equation

$$\begin{aligned} y_0 &= b_0 + b_1(x_0 - x_0) + b_2(x_0 - x_0)(x_0 - x_1) \\ y_1 &= b_0 + b_1(x_1 - x_0) + b_2(x_1 - x_0)(x_1 - x_1) \\ y_2 &= b_0 + b_1(x_2 - x_0) + b_2(x_2 - x_0)(x_2 - x_1) \end{aligned} \quad \Rightarrow \quad \begin{aligned} y_0 &= b_0 \\ y_1 &= b_0 + b_1(x_1 - x_0) \\ y_2 &= b_0 + b_1(x_2 - x_0) + b_2(x_2 - x_0)(x_2 - x_1) \end{aligned}$$

which can be solved for b_0, b_1, and b_2

b_1: Finite-divided difference for $f'(x)$

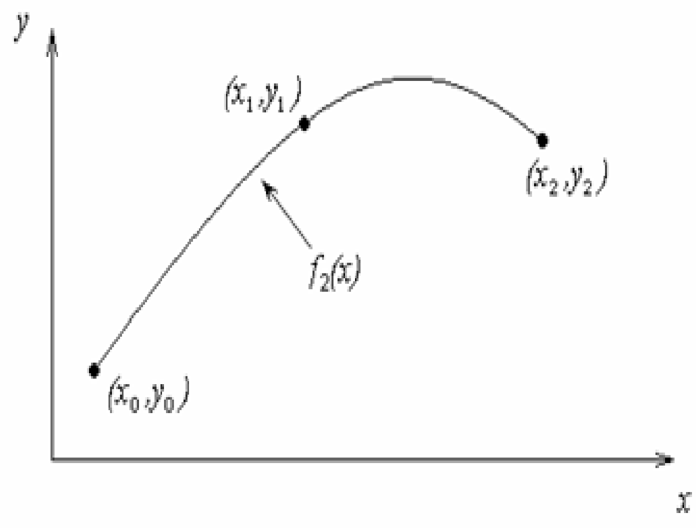
b_2: Finite-divided difference for $f''(x)$

Divided difference

$$x = x_0;\ b_0 = f(x_0)$$

$$x = x_1;\ b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$x = x_2;\ b_2 = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$



- The advantage is that b_0, b_1, and b_2 can be calculated conveniently.
- There is only one unique 2nd-order polynomial that passes through three points.
- The formula can be rewritten in the conventional form. i.e., as

$$P_2(x) = a_0 + a_1 x + a_2 x^2$$

Comparing Linear and Quadratic Interpolation

Linear interpolation

$$P_1(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x - x_0}(x - x_0)$$

Quadratic interpolation

$$P_2(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x - x_0}(x - x_0) + \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}(x - x_0)(x - x_1)$$

The quadratic interpolation formula includes an additional term which represents the 2nd-order curvature.

Newton's equation of a function that passes through four points can be written by adding a fourth term .

$$P_3(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1) + b_3(x - x_0)(x - x_1)(x - x_2)$$

The fourth term will vanish at all three previous points and, therefore, leaving all three previous coefficients intact.

Divided differences and the coefficients

The divided difference of a function, f with respect to x_i called as *zeroth divided difference*, is denoted as $f[x_i]$ and is simply the value of the function f at x_i

$$f[x_i] = f(x_i)$$

The divided difference of a function, f with respect to x_i and x_{i+1} called as the *first divided difference*, is denoted as

$$f[x_{i+1}, x_i]$$

where $$f\left[x_{i+1}, x_i\right] = \frac{f\left[x_{i+1}\right] - f\left[x_i\right]}{x_{i+1} - x_i}$$

The divided difference of a function, f with respect to x_i, x_{i+1} and x_{i+2} called as the *second divided difference*, is denoted as $f\left[x_{i+2}, x_{i+1}, x_i\right]$

$$f\left[x_{i+2}, x_{i+1}, x_i\right] = \frac{f\left[x_{i+2}, x_{i+1}\right] - f\left[x_{i+1}, x_i\right]}{x_{i+2} - x_i}$$

The *third divided difference* with respect to x_i, x_{i+1}, x_{i+2} and x_{i+3}

$$f\left[x_{i+3}, x_{i+2}, x_{i+1}, x_i\right] = \frac{f\left[x_{i+3}, x_{i+2}, x_{i+1}\right] - f\left[x_{i+2}, x_{i+1}, x_i\right]}{x_{i+3} - x_i}$$

These 1st, 2nd... and kth order differences are denoted by Δf, $\Delta^2 f$, …, $\Delta^k f$.

Newton's Divided differences

- The computations are organized in the divided-difference table as below.

i	x_i	$f(x_i)$	First	Second	Third
0	x_0	$f(x_0)$	$f[x_1, x_0]$	$f[x_2, x_1, x_0]$	$f[x_3, x_2, x_1, x_0]$
1	x_1	$f(x_1)$	$f[x_2, x_1]$	$f[x_3, x_2, x_1]$	
2	x_2	$f(x_2)$	$f[x_3, x_2]$		
3	x_3	$f(x_3)$			

Invariance Theorem

- Note that, the order of the data points does not matter.
- It is not necessary the data points be equally spaced but must be distinct.
- Hence, the divided difference $f[x_0, x_1, \ldots, x_k]$ is invariant under all permutations of the x_i's.

The third order polynomial, given (x_0, y_0), (x_1, y_1), (x_2, y_2), and (x_3, y_3), is

$$P_3(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1)$$
$$+ f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2)$$

For 4 points

$$\begin{array}{cccccc}
 & b_0 & & & & \\
x_0 & f(x_0) & & b_1 & & \\
 & & f[x_1, x_0] & & b_2 & \\
x_1 & f(x_1) & & f[x_2, x_1, x_0] & & b_3 \\
 & & f[x_2, x_1] & & f[x_3, x_2, x_1, x_0] & \\
x_2 & f(x_2) & & f[x_3, x_2, x_1] & & \\
 & & f[x_3, x_2] & & & \\
x_3 & f(x_3) & & & &
\end{array}$$

These equations are recursive, i.e. higher order differences are computed by taking differences of lower-order differences.

For 6 points

$f(x)$	First divided differences	Second divided differences	Third divided differences
$f[x_0]$			
	$f[x_0,x_1]=\dfrac{f[x_1]-f[x_0]}{x_1-x_0}$		
$f[x_1]$		$f[x_0,x_1,x_2]=\dfrac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$	
	$f[x_1,x_2]=\dfrac{f[x_2]-f[x_1]}{x_2-x_1}$		$f[x_0,x_1,x_2,x_3]=\dfrac{f[x_1,x_2,x_3]-f[x_0,x_1,x_2]}{x_3-x_0}$
$f[x_2]$		$f[x_1,x_2,x_3]=\dfrac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$	
	$f[x_2,x_3]=\dfrac{f[x_3]-f[x_2]}{x_3-x_2}$		$f[x_1,x_2,x_3,x_4]=\dfrac{f[x_2,x_3,x_4]-f[x_1,x_2,x_3]}{x_4-x_1}$
$f[x_3]$		$f[x_2,x_3,x_4]=\dfrac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$	
	$f[x_3,x_4]=\dfrac{f[x_4]-f[x_3]}{x_4-x_3}$		$f[x_2,x_3,x_4,x_5]=\dfrac{f[x_3,x_4,x_5]-f[x_2,x_3,x_4]}{x_5-x_2}$
$f[x_4]$		$f[x_3,x_4,x_5]=\dfrac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}$	
	$f[x_4,x_5]=\dfrac{f[x_5]-f[x_4]}{x_5-x_4}$		
$f[x_5]$			

General Form of Newton's Polynomials

- Consider our data set of $n+1$ points $y_i = f(x_i)$ at $x_0, x_1 \ldots x_i, \ldots x_n : x_n > x_0$
- Since $P_n(x)$ is the unique polynomial $P_n(x)$ of order n, write it:

$$\begin{aligned} P_n(x) = f(x_0) + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0] \\ + \cdots + (x - x_0)(x - x_1) \cdots (x - x_{n-1}) f[x_n, x_{n-1}, \cdots, x_0] \end{aligned}$$

$$\left.\begin{aligned} f[x_1, x_0] &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} \\ f[x_2, x_1, x_0] &= \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0} \\ &\vdots \\ f[x_n, x_{n-1}, \ldots, x_1, x_0] &= \frac{f[x_n, x_{n-1}, \ldots, x_1] - f[x_{n-1}, x_{n-2}, \ldots, x_0]}{x_n - x_0} \end{aligned}\right\} \text{Finite divided difference}$$

- If we take x_i in $P_n(x)$ we get $P_n(x_i) = f(x_i)$, then $P_n(x)$ is an interpolating point.

Example: Estimate the value of ln(*x*) using linear interpolation

1. Find *f*(2) in between 1 and 6

2. Find *f*(2) between 1 and 4 (smaller interval)

Solution:

1) Using the formula

$$f_1(2) = f(1) + \frac{f(6) - f(1)}{6-1}(2-1) = 0 + \frac{1.791759 - 0}{6-1}(1) = 0.3583518$$

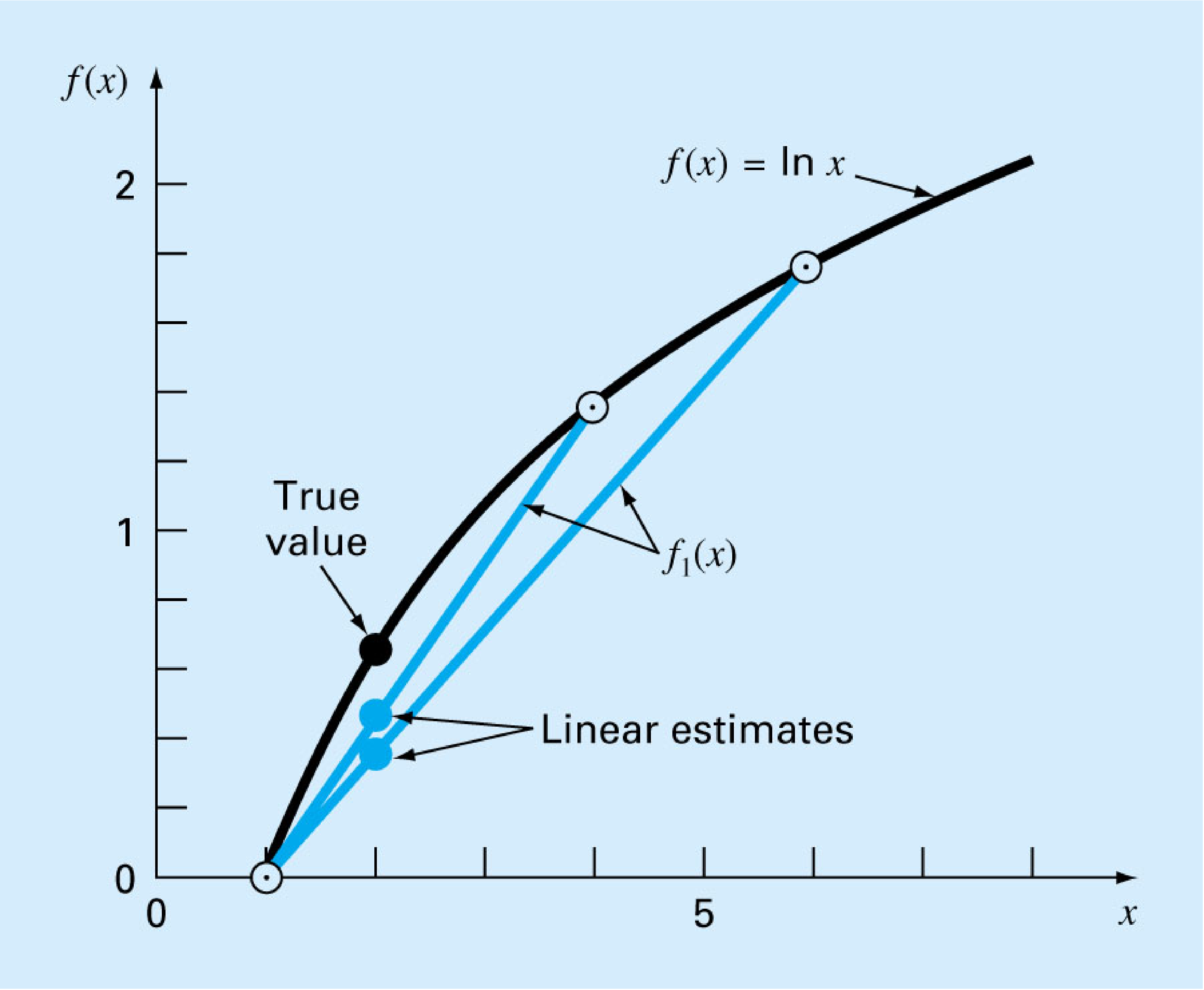
$$\varepsilon_t = \frac{\ln 2 - 0.3583518}{\ln 2} 100\% = 48.3\%$$

2) Using the formula

$$f_1(2) = f(1) + \frac{f(4) - f(1)}{4-1}(2-1) = 0 + \frac{1.386294 - 0}{4-1}(1) = 0.462098$$

$$\varepsilon_t = \frac{\ln 2 - 0.462098}{\ln 2} 100\% = 33.3\%$$

Two linear interpolations of $f(x) = \ln(x)$ on two different intervals.



Example: Estimate the value of ln(x) at x=2 using quadratic interpolation for x = 1, 4, and 6.

Solution:

$$x_0 = 1, f(x_0) = 0$$

$$x_1 = 4, f(x_1) = 1.386294$$

$$x_2 = 6, f(x_2) = 1.791759$$

$$b_0 = 0$$

$$b_1 = 0.4620981$$

$$b_2 = -0.0518731$$

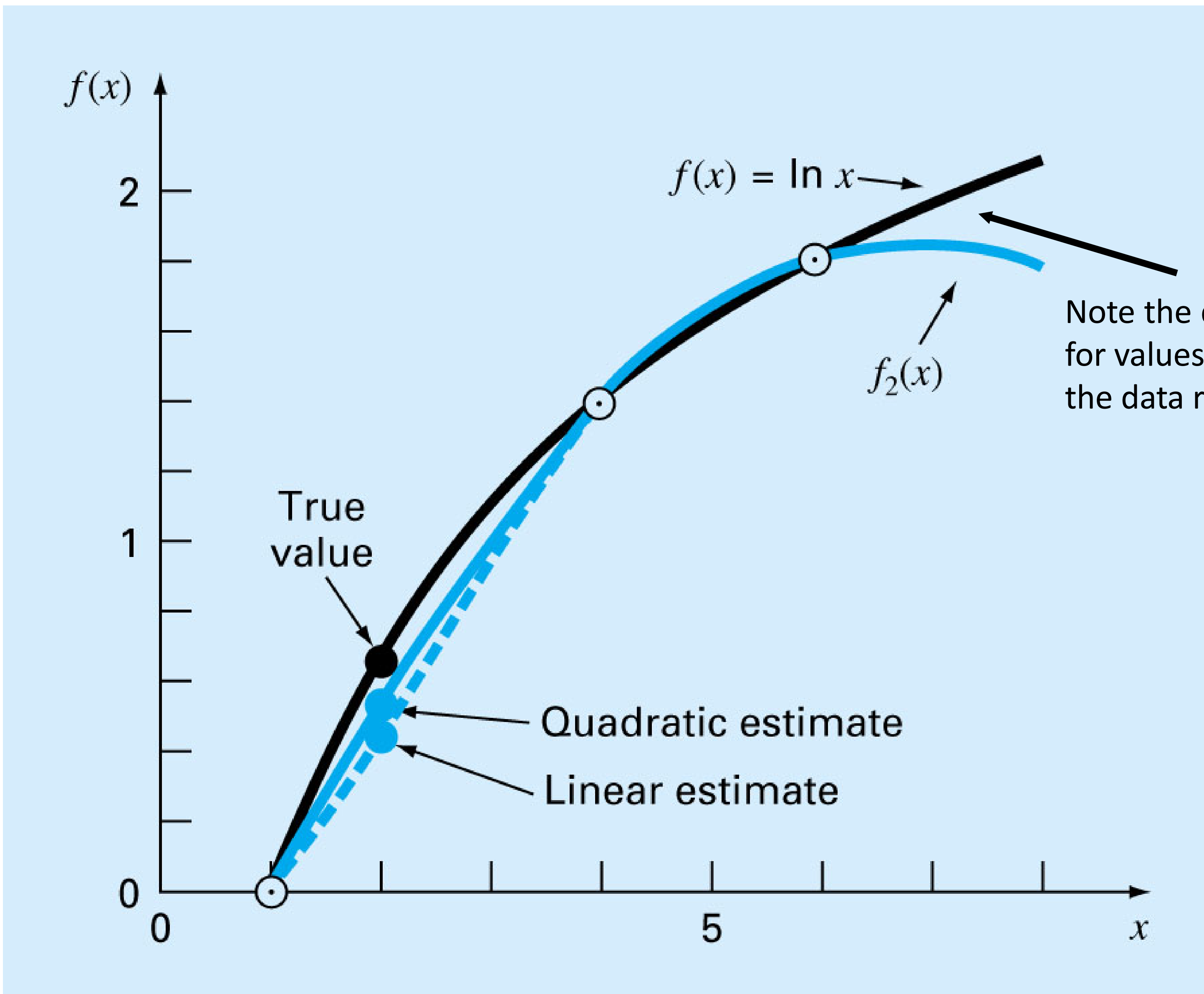
$$P_2(x) = 0 + 0.4620981(x-1) - 0.0518731(x-1)(x-4)$$

$$f_2(2) = 0.5658444$$

$$\varepsilon_t = 18.4\%$$

The quadratic interpolation produces a better estimate over the linear interpolation

Comparison of Linear and quadratic interpolation of $f(x) = \ln(x)$



Note the divergence for values outside of the data range.

Example: Find the interpolating polynomial of $\ln(x)$ for $x_0 = 1$, $x_1 = 4$, $x_2 = 6$, and $x_3 = 5$ and use the polynomial to estimate $\ln 2$.

Solution:

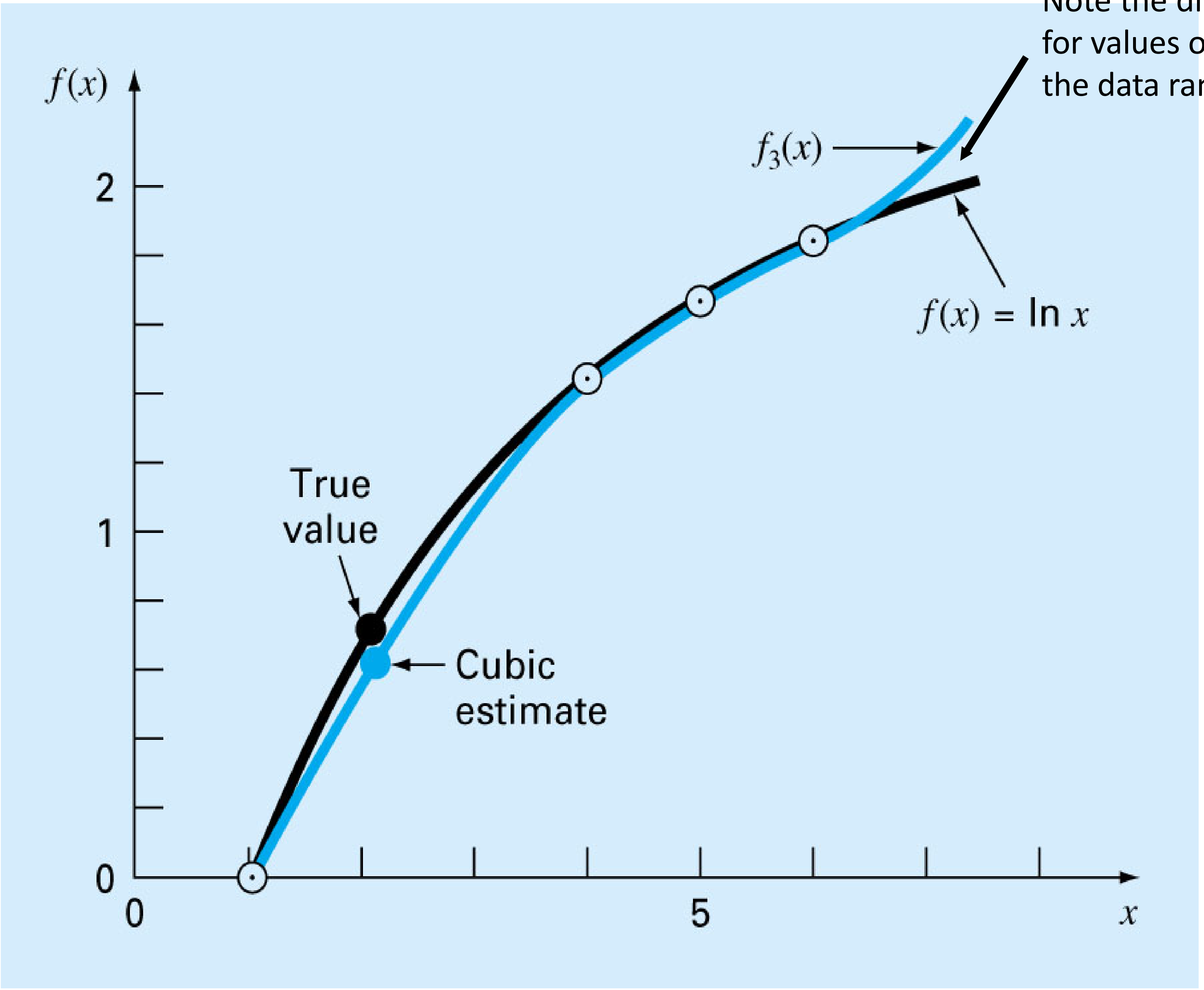
i	x_i	$f(x_i)$	First	Second	Third
0	1	0	0.462098	-0.05187	0.007865
1	4	1.386294	0.202733	-0.02041	
2	6	1.791759	0.182321		
3	5	1.609438			

- The interpolating polynomial is

$$P_3(x) = 0 + 0.462098(x-1) - 0.05187(x-1)(x-4) +$$
$$0.007865(x-1)(x-4)(x-6)$$

- For $x = 2$, $f_3(2) = 0.6287686$.
- $\varepsilon_t = 9.3\%$

Cubic interpolation of $f(x) = \ln(x)$



Note the divergence for values outside of the data range.

Example: Find Newton's interpolating polynomial to approximate a function whose 5 data points are given below.

i	x_i	$f[x_i]$	$f[x_{i+1}, x_i]$	$f[x_{i+2}, x_{i+1}, x_i]$	$f[x_{i+3}, \cdots, x_i]$	$f[x_{i+4}, \cdots, x_i]$
0	2.0	0.85467				
			-0.32617			
1	2.3	0.75682		-1.26505		
			-1.08520		2.13363	
2	2.6	0.43126		0.65522		-2.02642
			-0.69207		-0.29808	
3	2.9	0.22364		0.38695		
			-0.45990			
4	3.2	0.08567				

The 5 coefficients of the Newton's interpolating polynomial are:

$$b_0 = f[x_0] = 0.85467 \quad b_1 = f[x_1, x_0] = -0.32617 \quad b_2 = f[x_2, x_1, x_0] = -1.26505$$

$$b_3 = f[x_3, x_2, x_1, x_0] = 2.13363 \quad b_4 = f[x_4, x_3, x_2, x_1, x_0] = -2.02642$$

$$P_4(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1) + b_3(x - x_0)(x - x_1)(x - x_2)$$
$$+ b_4(x - x_0)(x - x_1)(x - x_2)(x - x_3)$$

$$P_4(x) = 0.85467 - 0.32617(x - 2.0) - 1.26505(x - 2.0)(x - 2.3)$$
$$+2.13363(x - 2.0)(x - 2.3)(x - 2.6) - 2.02642(x - 2.0)(x - 2.3)(x - 2.6)(x - 2.9)$$

$P(x)$ can now be used to estimate the value of the function $f(x)$ say at $x = 2.8$.

$$f(2.8) = 0.85467 - 0.32617(2.8 - 2.0) - 1.26505(2.8 - 2.0)(2.8 - 2.3)$$
$$+2.13363(2.8 - 2.0)(2.8 - 2.3)(2.8 - 2.6) - 2.02642(2.8 - 2.0)(2.8 - 2.3)(2.8 - 2.6)(2.8 - 2.9)$$

$$f(2.8) \approx P_4(x = 2.8) = 0.275$$

Example: What are the coefficients of the polynomial and what is the value of $P_4(2.3)$? Where The true function of the points is $f(x) = 2^x$

X	Y	d	dd	ddd	dddd
0	1				
		$\frac{y_2 - y_1}{x_2 - x_1} = \frac{2-1}{1-0} = 1$			
1	2		$\frac{d_2 - d_1}{x_3 - x_1} = \frac{2-1}{2-0} = 0.5$		
		$\frac{y_3 - y_2}{x_3 - x_2} = \frac{4-2}{2-1} = 2$		$\frac{dd_2 - dd_1}{x_4 - x_1} = \frac{1-0.5}{3-0} = 0.1667$	
2	4		$\frac{d_3 - d_2}{x_4 - x_2} = \frac{4-2}{3-1} = 1$		$\frac{ddd_2 - ddd_1}{x_5 - x_1} = \frac{0.33-0.167}{4-0} = 0.04167$
		$\frac{y_4 - y_3}{x_4 - x_3} = \frac{8-4}{3-2} = 4$		$\frac{dd_3 - dd_2}{x_5 - x_2} = \frac{2-1}{4-1} = 0.3333$	
3	8		$\frac{d_4 - d_3}{x_5 - x_3} = \frac{8-4}{4-2} = 2$		
		$\frac{y_5 - y_4}{x_5 - x_4} = \frac{16-8}{4-3} = 8$			
4	16				

The coefficients are the top row of the chart:

$$P_4(x) = y_1 + c_1 * (x - x_1) + c_2 * (x - x_1)(x - x_2) + c_3 * (x - x_1)(x - x_2)(x - x_3)$$
$$+ c_4 * (x - x_1)(x - x_2)(x - x_3)(x - x_4)$$

$$P_4(x) = 1 + 1*(x-0) + 0.5*(x-0)(x-1) + 0.1667*(x-0)(x-1)(x-2)$$
$$+ 0.042167*(x-0)(x-1)(x-2)(x-3)$$

The values are evaluated

$P_4(x) = 1 + (x-0)$

$+0.5*(x-0)(x-1)$

$+0.1667*(x-0)(x-1)(x-2)$

$+0.04167*(x)(x-1)(x-2)(x-3)$

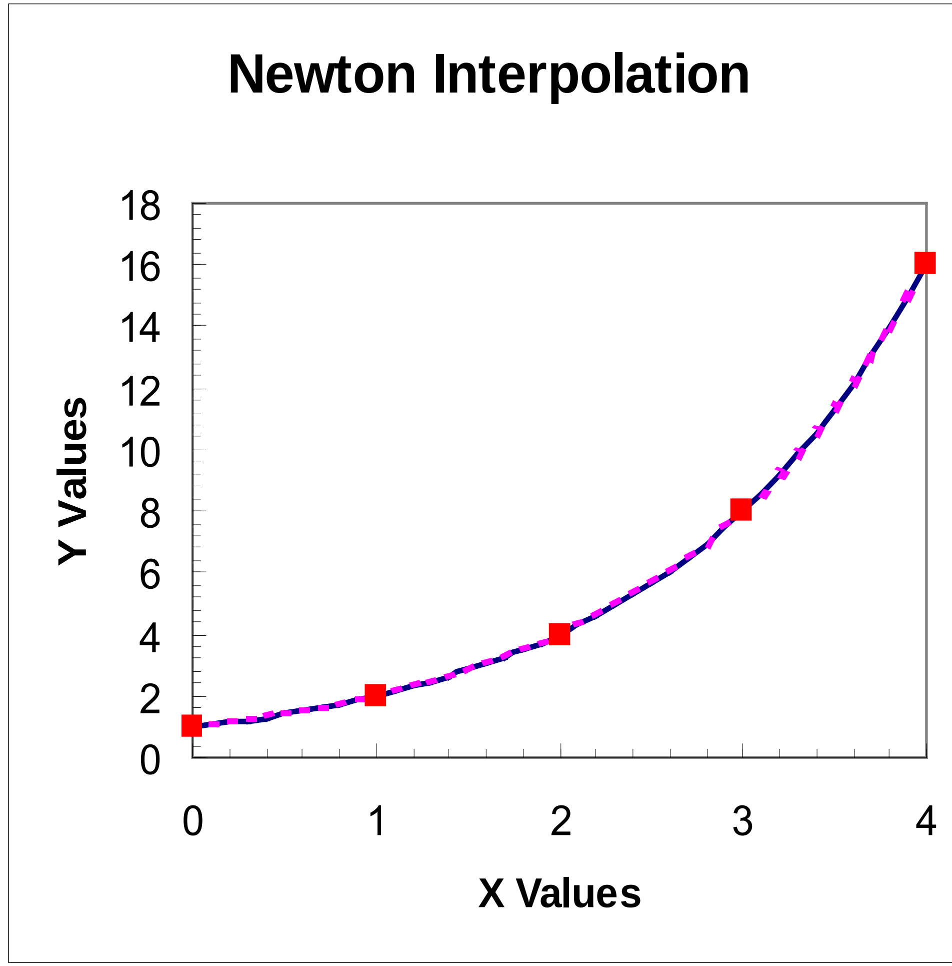
$f(2.3) = 1 + (2.3)$

$+0.5*(2.3)(1.3)$

$+0.1667*(2.3)(1.3)(0.3)$

$+0.04167*(2.3)(1.3)(0.3)(-0.7)$

$= 4.9183\ (4.9246)$



Example: The upward velocity of a rocket is given as a function of time in **Table 1**.

Find the velocity at ***t* =16** seconds using the Newton Divided Difference method for linear interpolation.

t	v(t)
s	m/s
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

Table 1: Velocity as a function of time

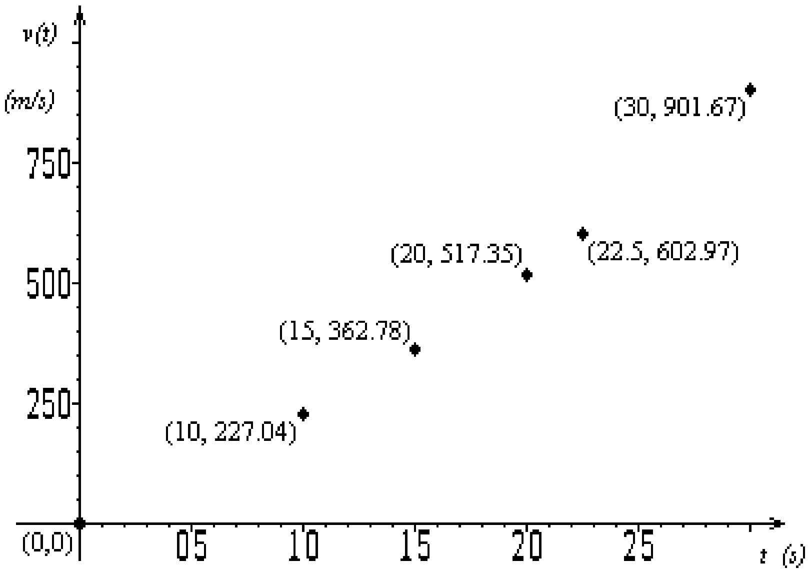


Figure 2: Velocity vs. time data for the rocket example

Linear Interpolation

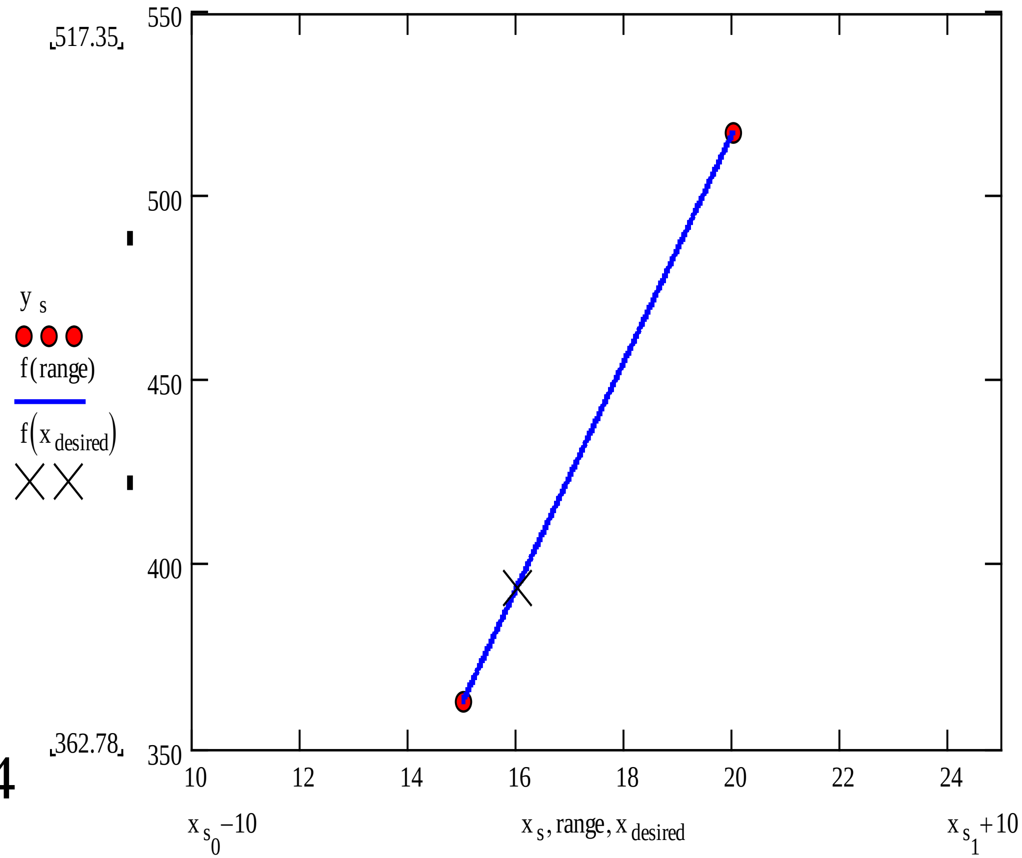
$$v(t) = b_0 + b_1(t - t_0)$$

$$t_0 = 15,\ v(t_0) = 362.78$$

$$t_1 = 20,\ v(t_1) = 517.35$$

$$b_0 = v(t_0) = 362.78$$

$$b_1 = \frac{v(t_1) - v(t_0)}{t_1 - t_0} = 30.914$$



$$v(t) = b_0 + b_1(t - t_0) = 362.78 + 30.914(t - 15),\ 15 \le t \le 20$$

At $t = 16$

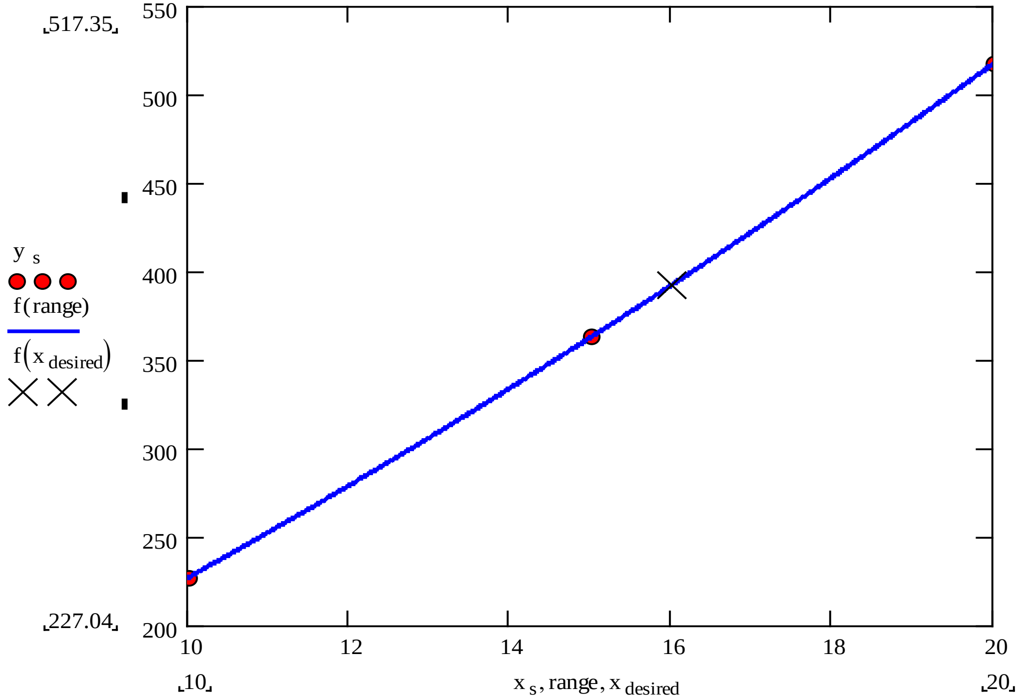
$$v(16) = 362.78 + 30.914(16 - 15) = 393.69 \text{ m/s}$$

Quadratic Interpolation

$$\boxed{t_0 = 10,\ v(t_0) = 227.04}$$

$$t_1 = 15,\ \ v(t_1) = 362.78$$

$$t_2 = 20,\ v(t_2) = 517.35$$



$$b_0 = v(t_0)$$

$$= 227.04$$

$$b_1 = \frac{v(t_1) - v(t_0)}{t_1 - t_0} = \frac{362.78 - 227.04}{15 - 10}$$

$$= 27.148$$

$$b_2 = \frac{\dfrac{v(t_2) - v(t_1)}{t_2 - t_1} - \dfrac{v(t_1) - v(t_0)}{t_1 - t_0}}{t_2 - t_0} = \frac{\dfrac{517.35 - 362.78}{20 - 15} - \dfrac{362.78 - 227.04}{15 - 10}}{20 - 10}$$

$$= \frac{30.914 - 27.148}{10}$$

$$= 0.37660$$

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1)$$

$$= 227.04 + 27.148(t - 10) + 0.37660(t - 10)(t - 15), \qquad 10 \le t \le 20$$

At $t = 16$,

$$v(16) = 227.04 + 27.148(16 - 10) + 0.37660(16 - 10)(16 - 15) = 392.19 \text{ m/s}$$

The absolute relative approximate error $|\in_a|$ obtained between the results from the first order and second order polynomial is

$$|\in_a| = \left|\frac{392.19 - 393.69}{392.19}\right| \text{x} 100 = 0.38502\ \%$$

If the velocity profile is chosen as

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1) + b_3(t - t_0)(t - t_1)(t - t_2)$$

we need to choose four data points that are closest to $t = 16$

$t_0 = 10, \quad v(t_0) = 227.04 \qquad t_1 = 15, \quad v(t_1) = 362.78$

$t_2 = 20, \quad v(t_2) = 517.35 \qquad \boxed{t_3 = 22.5, \quad v(t_3) = 602.97}$

The values of the constants are found as:

$b_0 = 227.04$; $b_1 = 27.148$; $b_2 = 0.37660$; $b_3 = 5.4347*10^{-3}$

	b_0	b_1	b_2	b_3
$t_0 = 10$	227.04			
		27.148		
$t_1 = 15,$	362.78		0.37660	
		30.914		$5.4347x10^{-3}$
$t_2 = 20,$	517.35		0.44453	
		34.248		
$t_3 = 22.5,$	602.97			

$b_0 = 227.04$; $b_1 = 27.148$; $b_2 = 0.37660$; $b_3 = 5.4347*10^{-3}$

Hence

$$v(t) = b_0 + b_1(t - t_0) + b_2(t - t_0)(t - t_1) + b_3(t - t_0)(t - t_1)(t - t_2)$$
$$= 227.04 + 27.148(t - 10) + 0.37660(t - 10)(t - 15)$$
$$+ 5.4347 * 10^{-3}(t - 10)(t - 15)(t - 20)$$

At t =16

$$v(16) = 227.04 + 27.148(16-10) + 0.37660(16-10)(16-15)$$
$$+ 5.4347 * 10^{-3}(16-10)(16-15)(16-20)$$

$$= 392.06 \text{ m/s}$$

The absolute relative approximate error $|\in_a|$ obtained is

$$|\in_a| = \left|\frac{392.06-392.19}{392.06}\right| x100 = 0.033427\ \%$$

Order of Polynomial	1	2	3
v(t=16) m/s	393.69	392.19	392.06
Absolute Relative Approximate Error	----------	0.38502 %	0.033427 %

Distance from Velocity Profile

Find the distance covered by the rocket from $t = 11s$ to $t = 16s$?

$$v(t) = 227.04 + 27.148(t-10) + 0.37660(t-10)(t-15) + 5.4347*10^{-3}(t-10)(t-15)(t-20) \qquad 10 \le t \le 22.5$$

$$= -4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3 \qquad 10 \le t \le 22.5$$

So

$$s(16) - s(11) = \int_{11}^{16} v(t)dt$$

$$= \int_{11}^{16} (-4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3)dt$$

$$= \left[-4.2541t + 21.265\frac{t^2}{2} + 0.13204\frac{t^3}{3} + 0.0054347\frac{t^4}{4}\right]_{11}^{16}$$

$$= 1605\, m$$

Acceleration from Velocity Profile

Find the acceleration of the rocket at $t = 16s$ given that

$$v(t) = -4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3$$

$$a(t) = \frac{d}{dt}v(t) = \frac{d}{dt}\left(-4.2541 + 21.265t + 0.13204t^2 + 0.0054347t^3\right)$$

$$= 21.265 + 0.26408t + 0.016304t^2$$

$$a(16) = 21.265 + 0.26408(16) + 0.016304(16)^2$$

$$= 29.664\, m/s^2$$

EXAMPLE Using the following table, find $y'(4)$ and the maximum value of y.

x	0	1	2	5
y	2	3	12	147

Solution Since x values are not equally-spaced, so we apply Newton's divided difference formula.

The divided difference table is:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
0	2			
		1		
1	3		4	
		9		1
2	12		9	
		45		
5	147			

Newton's divided difference interpolation formula is

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

Here, $$(x_0, x_1) = 1$$
$$(x_0, x_1, x_2) = 4$$
$$(x_0, x_1, x_2, x_3) = 1$$

and $$y_0 = 2$$

Also $$x_0 = 0$$
$$x_1 = 1$$
$$x_2 = 2$$
$$x_3 = 5$$

Substituting these values

$$y = f(x) = 2 + (x-0)1 + (x-0)(x-1)4 + (x-0)(x-1)(x-2)\cdot 1$$

$$y(x) = x^3 + x^2 - x + 2$$

$$y'(x) = 3x^2 + 2x - 1$$

$$y'(4) = 55$$

We know that $y(x)$ is maximum if $y'(x) = 0$ and $y''(x) = 0$.

$\therefore \quad y'(x) = 3x^2 + 2x - 1 = 0 \Rightarrow (-1, 1/3)$

Also $\quad y''(x) = 6x + 2 \Rightarrow y''(-1) < 0$. 1.814

$\therefore$ The maximum value of y occur at -1.

Maximum value of y is

$$y(-1) = (-1)^3 + (-1)^2 + (1) + 2 = 3$$

An example with actual values (not in order):

x_i	f_i	$f[x_i, x_{i+1}]$	$f[x_i, \ldots, x_{i+2}]$	$f[x_i, \ldots, x_{i+3}]$	$f[x_i, \ldots, x_{i+4}]$
3.2	22.0	8.400	2.856	−0.528	0.256
2.7	17.8	2.118	2.012	0.0865	
1.0	14.2	6.342	2.263		
4.8	38.3	16.750			
5.6	51.7				

- The *3rd* degree polynomial fitting all points from $x_0 = 3.2$ to $x_3 = 4.8$ is given by

  $P_3(x) = 22.0 + 8.400(x - 3.2) + 2.856(x - 3.2)(x - 2.7) - 0.528(x - 3.2)(x - 2.7)(x - 1.0)$
- The *4th* degree polynomial fitting all points is given by

  $P_4(x) = P_3(x) + 0.256(x - 3.2)(x - 2.7)(x - 1.0)(x - 4.8)$
- The interpolated value at $x = 3.0$ gives $f_3(x) = 20.2120$.

Calculating the Divided-Differences

- A *divided-difference* table can easily be constructed incrementally. Consider the function ln(*x*).

$$f[i+1,i] = \frac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)}$$

$$f[i+2,i+1,i] = \frac{f[i+2,i+1] - f[i+1,i]}{(x_{i+2} - x_i)}$$

$$f[i+3,\ldots,i] = \frac{f[i+3,i+2,i+1] - f[i+2,i+1,i]}{(x_{i+3} - x_i)}$$

$$f[i+4,\ldots,i] = \frac{f[i+4,\ldots,i] - f[i+3,\ldots,i]}{(x_{i+4} - x_i)}$$

$$f[i+5,\ldots,i] = \frac{f[i+5,\ldots,i] - f[i+4,\ldots,i]}{(x_{i+5} - x_i)}$$

$$f[i+6,\ldots,i] = \frac{f[i+6,\ldots,i] - f[i+5,\ldots,i]}{(x_{i+6} - x_i)}$$

$$f[i+7,\ldots,i] = \frac{f[i+7,\ldots,i] - f[i+6,\ldots,i]}{(x_{i+7} - x_i)}$$

Calculating the Divided-Differences

All of the coefficients for the resulting polynomial are in bold.

b_0 b_4 b_7

x	ln(x)	f[I,I+1]						f[I,I+1,…,I+7]
1	**0.000000**							
2	0.693147	**0.693147**						
3	1.098612	0.405465	**-0.143841**					
4	1.386294	0.287682	-0.058892	**0.028317**				
5	1.609438	0.223144	-0.032269	0.008874	**-0.004861**			
6	1.791759	0.182322	-0.020411	0.003953	-0.001230	**0.000726**		
7	1.945910	0.154151	-0.014085	0.002109	-0.000461	0.000154	**-0.000095**	
8	2.079442	0.133531	-0.010310	0.001259	-0.000212	0.000050	-0.000017	**0.000011**
x	ln(x)	b10-b9)/(A10-A9	(c10-c9)/(a10-a8	d10-d9)/(a10-a7	d10-d9)/(a10-a6	e10-e9)/(a10-a5	f10-f9)/(a10-a4	(g10-g9)/(a10-a3)

The resulting polynomial comes from the divided-differences and the corresponding product terms:

$$\begin{aligned}
P_7(x) = {} & 0 + 0.693(x-1) - 0.144(x-1)(x-2) + 0.28(x-1)(x-2)(x-3) \\
& -0.0049(x-1)(x-2)(x-3)(x-4) + 7.26\times 0^{-4}(x-1)(x-2)(x-3)(x-4)(x-5) \\
& -9.5\times 10^{-5}(x-1)(x-2)(x-3)(x-4)(x-5)(x-6) \\
& +1.1\times 10^{-5}(x-1)(x-2)(x-3)(x-4)(x-5)(x-6)(x-7)
\end{aligned}$$

Many polynomials

- Note that, the order of the numbers (x_i,y_i)'s only matters when writing the polynomial down.
  - The first column represents the set of lines between two adjacent points.
  - The second column gives us quadratics thru three adjacent points.
- Adding an additional point, simply adds an additional term to the existing polynomial.
  - Hence, only n additional divided-differences need to be calculated for the $n+1$-data point.

x	ln(x)	f[I,I+1]						f[I,I+1,…,I+7]	
1.0000000	**0.0000000**								
2.0000000	0.6931472	**0.6931472**							
3.0000000	1.0986123	0.4054651	**-0.1438410**						
4.0000000	1.3862944	0.2876821	-0.0588915	**0.0283165**					
5.0000000	1.6094379	0.2231436	-0.0322693	0.0088741	**-0.0048606**				
6.0000000	1.7917595	0.1823216	-0.0204110	0.0039528	-0.0012303	**0.0007261**			
7.0000000	1.9459101	0.1541507	-0.0140854	0.0021085	-0.0004611	0.0001539	**-0.0000954**		
8.0000000	2.0794415	0.1335314	-0.0103096	0.0012586	-0.0002125	0.0000497	-0.0000174	**0.0000111**	
1.5000000	0.4054651	0.2575348	-0.0225461	0.0027192	-0.0004173	0.0000819	-0.0000215	0.0000082	**-0.0000058**

b_8

Errors of Newton's Interpolating Polynomials

- Structure of interpolating polynomials is similar to the *Taylor series expansion* in the sense that finite divided differences are added sequentially to capture the higher order derivatives.

Taylor Series

$$f(x) = p(x) + r(x) = f(x_0) + \sum_{i=1}^{n} \frac{f^{(i)}(x_0)}{(i+1)!}(x - x_0)^i + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}$$

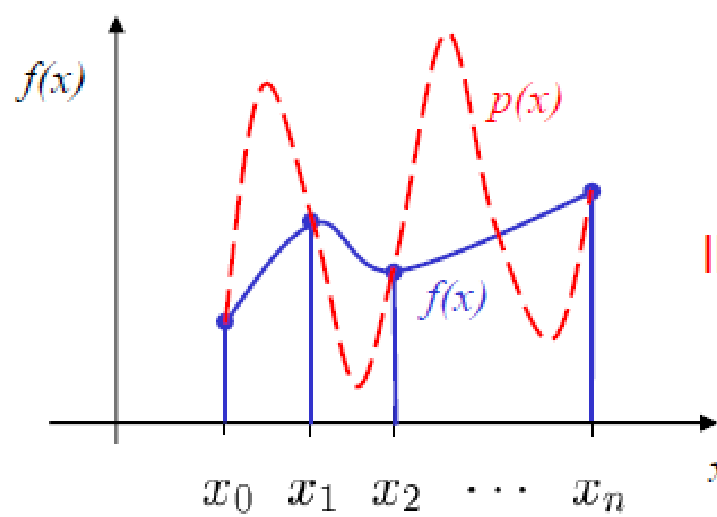
Remainder

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)^{n+1}$$

Requirement $\quad f^{(n+1)}(\xi) \ll 1$

Ill-conditioned for large n

Polynomial is unique, but how do we calculate the coefficients?



Ill-

- Define the error term as: $\varepsilon_n(x) = f(x) - p_n(x)$
- Intuitively, the first $n+1$ terms of the Taylor Series is also an $n^{\underline{th}}$ degree polynomial. If $f(x)$ is an $n^{\underline{th}}$ *order* polynomial $p_n(x)$ is of course exact.
- For an n^{th}-order interpolating polynomial, an analogous relationship for the error is:

$$\varepsilon_n(x) = f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \prod_{i=0}^{n} (x - x_i) \quad ; \quad x \in [a,b], \xi \in (a,b)$$

or

$$R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1)\cdots(x - x_n)$$

- For non differentiable functions, if an additional point $f(x_{n+1})$ is available, an alternative formula can be used.

$$x \notin \{x_0, x_1, \ldots x_n\}$$

$$\varepsilon_n(x) = f(x) - p_n(x) = f[x_{n+1}, x_n, x_{n-1} \ldots x_0]\prod_{i=0}^{n}(x - x_i)$$

or $$R_n \cong f[x_{n+1}, x_n, x_{n-1}, \ldots, x_0](x - x_0)(x - x_1)\cdots(x - x_n)$$

- Combining the last two statements, we can also get what these divided differences represent.

$$f[x_0, x_1, \ldots x_n] = \frac{1}{n!} f^{(n)}(\xi)$$

- **Corollary 1**: If $f(x)$ is a polynomial of degree $m<n$, then all $(m+1)^{st}$ divided differences and higher are zero.

Advantages

There are advantages using Newton Divided Difference polynomial for interpolation over the Lagrange Polynomial.

- It involves less arithmetic operations than does the Lagrange Polynomial.
- If we desire to add or subtract a point from the set to construct the polynomial, we do not have to start over in the computations unlike the Lagrange Polynomial.
- Suppose $f(x)$ is a polynomial of degree m, where $m<n$ such as $f(x) = 3x-2$ and we want to approximate $f(x)$ at five locations,$(-2,-8)$, $(-1,-5)$, $(0,-2)$, $(1,1)$, $(2,4)$, that means $n+1=5$. Using Divided Difference, all $(m+1)^{st}$ divided differences and higher are zero but the Lagrange Polynomial is not the case(over fit).

Disadvantages

Tabular data have a finite number of digits. The last digit is typically rounded off. Round off has an effect on the accuracy of the higher-order differences.

Newton Interpolation Program

The Newton interpolation is broken up into two programs to evaluate the new polynomial.

- a = newtonCoeff(x,y), which evaluates the coefficients of the Newton technique
- p = newtonPoly(a,x,k), which uses the coefficients a and x values to evaluate the polynomial

■ newtonCoeff

Machine computations are best carried out within a one-dimensional array **a** employing the following algorithm:

```
function a = newtonCoeff(xData,yData)
% Returns coefficients of Newton's polynomial.
% USAGE: a = newtonCoeff(xData,yData)
% xData = x-coordinates of data points.
% yData = y-coordinates of data points.
```

```
    n = length(xData);
    a = yData;
    for k = 2:n
        a(k:n) = (a(k:n) - a(k-1))./(xData(k:n) - xData(k-1));
    end
```

■ newtonPoly

Denoting the x-coordinate array of the data points by xData, and the number of data points by n, we have the following algorithm for computing $P_{n-1}(x)$:

```
function p = newtonPoly(a,xData,x)
% Returns value of Newton's polynomial at x.
% USAGE: p = newtonPoly(a,xData,x)
% a     = coefficient array of the polynomial;
%         must be computed first by newtonCoeff.
% xData = x-coordinates of data points.

n = length(xData);
p = a(n);
for k = 1:n-1;
    p = a(n-k) + (x - xData(n-k))*p;
end
```

Coefficients of an Interpolating Polynomial

- Lagrange and Newton polynomials are well suited for determining intermediate values between points.
- However, they do not provide a polynomial in the conventional form:

$$P_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

- To calculate $a_0, a_1, \ldots, a_n$, we can use simultaneous linear systems of equations at given $n+1$ points, $(x_0, f(x_0))$, $(x_1, f(x_1))$, …, $(x_n, f(x_n))$.

$$f(x_0) = a_0 + a_1 x_0 + a_2 x_0^2 \cdots + a_n x_0^n$$

$$f(x_1) = a_0 + a_1 x_1 + a_2 x_1^2 \cdots + a_n x_1^n$$

$$\vdots$$

$$f(x_n) = a_0 + a_1 x_n + a_2 x_n^2 \cdots + a_n x_n^n$$

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ 1 & x_2 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_n) \end{bmatrix}$$

- Solve this system of linear equations for a_0, a_1, …, a_n.
- Solving the system of linear equations directly is not the most efficient method.
- This system is typically ill-conditioned.
  - The resulting coefficients can be highly inaccurate when n is large.

INTERPOLATION FOR EQUALLY SPACED POINTS

Let $(X_0, Y_0), (X_1, Y_1), \ldots, (X_n, Y_n)$ be the given points with

$X_{i+1} = X_i + h, \quad i = 0,1,2,\ldots,(n-1).$

Finite Difference Operators

$$\boxed{f[x_0, x_1, \ldots, x_k] = \frac{1}{k!h^k}\Delta^k f(x_0).}$$

Forward difference operator $\Delta f(x_i) = f(x_i + h) - f(x_i)$

x	y	Δ	Δ^2	Δ^3
x_0	y_0			
		$\Delta y_0 = y_1 - y_0$		
x_1	y_1		$\Delta^2 y_0 = \Delta y_1 - \Delta y_0$	
		$\Delta y_1 = y_2 - y_1$		$\Delta^3 y_0 = \Delta^2 y_1 - \Delta^2 y_0$
x_2	y_2		$\Delta^2 y_1 = \Delta y_2 - \Delta y_1$	
		$\Delta y_2 = y_3 - y_2$		
x_3	y_3			

Backward difference operator $\nabla f(x_i) = f(x_i) - f(x_i - h)$

x	y	∇	∇^2	∇^3	∇^4
x_0	y_0				
		∇y_1			
x_1	y_1		$\nabla^2 y_2$		
		∇y_2		$\nabla^3 y_3$	
x_2	y_2		$\nabla^2 y_3$		$\nabla^4 y_4$
		∇y_3		$\nabla^3 y_4$	
x_3	y_3		$\nabla^2 y_4$		
		∇y_4			
x_4	y_4				

Shift operators

$$Ef(x) = f(x + h)$$

$$E^2 f(x) = f(x + 2h)$$

$$E^3 f(x) = f(x + 3h)$$

$$E^n f(x) = f(x + nh)$$

Central difference operator

$$\delta y_x = y_{x+(h/2)} - y_{x-(h/2)} = f(x + h/2) - f(x - h/2)$$

x	y	δy	$\delta^2 y$	$\delta^3 y$	$\delta^4 y$	$\delta^5 y$
x_0	y_0					
		$\delta y_{1/2}$				
x_1	y_1		$\delta^2 y_1$			
		$\delta y_{3/2}$		$\delta^3 y_{3/2}$		
x_2	y_2		$\delta^2 y_2$		$\delta^4 y_2$	
		$\delta y_{5/2}$		$\delta^3 y_{5/2}$		$\delta^5 y_{5/2}$
x_3	y_3		$\delta^2 y_3$		$\delta^4 y_3$	
		$\delta y_{7/2}$		$\delta^3 y_{7/2}$		
x_4	y_4		$\delta^2 y_4$			
		$\delta y_{9/2}$				
x_5	y_5					

NEWTON FORWARD INTERPOLATION

For convenience we put $p = \frac{x - x_0}{h}$ and $f_0 = y_0$.

Then we have

$$y(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2) + \ldots + a_n(x - x_0)(x - x_1)\ldots(x - x_{n-1})$$

$$f(x_0 + ph) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \ldots\ldots\ldots + \frac{p(p-1)\ldots\ldots(p-(n-1))}{n!}\Delta^n y_0$$

NEWTON BACKWARD INTERPOLATION

For convenience we put $p = \frac{x - x_n}{h}$ and $f_0 = y_0$.

Then we have

$$y(x) = a_0 + a_1(x - x_n) + a_2(x - x_n)(x - x_{n-1}) + a_3(x - x_n)(x - x_{n-1})(x - x_{n-2}) + \ldots + a_n(x - x_n)(x - x_{n-1})\ldots(x - x_1)$$

$$f(x_n + ph) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \ldots\ldots\ldots + \frac{p(p+1)\ldots\ldots(p+(n-1))}{n!}\nabla^n y_n$$

EXAMPLE Estimate the value of sin θ at $\theta = 25°$, using the Newton–Gregory forward difference formula with the help of the following table.

θ	10	20	30	40	50
sin θ	0.1736	0.3420	0.5000	0.6428	0.7660

Solution In order to use the Newton–Gregory forward difference formula, we need the values of $\Delta^i y_0$. These coefficients can be obtained from the difference table given below.

θ	$y = \sin\theta$	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
10	$\boxed{0.1736}$					
		$\boxed{0.1684}$				
20	0.3420		$\boxed{-0.0104}$			
		0.1580		$\boxed{0.0048}$		
30	0.5000		− 0.0152		$\boxed{-0.0004}$	–
		0.1428		0.0044		
40	0.6428		− 0.0196			
		0.1232				
50	0.7660					

Here $$x_0 = \theta_0 = 10$$

and $$h = 10$$

Therefore, $$p = \frac{x - x_0}{h}$$

$$= \frac{25 - 10}{10}$$

We have $$= 1.5$$

$$y = y_0 + p(\Delta y_0) + \left[\frac{p(p-1)}{1 \cdot 2}\right](\Delta^2 y_0) + \left[\frac{p(p-1)(p-2)}{1 \cdot 2 \cdot 3}\right](\Delta^3 y_0)$$

$$+ \left[\frac{p(p-1)(p-2)(p-3)}{1 \cdot 2 \cdot 3 \cdot 4}\right](\Delta^4 y_0)$$

Here $y_0 = 1.1736, \quad \Delta y_0 = 0.1684, \quad \Delta^2 y_0 = -\,0.0104$

$$\Delta^3 y_0 = 0.0048, \quad \Delta^4 y_0 = -\,0.0004$$

$$y_p = 1.1736 + 1.5 \times 0.1684 + \frac{(1.5)\,(1.5-1)}{1.2}(-0.0104)$$

$$+ \frac{1.5\,(1.5-1)\,(1.5-2)}{1 \cdot 2 \cdot 3}(0.0048)$$

$$+ (1.5)\,(1.5-1)\,\frac{(1.5-2)\,(1.5-3)}{1 \cdot 2 \cdot 3 \cdot 4}(-0.0004)$$

Thus, sin 25 = 0.4220, which is accurate to four decimal places.

EXAMPLE The following data gives the melting point of an alloy of lead and zinc, where y is the temperature in °C and x is the percentage of lead in the alloy.

x	40	50	60	70	80	90
y	184	204	226	250	276	304

Using Newton's interpolation formula, find the melting point of the alloy containing 84% of lead.

Solution Since the value 84 of x is near the end of the table, so we use Newton's backward formula.

The backward differences are calculated and tabulated below.

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
40	184					
		20				
50	204		2			
		22		0		
60	206		2		0	
		24		0		$\boxed{0}$
70	250		2		$\boxed{0}$	
		26		$\boxed{0}$		
80	276		$\boxed{2}$			
		$\boxed{28}$				
90	$\boxed{304}$					

Newton's backward formula gives

$$y_p = y_n + p(\nabla y_n) + \left[\frac{p(p+1)}{2!}\right](\nabla^2 y_n) + \left[\frac{p(p+1)(p+2)}{3!}\right](\nabla^3 y_n)$$

$$+\left[\frac{p(p+1)(p+2)(p+3)}{4!}\right](\nabla^4 y_n) + \ldots$$

Here, $x_n = 90, \quad y_n = 304, \quad \nabla y_n = 28, \quad \nabla^2 y_n = 2, \quad h = 10$

$$p = \frac{x - x_n}{h}$$

$$= \frac{84 - 90}{10}$$

$$= -0.6$$

$$y_p = 304 + (-0.6 \times 28) + \left[\frac{(-0.6)(-0.6+1)}{2!}\right](2) + 0$$

$$= 304 - 16.8 - 0.24$$

$$= 287 \text{ nearly}$$

INTERPOLATION USING CENTRAL DIFFERENCES

- Suppose the values of the function $f(x)$ are known at the points $a - 3h$, $a - 2h$, $a - h$, a, $a + h$, $a + 2h$, $a + 3h$, ... etc. Let these values be y_{-3}, y_{-2}, y_{-1}, y_0, y_1, y_2, y_3 ..., and so on. Then we can form the central difference table as:

x	f(x)	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$	$\Delta^6 f$
a-3h	y_{-3}						
		Δy_{-3}					
a-2h	y_{-2}		$\Delta^2 y_{-3}$				
		Δy_{-2}		$\Delta^3 y_{-3}$			
a-h	y_{-1}		$\Delta^2 y_{-2}$		$\Delta^4 y_{-3}$		
		Δy_{-1}		$\Delta^3 y_{-2}$		$\Delta^5 y_{-3}$	
a	y_0		$\Delta^2 y_{-1}$		$\Delta^4 y_{-2}$		$\Delta^6 y_{-3}$
		Δy_0		$\Delta^3 y_{-1}$		$\Delta^5 y_{-2}$	
a+h	y_1		$\Delta^2 y_0$		$\Delta^4 y_{-1}$		
		Δy_1		$\Delta^3 y_0$			
a+2h	y_2		$\Delta^2 y_1$				
		Δy_2					
a+3h	y_3						

We can relate the central difference operator δ with Δ and E using the operator relation $\delta = \Delta E^{½}$.

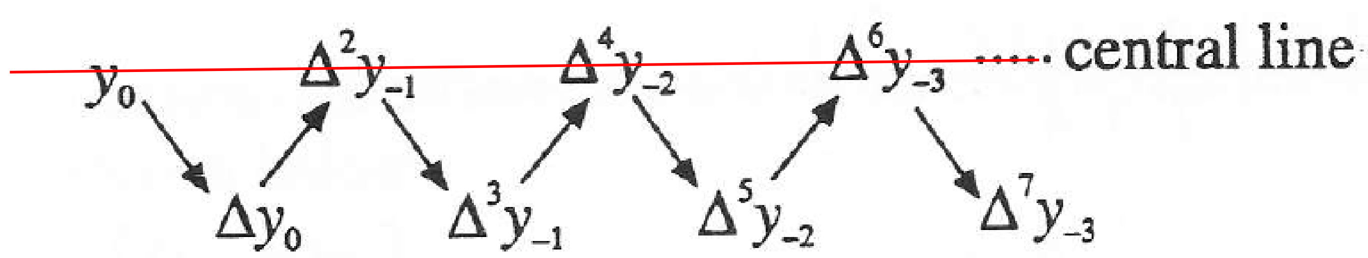
GAUSS FORWARD INTERPOLATION FORMULA

- The value p is measured forwardly from the origin and $0<p<1$.

$$y_p = y_0 + p\,\Delta y_0 + \left[\frac{p(p-1)}{1\cdot 2}\right](\Delta^2 y_{-1}) + \left[\frac{(p+1)\,p(p-1)}{1\cdot 2\cdot 3}\right](\Delta^3 y_{-1})$$

$$+\left[\frac{(p+1)p\,(p-1)\,(p-2)}{1\cdot 2\cdot 3\cdot 4}\right](\Delta^4 y_{-2}) + \ldots$$

- The above formula involves odd differences below the central horizontal line and even differences on the line. This is explained in the following figure.



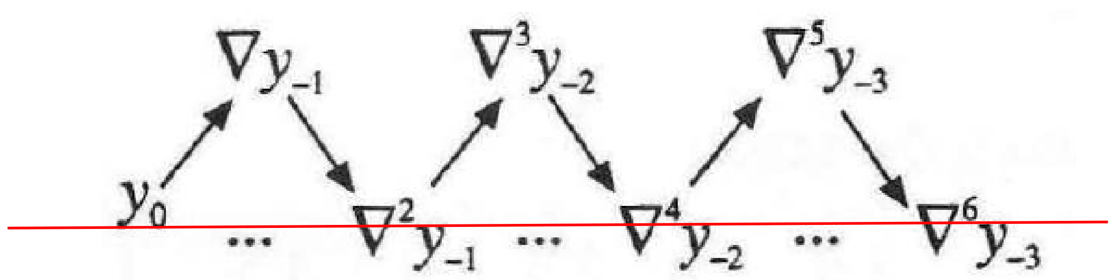
GAUSS BACKWARD INTERPOLATION FORMULA

- The value p is measured forwardly from the origin and $-1<p<0$.

$$y_p = y_0 + (p)\Delta y_{-1} + \left[\frac{(p+1)p}{1\cdot 2}\right](\Delta^2 y_{-1}) + \left[\frac{(p+1)\,p(p-1)}{1\cdot 2\cdot 3}\right](\Delta^3 y_{-2})$$

$$+ \left[\frac{(p+2)\,(p+1)\,p(p-1)}{1\cdot 2\cdot 3\cdot 4}\right](\Delta^4 y_{-2}) + \dots$$

- The above formula involves odd differences above the central horizontal line and even differences on the line.



EXAMPLE Apply Gauss's forward formula to obtain $f(x) = x \sin x + 2$, at $x = 3.5$, from the following table.

x	2	3	4	5
$f(x)$	3.818	2.423	–1.027	–2.794

Solution

Here $h = 1$

Taking $x_0 = 3$

Therefore, the central difference table is

p	x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
– 1	2	3.818			
			– 1.395		
0	3	$\boxed{2.423}$		$\boxed{-2.055}$	
			$\boxed{-3.45}$		$\boxed{3.738}$
1	4	– 1.027		1.683	
			– 1.767		
2	5	– 2.794			

$$p = \frac{x - x_0}{h} = \frac{3.5 - 3}{1} = 0.5$$

Gauss's forward formula is

$$y_p = y_0 + p(\Delta y_0) + \left[\frac{p(p-1)}{2!}\right](\Delta^2 y_{-1}) + \left[\frac{(p+1)\,p(p-1)}{3!}\right](\Delta^3 y_{-1})$$

$$+ \left[\frac{(p+1)\,p(p-1)\,(p-2)}{4!}\right](\Delta^4 y_{-2}) + \ldots$$

$$= 2.423 + 0.5(-3.45) + \left[\frac{(0.5)\,(0.5-1)}{2!}\right](-2.055)$$

$$+ \left[\frac{(0.5+1)\,(0.5)\,(0.5-1)}{3!}\right](3.738)$$

$$= 0.254$$

EXAMPLE Given the table:

x	1.5	2.5	3.5	4.5
$y = xe^x$	8.963	24.364	66.230	180.034

Find the value of y, at $x = 2$___ , by Gauss's backward difference formula.

Let us form the central difference table

p	x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
−1	1.5	8.963			
			$\boxed{15.401}$		
0	2.5	$\boxed{24.364}$		$\boxed{26.465}$	
			41.866		45.473
1	3.5	66.230		71.938	
			113.804		
2	4.5	180.034			

Solution

Here $h = 1$

Taking $x_0 = 2.5$

$$p = \frac{x - x_0}{h} = -0.5$$

Gauss's backward formula is

$$y_p = y_0 + p(\Delta y_{-1}) + \left[\frac{p(p+1)}{2!}\right](\Delta^2 y_{-1}) + \left[\frac{(p+1)\,p(p-1)}{3!}\right](\Delta^3 y_{-2}) + \ldots$$

$$= 24.364 + (-0.5)\,(15.401) + \left[\frac{(-0.5)\,(-0.5+1)}{2!}\right](26.465)$$

$$= 13.355$$

EXAMPLE Apply Gauss's forward formula to find the value of $f(x)$, at $x = 3.75$, from the following table:

x	2.5	3.0	3.5	4.0	4.5	5.0
$f(x)$	24.145	22.043	20.225	18.644	17.262	16.047

Solution

Taking $x_0 = 3.5$ and $h = 0.5$ $\qquad p = \dfrac{x - 3.5}{0.5}$

Therefore, the central difference table is

p	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
– 2	24.145					
		– 2.102				
– 1	22.043		0.284			
		– 1.818		– 0.047		
0	20.225		0.237		0.009	
		– 1.581		– 0.038		– 0.003
1	18.644		0.199		0.006	
		– 1.382		– 0.032		
2	17.262		0.167			
		– 1.215				
3	16.047					

Gauss's forward formula is

$$y_p = y_0 + p(\Delta y_0) + \left[\frac{p(p-1)}{1\cdot 2}\right](\Delta^2 y_{-1}) + \left[\frac{(p+1)\,p(p-1)}{1\cdot 2\cdot 3}\right](\Delta^3 y_{-1})$$

$$+ \left[\frac{(p+1)\,p(p-1)\,(p-2)}{1\cdot 2\cdot 3\cdot 4}\right](\Delta^4 y_{-2})$$

$$+ \left[\frac{(p+2)\,(p+1)\,p(p-1)\,(p-2)}{1\cdot 2\cdot 3\cdot 4\cdot 5}\right](\Delta^5 y_{-2}) + \ldots$$

when $x = 3.75$ $\qquad p = \dfrac{3.75 - 3.5}{0.5} = 0.5$

Hence, $\quad y_0 = 20.225, \quad \Delta^2 y_{-1} = 0.237, \quad \Delta^4 y_{-2} = 0.009,$

$\Delta y_0 = -1.581, \quad \Delta^3 y_{-1} = -0.038, \quad \Delta^5 y_{-2} = -0.003$

$$y_p = 20.225 + (0.5)\,(-1.581) + \left[\frac{(0.5)\,(0.5-1)}{1\cdot 2}\right](0.237)$$

$$+ \left[\frac{(0.5+1)\,(0.5)\,(0.5-1)}{1\cdot 2\cdot 3}\right](-0.038)$$

$$+\left[\frac{(0.5+1)(0.5)(0.5-1)(0.5-2)}{1\cdot 2\cdot 3\cdot 4}\right](0.009)$$

$$+\left[\frac{(0.5+2)(0.5+1)(0.5)(0.5-1)(0.5-2)}{1\cdot 2\cdot 3\cdot 4}\right](-0.003)$$

$$= 20.225 - 0.7905 - 0.02925 + 0.002375 + 0.0002109375 - 0.00003515625$$

$= 19.407$, correct to three decimal places.

STIRLING'S FORMULA

This formula gives the average of the values obtained by Gauss forward and backward interpolation formulae. For using this formula we should have $-\frac{1}{2} < p < \frac{1}{2}$. We can get very good estimates if $-\frac{1}{4} < p < \frac{1}{4}$. The formula is:

$$y = y_0 + u\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{u^2}{2!}\Delta^2 y_{-1} + \frac{u(u^2-1)}{3!}\left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right] + \frac{u^2(u^2-1)}{4!}\Delta^4 y_{-2}$$

$$+\frac{u(u^2-1)(u^2-4)}{5!}\left[\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right] + \ldots\ldots\ldots$$

where $u = \dfrac{x - x_0}{h}$

Inverse Interpolation

- We want to find the value of x that will make $f_n(x)$ equal to a given value.

- For this purpose, Lagrange's interpolation is used.

$$x = \left[\frac{(y-y_1)(y-y_2)\ldots\ldots(y-y_n)}{(y_0-y_1)(y_0-y_2)\ldots\ldots(y_0-y_n)}\right](x_0)$$

$$+\left[\frac{(y-y_0)(y-y_2)\ldots\ldots(y-y_n)}{(y_1-y_0)(y_1-y_2)\ldots\ldots(y_1-y_n)}\right]$$

$$+ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$+\left[\frac{(y-y_0)(y-y_1)\ldots\ldots(y-y_{n-1})}{(y_n-y_0)(y_n-y_1)\ldots\ldots(y_n-y_{n-1})}\right](x_n)$$

EXAMPLE Use Lagrange's inverse interpolation formula to obtain the value of t, when $A = 85$ from the following table.

t	2	5	8	14
A	94.8	87.9	81.3	68.7

Solution

Here, $x_0 = 2 \quad x_1 = 5 \quad x_2 = 8 \quad x_3 = 14$

$$y_0 = 94.8 \quad y_1 = 87.9 \quad y_2 = 81.3 \quad y_3 = 68.7$$

The inverse interpolation formula is

Taking $y = 85$, we have

$$x(85) = \left[\frac{(85-87.9)(85-81.3)(85-68.7)}{(94.8-87.9)(94.8-81.3)(94.8-68.7)}\right](2)$$

$$+\left[\frac{(85-94.8)(85-81.3)(85-68.7)}{(87.9-94.8)(87.9-81.5)(87.9-68.7)}\right](5)$$

$$+\left[\frac{(85-94.8)(85-87.9)(85-68.7)}{(81.3-94.8)(81.3-87.9)(81.3-68.7)}\right](8)$$

$$+\left[\frac{(85-94.8)(85-87.9)(85-81.3)}{(68.7-94.8)(68.7-87.9)(68.7-81.3)}\right](14)$$

$$= 6.5928$$

EXAMPLE Find the value of x corresponding to $y = 100$, by using inverse interpolation, from the given data.

x	3	5	7	9
y	6	24	58	108

Solution

Here,
$$x_0 = 3, \quad x_1 = 5, \quad x_2 = 7, \quad x_3 = 9$$

$$y_0 = 6, \quad y_1 = 24, \quad y_2 = 58, \quad y_3 = 108$$

When $y = 100$, substituting above values in inverse interpolation formula, we get

$$x = \left[\frac{(100-24)(100-58)(100-108)}{(6-24)(6-58)(6-108)}\right](3)$$

$$+\left[\frac{(100-6)(100-58)(100-108)}{(24-6)(24-58)(24-108)}\right](5)$$

$$+\left[\frac{(100-6)(100-24)(100-108)}{(58-6)(58-24)(25-108)}\right](7)$$

$$+\left[\frac{(100-6)(100-24)(100-58)}{(108-6)(108-24)(108-58)}\right](9)$$

$$= 0.802413 + (-3.071895) + 4.52561 + 6.30352$$

$$= 8.559657$$

Maxima and Minima of a Tabulated Function

Recalling the Newton's forward interpolation

$$y = y_0 + p\Delta y_0 + \left[\frac{p(p-1)}{2!}\right](\Delta^2 y_0) + \left[\frac{p(p-1)(p-2)}{3!}\right](\Delta^3 y_0) + \ldots$$

where $p = \dfrac{x - x_0}{h}$

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-6p+2}{6}\Delta^3 y_0 + \ldots\right]$$

From elementary calculus, it is known that the maximum and minimum values of a function $y = f(x)$ are obtained by equating its first derivative with respect to x to zero and solving it for x. Same idea holds in the case of tabulated function too. Thus, we have

$$\Delta y_0 + \left[\frac{2p-1}{2}\right](\Delta^2 y_0) + \left[\frac{3p^2 - 6p + 2}{6}\right](\Delta^3 y_0) + \ldots = 0$$

EXAMPLE Find for what value of x, y is minimum, using the data given below.

x	3	4	5	6	7	8
y	0.205	0.240	0.259	0.262	0.250	0.224

Solution From the given data, it can be seen that the arguments are equally-spaced and, therefore, we construct the forward difference table as

Here,

$$p = \frac{x - x_0}{h} \qquad \Delta y_0 = 0.035 \qquad \Delta^3 y_0 = 0$$

$$\Delta^2 y_0 = -0.016 \qquad \Delta^4 y_0 = -0.001$$

$$p = (x - 3)$$

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
3	0.205				
		0.035			
4	0.240		– 0.016		
		0.019		0.00	
5	0.259		– 0.016		– 0.001
		0.003		– 0.001	
6	0.262		– 0.015		0.002
		– 0.012		0.001	
7	0.250		– 0.014		
		– 0.026			
8	0.224				

Newton's forward formula is

$$y = y_0 + p\Delta y_0 + \left[\frac{p(p-1)}{2!}\right](\Delta^2 y_0) + \left[\frac{p(p-1)(p-2)}{3!}\right](\Delta^3 y_0)$$

Substituting the value of p and the differences, we have

$$y = 0.205 + (x-3)(0.035) + \frac{(x-3)(x-4)(-0.016)}{2}$$

$$y = -0.008x^2 + 0.091x + 0.004$$

For maxima or minima, we require

$$\frac{dy}{dx} = -0.016x + 0.091 = 0 \Longrightarrow x = 5.6875$$

Thus, the maximum value of y at $x = 5.6875$ is

$$y = -0.008\,(32.3477) + 0.091\,(5.6875) + 0.004$$

$$= 0.26278$$

Hence, the maximum value at $x = 5.6875$ of the given tabulated function is 0.26278

What is Regression?

What is regression? Given n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = f(x)$ to the data. The best fit is generally based on minimizing the sum of the square of the residuals, S_r.

Residual at a point is

$$\varepsilon_i = y_i - f(x_i)$$

Sum of the square of the residuals

$$S_r = \sum_{i=1}^{n} (y_i - f(x_i))^2$$

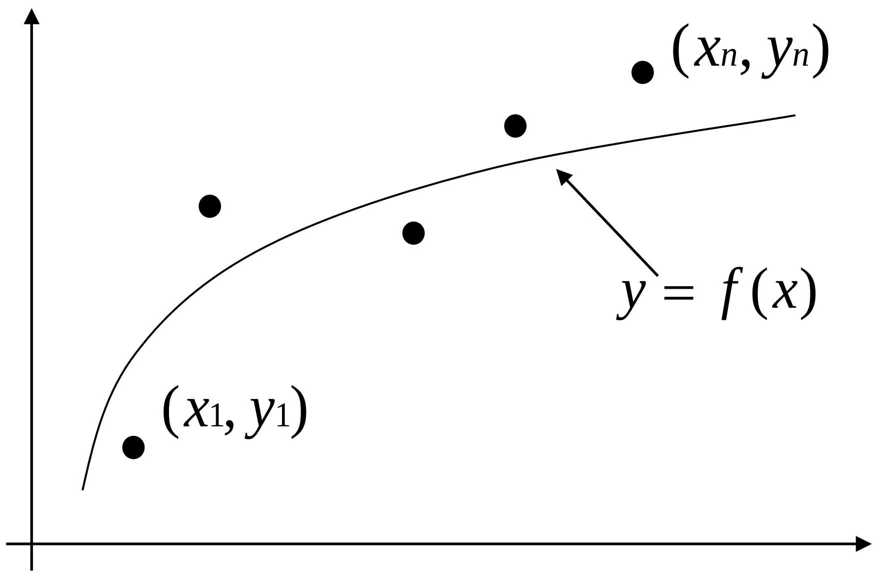


Figure. Basic model for regression

Linear Regression (Criterion 1)

Fitting a straight line to a set of paired observations:

$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit is $y = a_0 + a_1 x + e$

- a_0 - intercept
- a_1 - slope
- e - error or residual
- n - total number of points

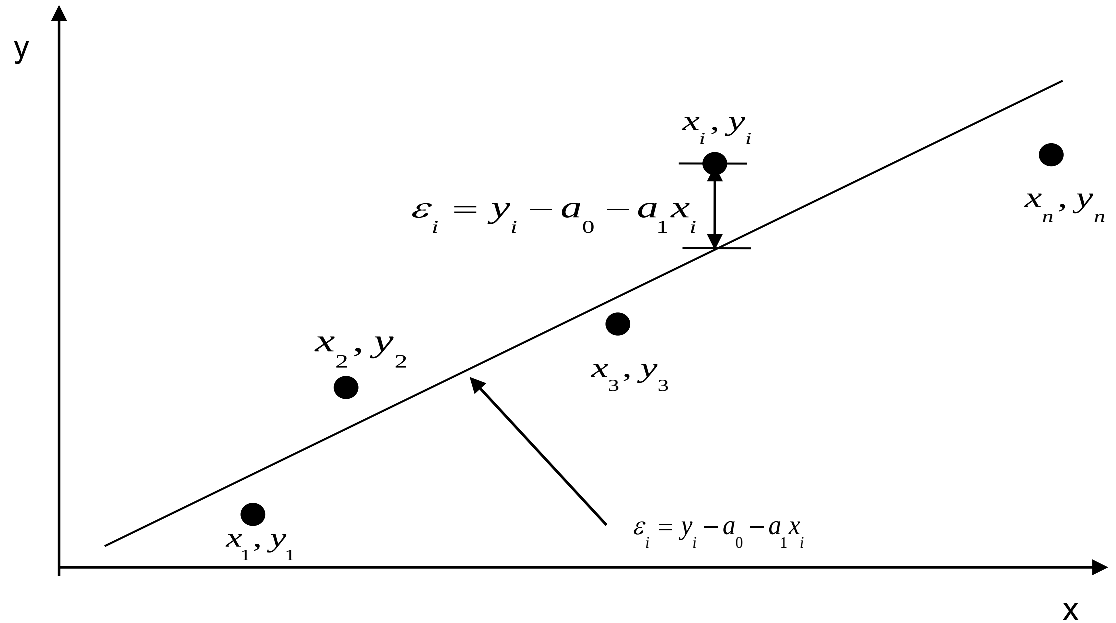


Figure. Linear regression of y-x data showing residuals at a typical x_i .

Minimize the sum of the residual errors for all available data as a criterion :

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - \boxed{a_o - a_1 x_i})$$

Least Squares

Finding Constants of Linear Model

Minimize the sum of the square of the residuals: $S_r = \sum_{i=1}^{n} \varepsilon_i^{\,2} = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)^2$

To find a_0 and a_1 we minimize S_r with respect to a_1 and a_0.

$$\frac{\partial S_r}{\partial a_0} = -2\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)\left(-1\right) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i\right)\left(-x_i\right) = 0$$

giving

$$\sum_{i=1}^{n} a_0 + \sum_{i=1}^{n} a_1 x_i = \sum_{i=1}^{n} y_i$$

$$\sum_{i=1}^{n} a_0 x_i + \sum_{i=1}^{n} a_1 x_i^{\,2} = \sum_{i=1}^{n} y_i x_i$$

Solving for a_0 and a_1 directly yields,

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

and

$$a_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

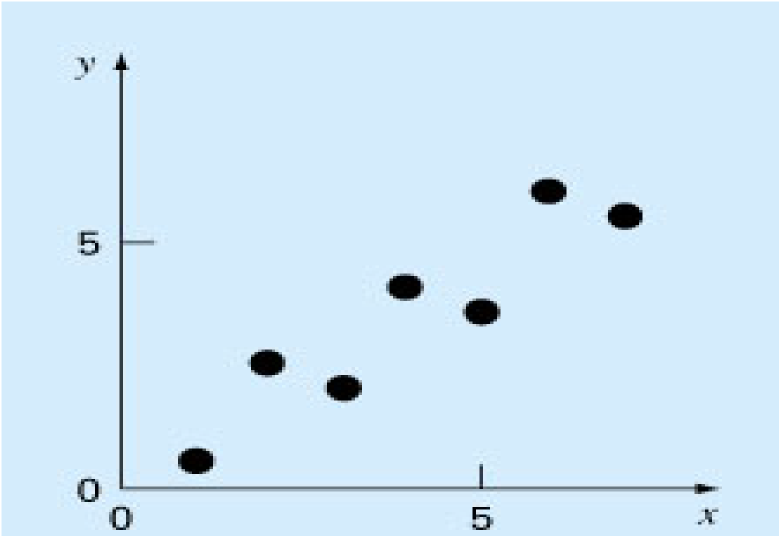
or $(a_0 = \bar{y} - a_1 \bar{x})$

Mean values

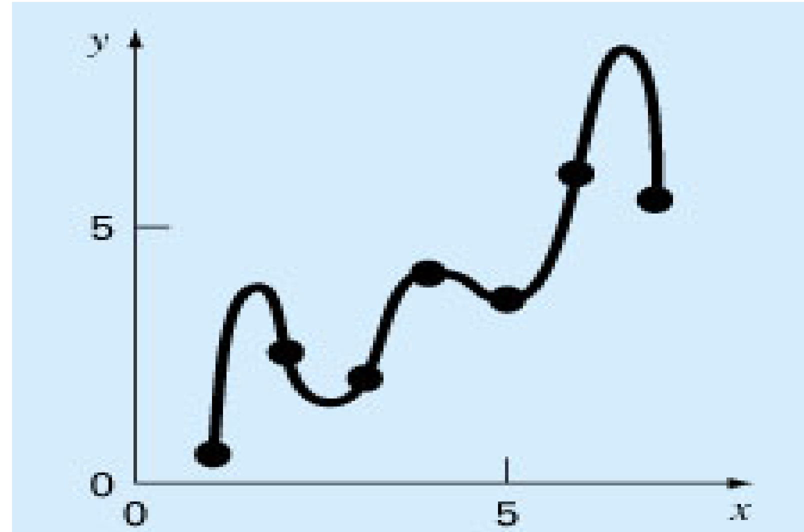
In matrix form: $\mathbf{x} = (A^T A)^{-1} A^T \mathbf{b}$

where

$$x = \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \qquad A = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \qquad b = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$



(a)



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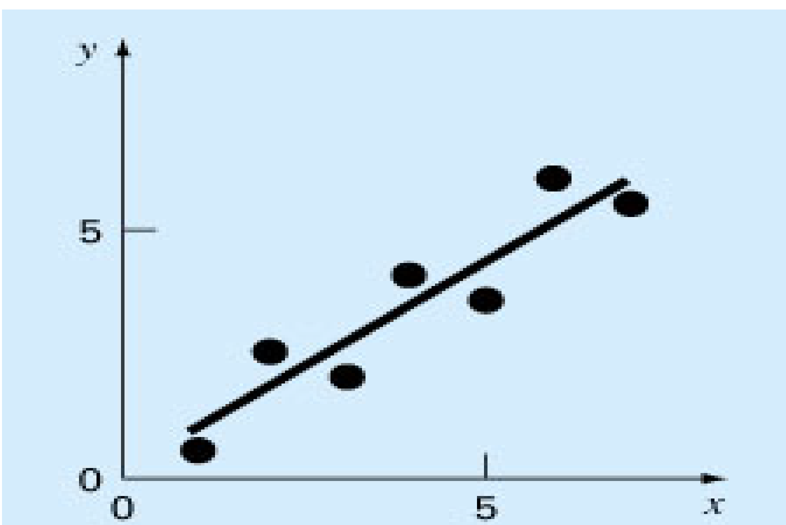

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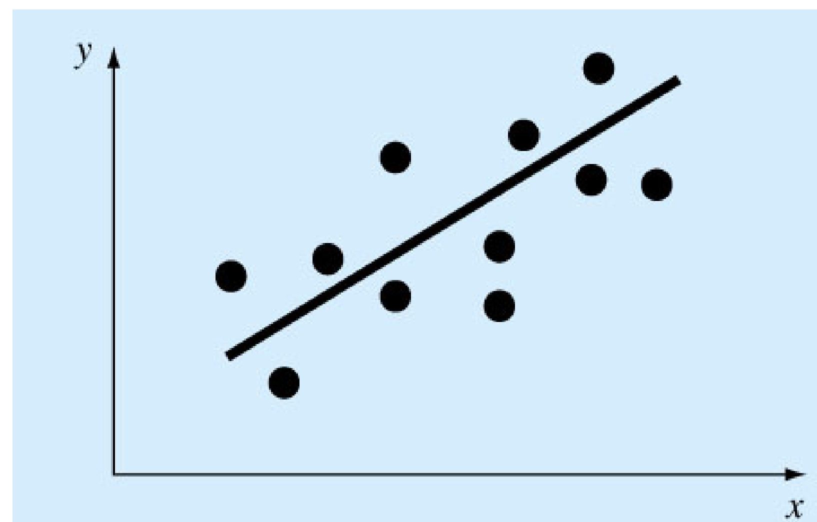


(d)

Error Quantification of Linear Regression

- Total sum of the squares around the mean for the dependent variable *y*, is $\boldsymbol{S_t}$

$$S_t = \sum_i^n (y_i - \bar{y})^2$$

- Sum of the squares of residuals around the regression line is $\boldsymbol{S_r}$

$$S_r = \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

- *Where* S_t-S_r quantifies the improvement or error reduction due to describing data in terms of a straight line rather than as an average value.

r : correlation coefficient

$$r^2 = \frac{S_t - S_r}{S_t}$$

For a perfect fit:

- $S_r = 0$ and $r = r^2 = 1$, signifying that the line explains 100 percent of the variability of the data.
- For $r = r^2 = 0$, $S_r = S_t$, the fit represents no improvement.

Example: Fit a straight line to the x and y values in the following Table:

x_i	y_i	$x_i y_i$	x_i^2
1	0.5	0.5	1
2	2.5	5	4
3	2	6	9
4	4	16	16
5	3.5	17.5	25
6	6	36	36
7	5.5	38.5	49
28	**24**	**119.5**	**140**

$$\sum x_i = 28 \qquad \sum y_i = 24.0$$

$$\sum x_i^2 = 140 \qquad \sum x_i y_i = 119.5$$

$$\bar{x} = \frac{28}{7} = 4$$

$$\bar{y} = \frac{24}{7} = 3.4285$$

$$a_0 = \bar{y} - a_1\bar{x}$$
$$= 3.428571 - 0.8392857 \times 4$$
$$= 0.07142857$$

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - (\sum x_i)^2}$$
$$= \frac{7\times 119.5 - 28\times 24}{7\times 140 - 28^2} = 0.8392857$$

Y = 0.07142857 + 0.8392857 x

x_i	y_i	$(y_i - \bar{y})^2$	$e_i^2 = (y_i - \hat{y})^2$
1	0.5	8.5765	0.1687
2	2.5	0.8622	0.5625
3	2.0	2.0408	0.3473
4	4.0	0.3265	0.3265
5	3.5	0.0051	0.5896
6	6.0	6.6122	0.7972
7	5.5	4.2908	0.1993
28	**24.0**	**22.7143**	**2.9911**

$$S_t = \sum (y_i - \bar{y})^2$$
$$= 22.7143$$

$$S_r = \sum e_i^2 = 2.9911$$

$$r^2 = \frac{S_t - S_r}{S_t} = 0.868$$

$$r = \sqrt{0.868} = 0.932$$

These results indicate that 86.8 percent of the original uncertainty has been explained by the linear model.

Example of Error Analysis

- The standard deviation (quantifies the spread around the mean):

$$s_y = \sqrt{\frac{S_t}{n-1}} = \sqrt{\frac{22.7143}{7-1}} = 1.9457$$

- The standard error of estimate (quantifies the spread around the regression line)

$$s_{y/x} = \sqrt{\frac{S_r}{n-2}} = \sqrt{\frac{2.9911}{7-2}} = 0.7735$$

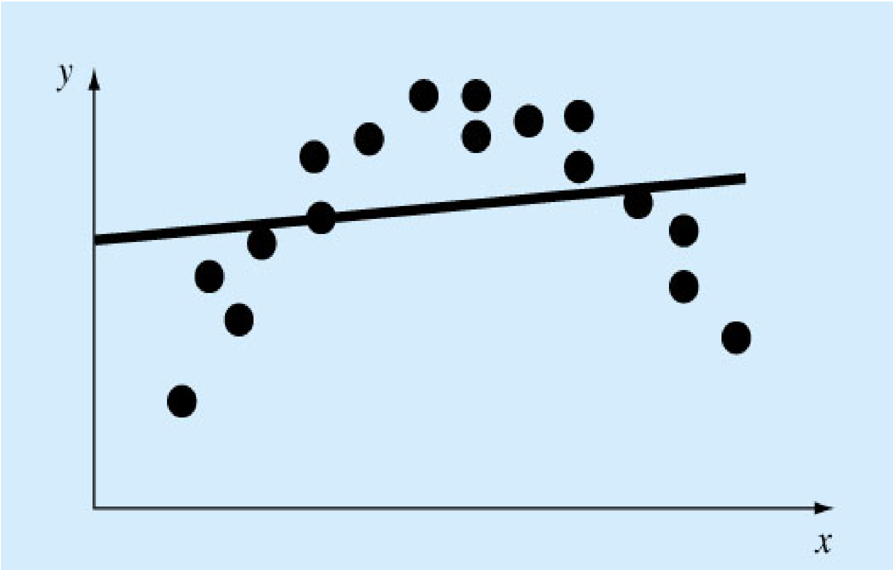
Because $S_{y/x} < S_y$, the linear regression model has good fitness

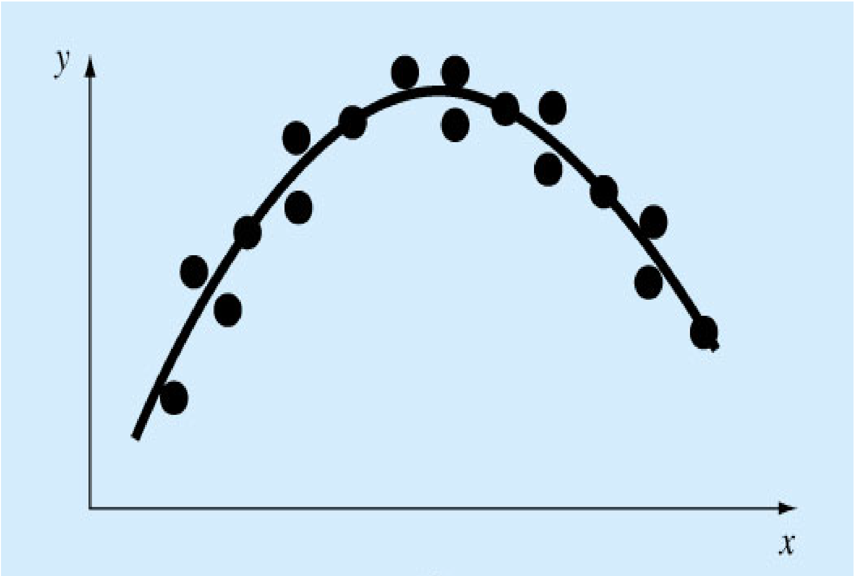
Algorithm for linear regression

```
SUB Regress(x, y, n, a1, a0, syx, r2)

  sumx = 0: sumxy = 0: st = 0
  sumy = 0: sumx2 = 0: sr = 0
  DO i = 1, n
    sumx = sumx + x_i
    sumy = sumy + y_i
    sumxy = sumxy + x_i*y_i
    sumx2 = sumx2 + x_i*x_i
  END DO
  xm = sumx/n
  ym = sumy/n
  a1 = (n*sumxy - sumx*sumy)/(n*sumx2 - sumx*sumx)
  a0 = ym - a1*xm
  DO i = 1, n
    st = st + (y_i - ym)^2
    sr = sr + (y_i - a1*x_i - a0)^2
  END DO
  syx = (sr/(n - 2))^0.5
  r2 = (st - sr)/st

END Regress
```

Polynomial Regression

- Some engineering data is poorly represented by a straight line. For these cases a curve is better suited to fit the data.
- The least squares method can readily be extended to fit the data to higher order polynomials.





A parabola is preferable

Polynomial Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = a_0 + a_1 x + \ldots + a_m x^m$ $(m \le n-2)$ to a given data set. The residual at each data point is given by

$$E_i = y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m$$

The sum of the square of the residuals then is

$$S_r = \sum_{i=1}^{n} E_i^2 = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m \right)^2$$

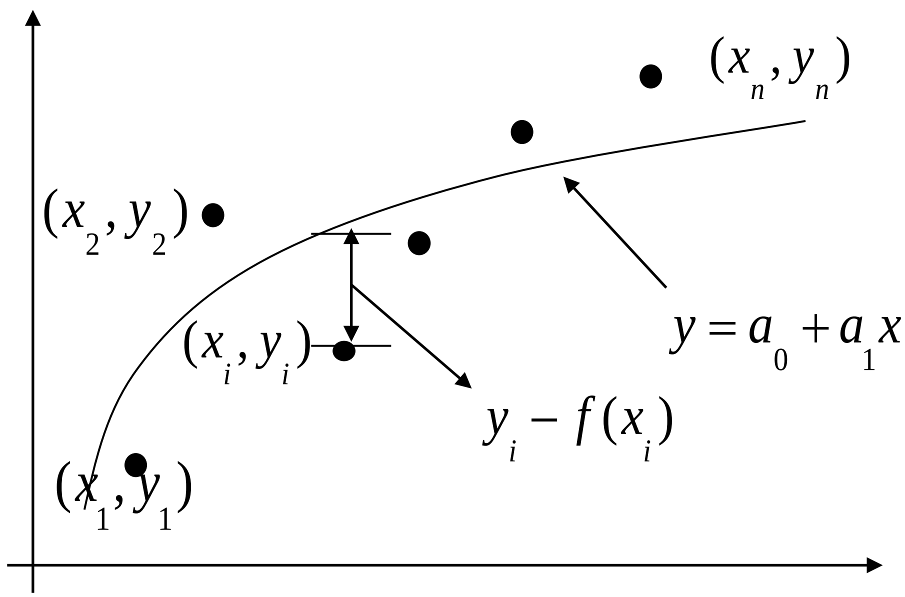


Figure. Polynomial model for nonlinear regression of y - x data

To find the constants of the polynomial model, we set the derivatives with respect to a_i where $i = 1, \ldots m,$ equal to zero.

$$\frac{\partial S_r}{\partial a_0} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m\right)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m\right)(-x_i) = 0$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$\frac{\partial S_r}{\partial a_m} = \sum_{i=1}^{n} 2.\left(y_i - a_0 - a_1 x_i - \ldots - a_m x_i^m\right)(-x_i^m) = 0$$

These equations in matrix form are given by

$$(\mathrm{A^T A})\mathrm{x} = \begin{bmatrix} n & (\sum_{i=1}^{n} x_i^1) & \cdots & (\sum_{i=1}^{n} x_i^m) \\ (\sum_{i=1}^{n} x_i^1) & (\sum_{i=1}^{n} x_i^2) & \cdots & (\sum_{i=1}^{n} x_i^{m+1}) \\ \vdots & \vdots & \ddots & \vdots \\ (\sum_{i=1}^{n} x_i^m) & (\sum_{i=1}^{n} x_i^{m+1}) & \cdots & (\sum_{i=1}^{n} x_i^{2m}) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i^1 y_i \\ \vdots \\ \sum_{i=1}^{n} x_i^m y_i \end{bmatrix} = \mathrm{A^T b}$$

The above equations are then solved for $a_0, a_1, \ldots, a_m$

Quadratic Polynomial Regression

- **A 2nd order polynomial (quadratic)** is defined by:

$$y = a_o + a_1 x + a_2 x^2 + e$$

- The residuals between the model and the data:

$$e_i = y_i - a_o - a_1 x_i - a_2 x_i^{\ 2}$$

- The sum of squares of the residual:

$$S_r = \sum e_i^{\ 2} = \sum \left(y_i - a_o - a_1 x_i - a_2 x_i^{\ 2} \right)^2$$

$$\frac{\partial S_r}{\partial a_o} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) x_i = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum (y_i - a_o - a_1 x_i - a_2 x_i^2) x_i^2 = 0$$

$$\left.\begin{aligned}\sum y_i &= n\cdot a_o + a_1\sum x_i + a_2\sum x_i^2\\ \sum x_i y_i &= a_o\sum x_i + a_1\sum x_i^2 + a_2\sum x_i^3\\ \sum x_i^2 y_i &= a_o\sum x_i^2 + a_1\sum x_i^3 + a_2\sum x_i^4\end{aligned}\right\}$$

3 linear equations with 3 unknowns (a_o,a_1,a_2), can be solved

- A system of 3x3 equations needs to be solved to determine the coefficients of the polynomial.

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix}\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{Bmatrix}$$

- The standard error & the coefficient of determination

$$s_{y/x} = \sqrt{\frac{S_r}{n-3}} \qquad r^2 = \frac{S_t - S_r}{S_t}$$

General form:

The m^th^-order polynomial:

$$y = a_o + a_1 x + a_2 x^2 + \ldots\ldots + a_m x^m + e$$

- A system of $(m+1)(m+1)$ linear equations must be solved for determining the coefficients of the **m**th-order polynomial.
- The standard error:

$$s_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

- The coefficient of determination:

$$r^2 = \frac{S_t - S_r}{S_t}$$

Example of Polynomial Regression: Fit a second order polynomial to data

x_i	y_i	x_i^2	x_i^3	x_i^4	$x_i y_i$	$x_i^2 y_i$
0	**2.1**	0	0	0	0	0
1	**7.7**	1	1	1	7.7	7.7
2	**13.6**	4	8	16	27.2	54.4
3	**27.2**	9	27	81	81.6	244.8
4	**40.9**	16	64	256	163.6	654.4
5	**61.1**	25	125	625	305.5	1527.5
15	**152.6**	**55**	**225**	**979**	**585.6**	**2489**

$$\sum x_i = 15$$

$$\sum y_i = 152.6$$

$$\sum x_i^2 = 55$$

$$\sum x_i^3 = 225$$

$$\sum x_i^4 = 979$$

$$\sum x_i y_i = 585.6$$

$$\sum x_i^{\,2} y_i = 2488.8$$

$$\bar{x} = \frac{15}{6} = 2.5$$

$$\bar{y} = \frac{152.6}{6} = 25.433$$

The system of simultaneous linear equations

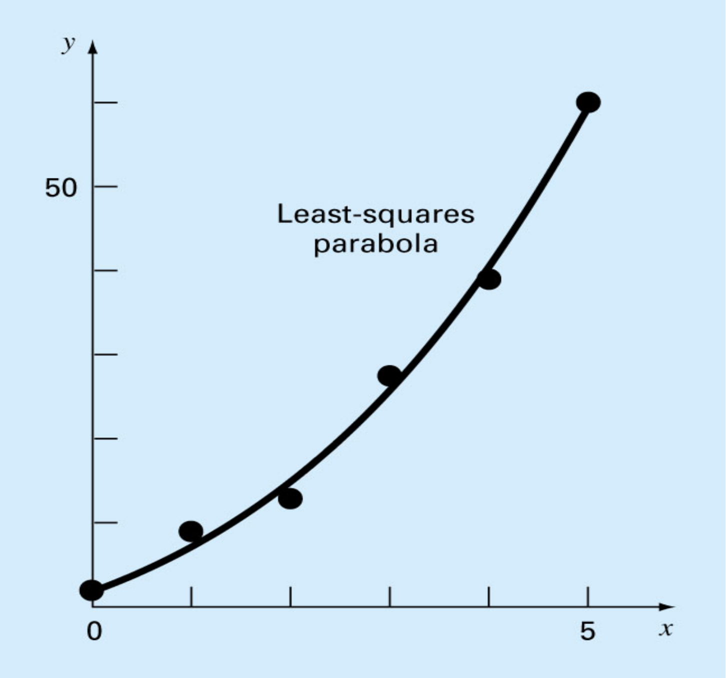
$$\begin{bmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 152.6 \\ 585.6 \\ 2488.8 \end{Bmatrix}$$

$$a_0 = 2.47857,\ a_1 = 2.35929,\ a_2 = 1.86071$$

$$y = 2.47857 + 2.35929\,x + 1.86071\,x^2$$

$$S_t = \sum (y_i - \bar{y})^2 = 2513.39 \qquad S_r = \sum e_i^{\ 2} = 3.74657$$

x_i	y_i	y_{model}	e_i^2	$(y_i\text{-}y\grave{})^2$
0	2.1	2.4786	0.14332	544.42889
1	7.7	6.6986	1.00286	314.45929
2	13.6	14.64	1.08158	140.01989
3	27.2	26.303	0.80491	3.12229
4	40.9	41.687	0.61951	239.22809
5	61.1	60.793	0.09439	1272.13489
15	**152.6**		**3.74657**	**2513.39333**



•The standard error of estimate: $s_{y/x} = \sqrt{\dfrac{3.74657}{6-3}} = 1.12$

•The coefficient of determination:

$$r^2 = \frac{2513.39 - 3.74657}{2513.39} = 0.99851, \quad r = \sqrt{r^2} = 0.99925$$

Example of Polynomial Model: Regress the thermal expansion coefficient vs. temperature data to a second order polynomial.

Temperature, T (°F)	Coefficient of thermal expansion, α (in/in/°F)
80	6.47×10^{-6}
40	6.24×10^{-6}
−40	5.72×10^{-6}
−120	5.09×10^{-6}
−200	4.30×10^{-6}
−280	3.33×10^{-6}
−340	2.45×10^{-6}

Table. Data points for temperature - α

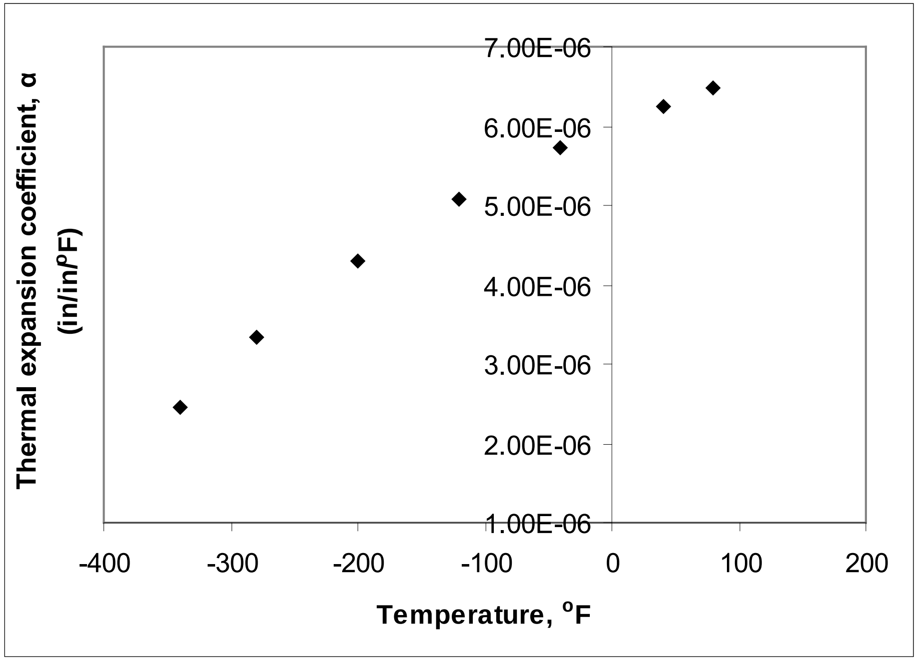


Figure. Data points for thermal expansion coefficient - temperature.

We are to fit the data to the polynomial regression model

$$\alpha = a_0 + a_1 T + a_2 T^2$$

The coefficients a_0, a_1, a_2 are found by differentiating the sum of the square of the residuals with respect to each variable and setting the values equal to zero to obtain

The necessary summations are as follows

$$\begin{bmatrix} n & \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) \\ \left(\sum_{i=1}^{n} T_i\right) & \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) \\ \left(\sum_{i=1}^{n} T_i^2\right) & \left(\sum_{i=1}^{n} T_i^3\right) & \left(\sum_{i=1}^{n} T_i^4\right) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{n} \alpha_i \\ \sum_{i=1}^{n} T_i \, \alpha_i \\ \sum_{i=1}^{n} T_i^2 \alpha_i \end{bmatrix}$$

$$\sum_{i=1}^{7} T_i^2 = 2.5580 \times 10^5 \quad \sum_{i=1}^{7} T_i^3 = -7.0472 \times 10^7$$

$$\sum_{i=1}^{7} T_i^4 = 2.1363 \times 10^{10} \quad \sum_{i=1}^{7} \alpha_i = 3.3600 \times 10^{-5}$$

$$\sum_{i=1}^{7} T_i \alpha_i = -2.6978 \times 10^{-3}$$

$$\sum_{i=1}^{7} T_i^2 \alpha_i = 8.5013 \times 10^{-1}$$

Using these summations, we can now calculate a_0, a_1, a_2

$$\begin{bmatrix} 7.0000 & -8.6000 \times 10^2 & 2.5800 \times 10^5 \\ -8.600 \times 10^2 & 2.5800 \times 10^5 & -7.0472 \times 10^7 \\ 2.5800 \times 10^5 & -7.0472 \times 10^7 & 2.1363 \times 10^{10} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 3.3600 \times 10^{-5} \\ -2.6978 \times 10^{-3} \\ 8.5013 \times 10^{-1} \end{bmatrix}$$

Solving the above system of simultaneous linear equations we have

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 6.0217 \times 10^{-6} \\ 6.2782 \times 10^{-9} \\ -1.2218 \times 10^{-11} \end{bmatrix}$$

The polynomial regression model is then

$$\begin{aligned} \alpha &= a_0 + a_1 T + a_2 T^2 \\ &= 6.0217 \times 10^{-6} + 6.2782 \times 10^{-9} \mathrm{T} - 1.2218 \times 10^{-11} \mathrm{T}^2 \end{aligned}$$

General Linear Least Squares

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

$z_0, z_1, \ldots, z_m$ are $m+1$ basis functions

$$\{Y\} = [Z]\{A\} + \{E\}$$

$[Z]$ – matrix of the calculated values of the basis functions at the measured values of the independent variable

$\{Y\}$ – observed valued of the dependent variable

$\{A\}$ – unknown coefficients

$\{E\}$ – residuals

$$S_r = \sum_{i=1}^{n} \left(y_i - \sum_{j=0}^{m} a_j z_{ji} \right)^2$$

Minimized by taking its partial derivative w.r.t. each of the coefficients and setting the resulting equation equal to zero

Nonlinear Regression

Some popular nonlinear regression models:

1. Exponential model: $(y = ae^{bx})$
2. Power model: $(y = ax^{b})$
3. Saturation growth model: $\left(y = \dfrac{ax}{b+x}\right)$
4. Polynomial model: $(y = a_0 + a_1 x + \ldots + a_m x^m)$

Given n data points $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = f(x)$ to the data, where $f(x)$ is a nonlinear function of x.

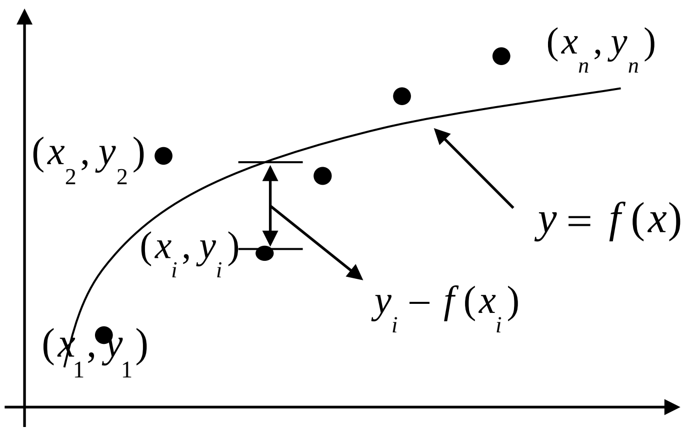


Figure. Nonlinear regression model for discrete y vs. x data

Exponential Model

Given $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ best fit $y = ae^{bx}$ to the data.

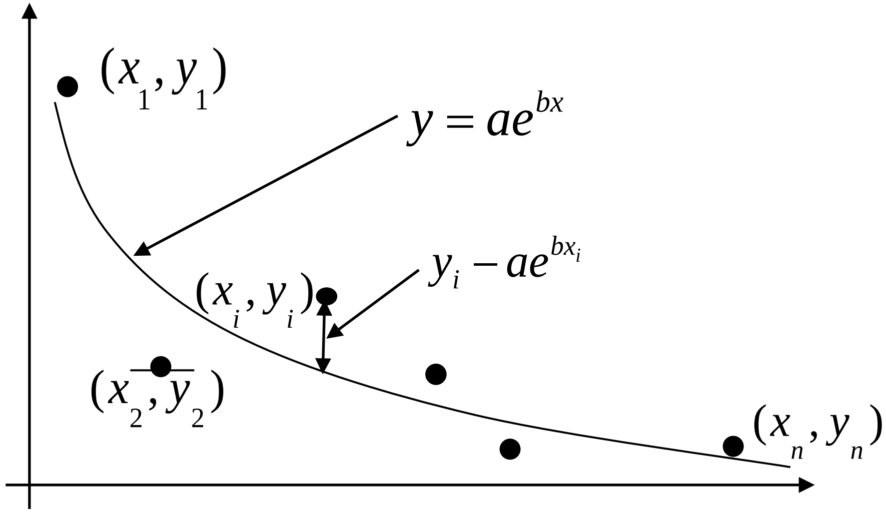


Figure. Exponential model of nonlinear regression for y vs. x data

The sum of the square of the residuals is defined as $S_r = \sum_{i=1}^{n} \left(y_i - ae^{bx_i}\right)^2$

Differentiate with respect to *a* and *b*

$$\frac{\partial S_r}{\partial a} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i}\right)\left(-e^{bx_i}\right) = 0$$

$$\frac{\partial S_r}{\partial b} = \sum_{i=1}^{n} 2\left(y_i - ae^{bx_i}\right)\left(-ax_ie^{bx_i}\right) = 0$$

Finding Constants of Exponential Model

Rewriting the equations, we obtain

$$-\sum_{i=1}^{n} y_i e^{bx_i} + a\sum_{i=1}^{n} e^{2bx_i} = 0$$

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - a\sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

Solving the first equation for *a* yields

$$a = \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}}$$

Substituting a back into the previous equation

$$\sum_{i=1}^{n} y_i x_i e^{bx_i} - \frac{\sum_{i=1}^{n} y_i e^{bx_i}}{\sum_{i=1}^{n} e^{2bx_i}} \sum_{i=1}^{n} x_i e^{2bx_i} = 0$$

The constant *b* can be found through numerical methods such as bisection method.

Transformation of Data

Linearization of Nonlinear Relationships

For mathematical convenience to find the constants of many nonlinear models, some of the data can be transformed. For example, the data for an exponential, power, saturation-growth-rate model can be transformed.

Suppose: $y = ae^{bx}$ Taking the natural log of both sides yields,

$$\ln y = \ln a + bx$$

Let $z = \ln y$ and $a_0 = \ln a$

We now have a linear regression model where $z = a_0 + a_1 x$ (implying) $a = e^{a_o}$ with $a_1 = b$

Using linear model regression methods,

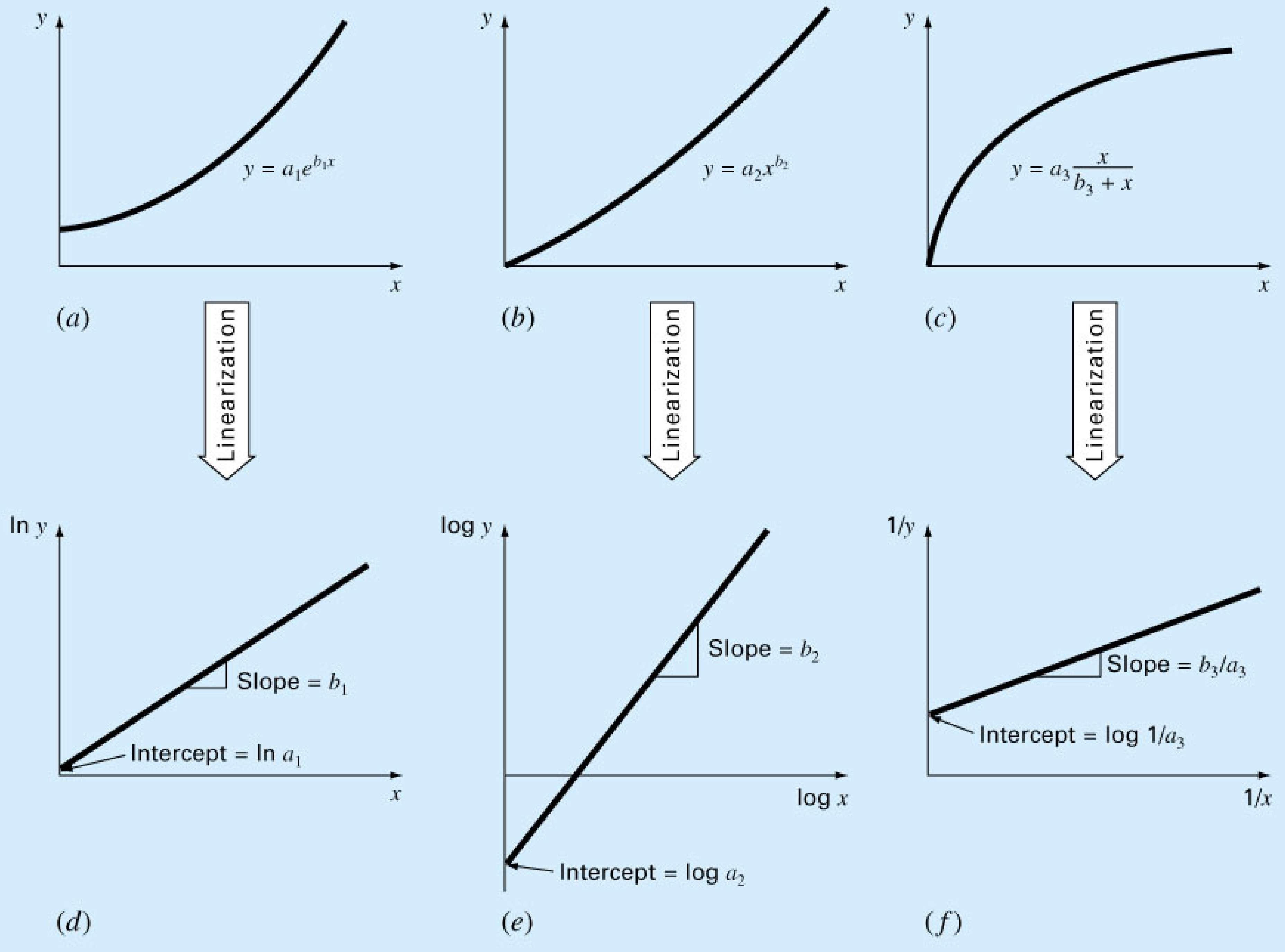
$$a_1 = \frac{n\sum_{i=1}^{n} x_i z_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} z_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2}$$

$$a_0 = \bar{z} - a_1 \bar{x}$$

Once a_o, a_1 are found, the original constants of the model are found as

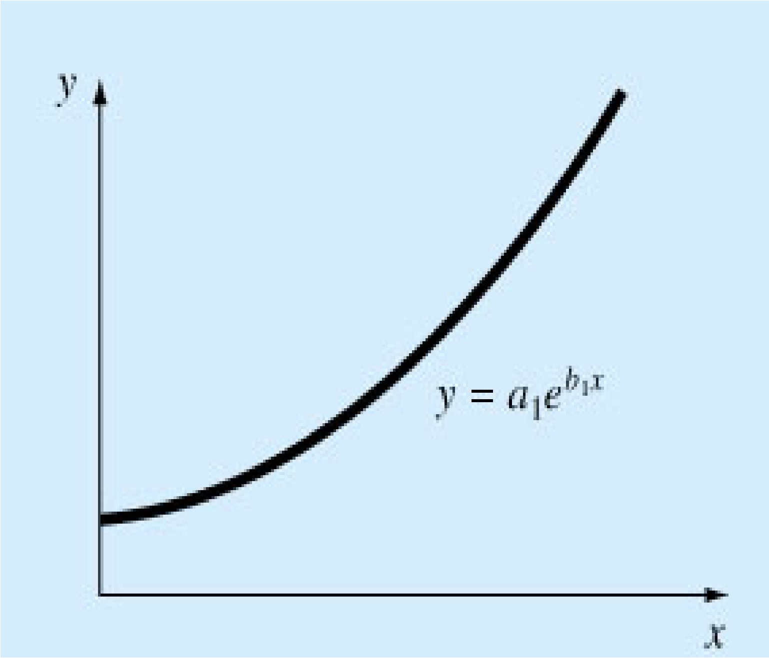
$$b = a_1$$

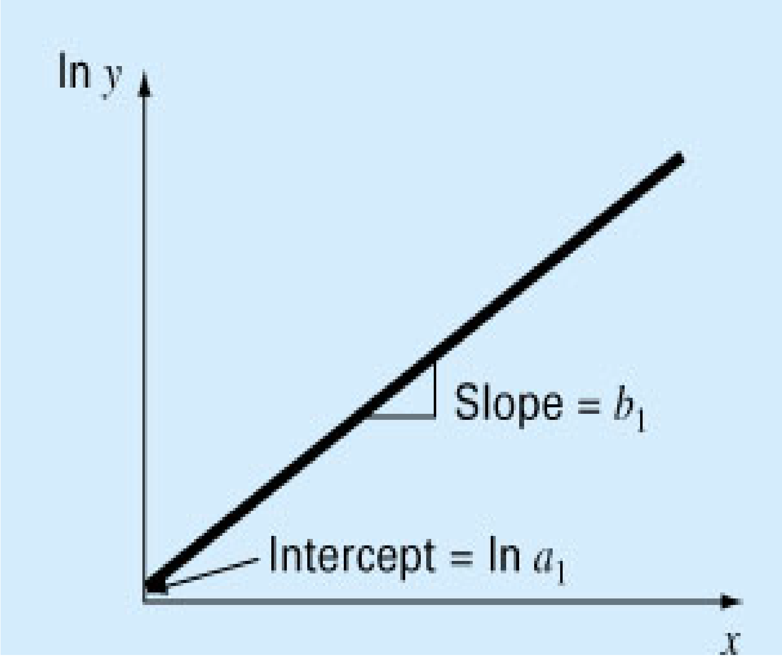
$$a = e^{a_0}$$



y
x
$y = a_1 e^{b_1 x}$
(a)
Linearization
y
x
$y = a_2 x^{b_2}$
(b)
Linearization
y
x
$y = a_3 \frac{x}{b_3 + x}$
(c)
Linearization
ln y
x
Slope = b_1
Intercept = ln a_1
(d)
log y
log x
Slope = b_2
Intercept = log a_2
(e)
1/y
1/x
Slope = b_3/a_3
Intercept = log $1/a_3$
(f)

Linearization of Nonlinear Relationships
1. The exponential equation



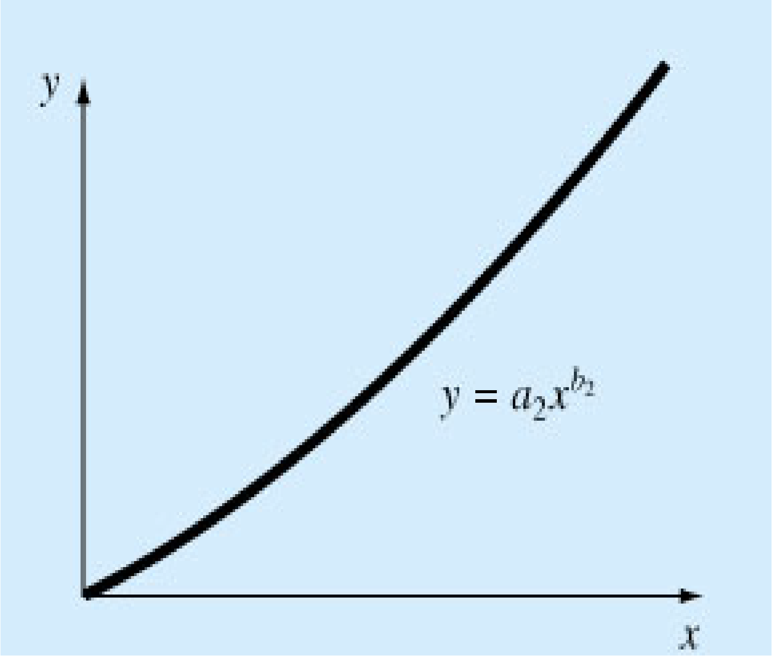


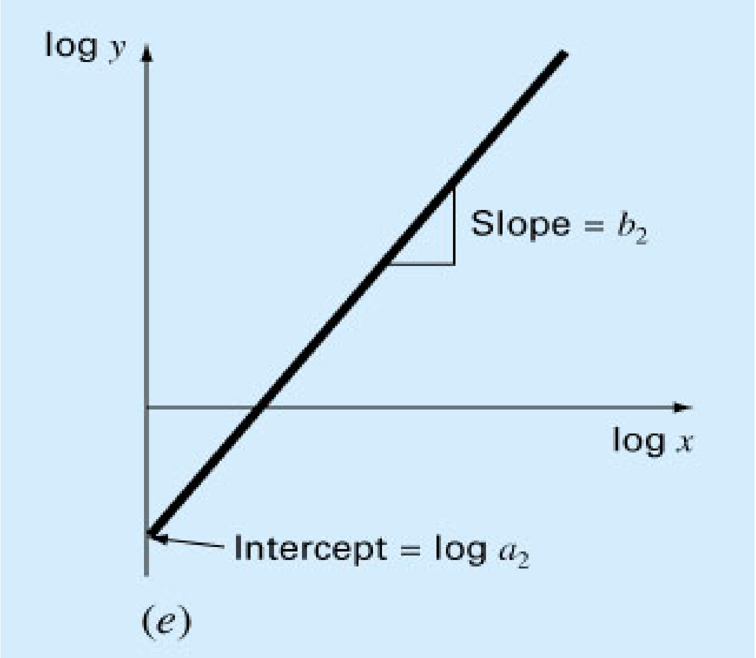
$$\ln y = \ln a_1 + b_1 x$$

$$y^* = a_o + a_1 x$$

Linearization of Nonlinear Relationships

2. The power equation

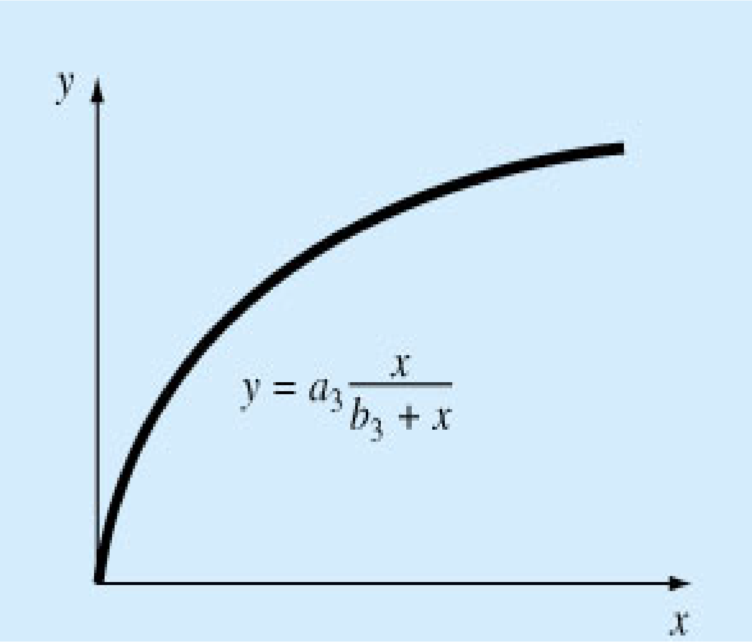


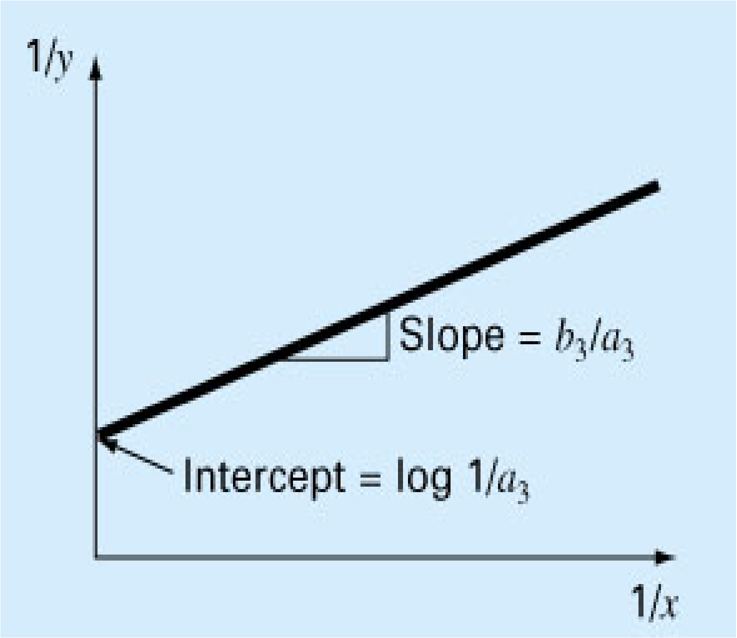


$$\log y = \log a_2 + b_2 \log x$$

$$y^* = a_o + a_1 x^*$$

Linearization of Nonlinear Relationships
3. The saturation-growth-rate equation





$$\frac{1}{y} = \frac{1}{a_3} + \frac{b_3}{a_3}\left(\frac{1}{x}\right)$$

$y^* = 1/y$

$a_o = 1/a_3$

$a_1 = b_3/a_3$

$x^* = 1/x$

Linearization

Take the natural log of the equations

$$y = \mathrm{b}x^{\mathrm{a}} \Rightarrow \ln y = \ln(\mathrm{b}) + \mathrm{a}\ln(x)$$
$$\Rightarrow y' = \mathrm{b}' + \mathrm{a}\,x'$$

and

$$y = \mathrm{b}e^{\mathrm{a}x} \Rightarrow \ln y = \ln(\mathrm{b}) + \mathrm{a}x$$
$$\Rightarrow y' = \mathrm{b}' + \mathrm{a}x$$

Example: Fit the following Equation: $y = a_2 x^{b_2}$

to the data in the following table:

x_i	y_i	$X^*=\log x_i$	$Y^*=\log y_i$
1	0.5	0	-0.301
2	1.7	0.301	0.226
3	3.4	0.477	0.534
4	5.7	0.602	0.753
5	8.4	0.699	0.922
15	19.7	2.079	2.141

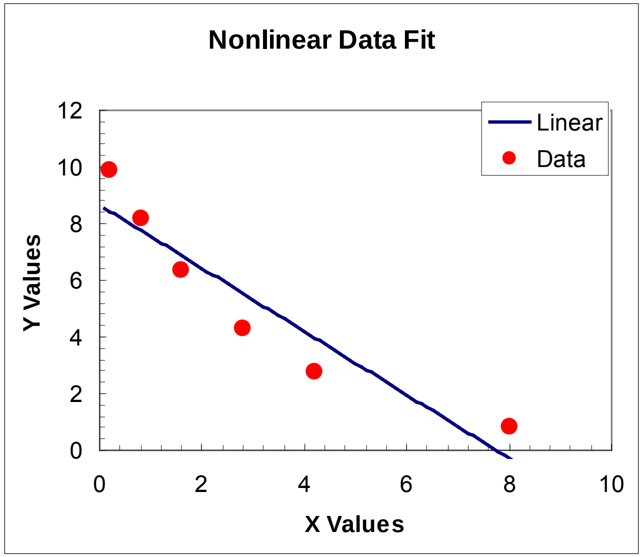
$$\log y = \log(a_2 x^{b_2})$$
$$\log y = \log a_2 + b_2 \log x$$
$$\text{let } Y^* = \log y,\ X^* = \log x,$$
$$a_0 = \log a_2,\ a_1 = b_2$$
$$Y^* = a_0 + a_1 X^*$$

Linear Least Square Approximations

Suppose we want to fit the data set.

Use: $y = ax + b$

x	Data	x^2	xy	ln(y)	x ln(y)	N
0.2	9.91	0.04	1.982	2.293544	0.458709	1
0.8	8.18	0.64	6.544	2.101692	1.681354	1
1.6	6.33	2.56	10.128	1.8453	2.95248	1
2.8	4.31	7.84	12.068	1.460938	4.090626	1
4.2	2.75	17.64	11.55	1.011601	4.248724	1
8	0.82	64	6.56	-0.19845	-1.58761	1
17.6	32.3	92.72	48.832	8.514625	11.84429	6



We would like to find the best straight line to fit the data?

y = -1.11733x + 8.66608

Use: $y = be^{ax}$

$$a = \frac{6(11.84429) - 17.6(8.514625)}{6(92.72) - (17.6)^2} = -0.31956$$

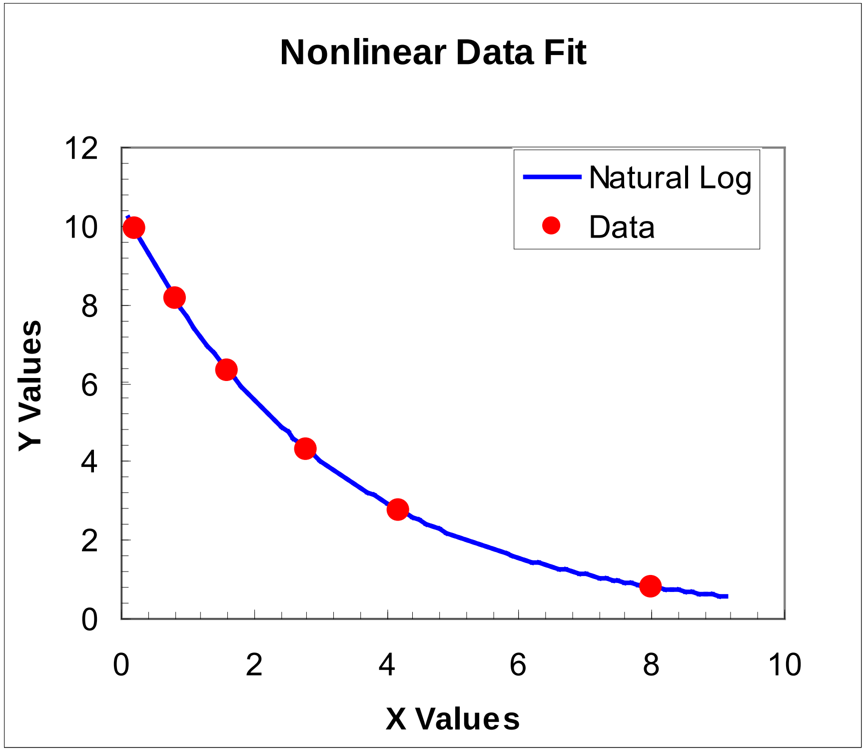
$$b = \frac{92.72(8.514625) - 17.6(11.84429)}{6(92.72) - (17.6)^2} = 2.356492$$

x	Data	x^2	xy	ln(y)	x ln(y)	N
0.2	9.91	0.04	1.982	2.293544	0.458709	1
0.8	8.18	0.64	6.544	2.101692	1.681354	1
1.6	6.33	2.56	10.128	1.8453	2.95248	1
2.8	4.31	7.84	12.068	1.460938	4.090626	1
4.2	2.75	17.64	11.55	1.011601	4.248724	1
8	0.82	64	6.56	-0.19845	-1.58761	1
17.6	32.3	92.72	48.832	8.514625	11.84429	6

The equation is:

$$y' = 2.356492 - 0.31965x$$

$$y = 10.55386\ e^{-0.31965\,x}$$



Use: $y = bx^a$

x	Data	x^2	xy	lnx	$(\ln x^2)$	ln(y)	x ln(y)	lnx lny	N
0.2	9.91	0.04	1.982	-1.60944	2.59029	2.293544	0.458709	-3.69132	1
0.8	8.18	0.64	6.544	-0.22314	0.049793	2.101692	1.681354	-0.46898	1
1.6	6.33	2.56	10.128	0.470004	0.220903	1.8453	2.95248	0.867298	1
2.8	4.31	7.84	12.068	1.029619	1.060116	1.460938	4.090626	1.50421	1
4.2	2.75	17.64	11.55	1.435085	2.059468	1.011601	4.248724	1.451733	1
8	0.82	64	6.56	2.079442	4.324077	-0.19845	-1.58761	-0.41267	1
17.6	32.3	92.72	48.832	3.181568	10.30465	8.514625	11.84429	-0.74972	6

The exponential approximation fits the data.

The power approximation does not fit the data.