CPE 310: Numerical Analysis for Engineers

Chapter 3: Interpolation and Curve Fitting

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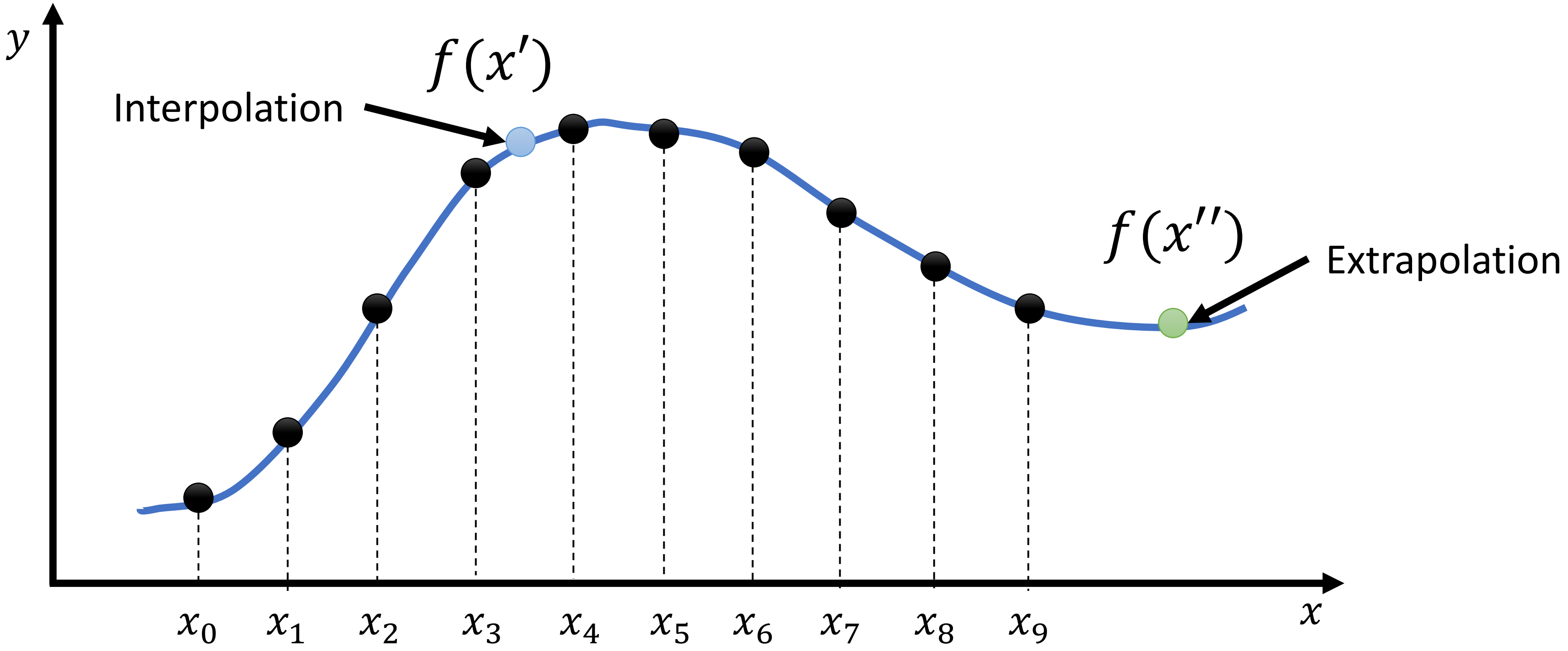
Given **values of an unknown function** corresponding to certain values of *x*

What is the behavior of the function?

In this chapter, we would like to answer the question "What is the function?" but this is always impossible to determine with a limited amount of data

Direct Interpolation | Lagrangian Polynomials | Divided Differences | Evenly-Spaced Data | Least-Squares Approximations

Interpolation versus Extrapolation



Extrapolation

An estimation of a value *beyond* the range of the known data points

Interpolation

An estimation of a value *between* the range of the known data points

The set of data points should be close to the data point we want to interpolate at

Fit a **cubic polynomial** through the **first four points** and use it to find the interpolated value for x = 3.0

x	$f(x)$
3.2	22.0
2.7	17.8
1.0	14.2
4.8	38.3
5.6	51.7

To find a polynomial that passes through the same points as our unknown function, we **set up a system of equations involving the coefficients of the polynomial**

The maximum degree of the polynomial is always **one less than the number of points**

Cubic Polynomial $ax^3 + bx^2 + cx + d$ requires 4 data points

We can write four equations involving the unknown coefficients *a*, *b*, *c*, and *d*

$$\text{If } x = 3.2: a(3.2)^3 + b(3.2)^2 + c(3.2) + d = 22.0$$

$$\text{If } x = 2.7: a(2.7)^3 + b(2.7)^2 + c(2.7) + d = 17.8$$

$$\text{If } x = 1.0: a(1.0)^3 + b(1.0)^2 + c(1.0) + d = 14.2$$

$$\text{If } x = 4.8: a(4.8)^3 + b(4.8)^2 + c(4.8) + d = 38.3$$

$$Ax = b$$

$$\begin{bmatrix} 3.2^3 & 3.2^2 & 3.2 & 1 \\ 2.7^3 & 2.7^2 & 2.7 & 1 \\ 1 & 1 & 1.0 & 1 \\ 4.8^3 & 4.8^2 & 4.8 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 22.0 \\ 17.8 \\ 14.2 \\ 38.3 \end{bmatrix}$$

→ Gaussian Elimination →

$$a = -0.5275, b = 6.4952, \\ c = -16.1177, d = 24.3499$$

Our Polynomial: $-0.5275x^3 + 6.4952x^2 - 16.1177x + 24.3499$

At x = 3.0, the estimated value is 20.21

Adding/Subtracting a point from the set used to construct the polynomial **requires starting over the computations**

Lagrangian Polynomials

The polynomial of lowest degree that passes the same points as our unknown function

The simplest way to exhibit the existence of a polynomial for interpolation with **unevenly spaced data**

Lagrangian Polynomials

We don't assume uniform spacing between the x-values, nor do we need the x-values arranged in a particular order, however, the x-values must all be distinct

x	$f(x)$
x_0	f_0
x_1	f_1
x_2	f_2
x_3	f_3

The Lagrangian polynomial of degree "3" is:

$$P_3(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f_0 + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f_1 + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}f_2 + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}f_3$$

The Lagrangian polynomial for degree *n* will have (*n*+1) terms

Lagrangian Polynomials

We don't assume uniform spacing between the x-values, nor do we need the x-values arranged in a particular order, however, the x-values must all be distinct

$\underline{x}$	$\underline{f(x)}$
x_0	f_0
x_1	f_1
x_2	f_2
x_3	f_3
x_4	f_4

The Lagrangian polynomial of degree "4" is:

$$P_4(x) = \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)} f_0 + \frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)} f_1$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_3)(x-x_4)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)(x_2-x_4)} f_2 + \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_4)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)(x_3-x_4)} f_3$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)} f_4$$

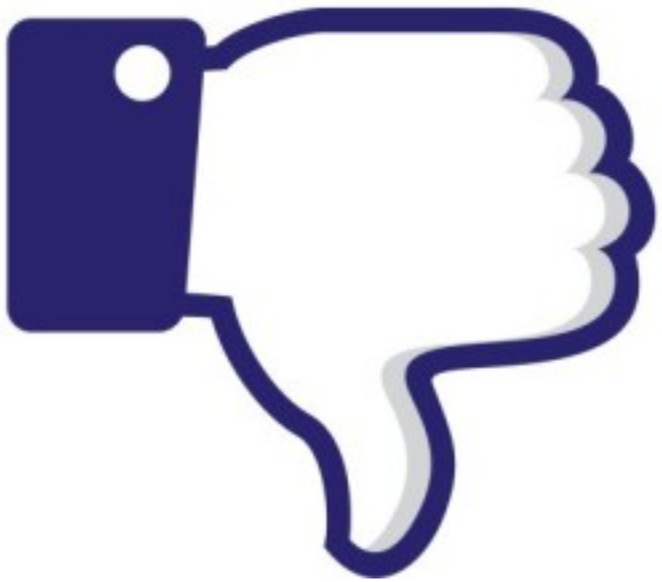
Fit a **cubic polynomial** through the **first four points** and use it to find the interpolated value for x = 3.0

x	$f(x)$
3.2	22.0
2.7	17.8
1.0	14.2
4.8	38.3
5.6	51.7

$$P_3(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f_0 + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f_1 + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}f_2 + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}f_3$$

$$P_3(3.0) = \frac{(3.0-2.7)(3.0-1.0)(3.0-4.8)}{(3.2-2.7)(3.2-1.0)(3.2-4.8)}(22.0) + \frac{(3.0-3.2)(3.0-1.0)(3.0-4.8)}{(2.7-3.2)(2.7-1.0)(2.7-4.8)}(17.8) + \frac{(3.0-3.2)(3.0-2.7)(3.0-4.8)}{(1.0-3.2)(1.0-2.7)(1.0-4.8)}(14.2) + \frac{(3.0-3.2)(3.0-2.7)(3.0-1.0)}{(4.8-3.2)(4.8-2.7)(4.8-1.0)}(38.3)$$

$$P_3(3.0) = 20.21$$



Lagrangian involves **more arithmetic operations** than does the other methods

Adding/Subtracting a point from the set used to construct the polynomial **requires starting over the computations**

Divided Differences

Divided Differences

We don't assume uniform spacing between the x-values, ***nor*** *do we need the x-values arranged in a particular order,* but some ordering may be *advantageous*

The polynomial for degree *n* will have (*n*+1) terms

$$P_n(x) = a_0 + (x - x_0)a_1 + (x - x_0)(x - x_1)a_2 + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})a_n$$

Divided Differences

We don't assume *uniform spacing between* *the x-values,* ***nor*** *do we need the x-values arranged in a* *particular order,* but some ordering may be *advantageous*

The polynomial for degree *n* will have (*n*+1) terms

$$P_n(x) = a_0 + (x - x_0)a_1 + (x - x_0)(x - x_1)a_2 + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})a_n$$

$$P_n(x) = \boldsymbol{f_0^{[0]}} + (x - x_0)\boldsymbol{f_0^{[1]}} + (x - x_0)(x - x_1)\boldsymbol{f_0^{[2]}} + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})\boldsymbol{f_0^{[n]}}$$

$$f_i^{[0]} = f[x_i] = f_i$$

Zero Order Divided Difference

$$f_i^{[1]} = f[x_i, x_{i+1}] = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

First Order Divided Difference

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

Second Order Divided Difference

$$f_i^{[n]} = f[x_0, x_1, \cdots x_n] = \frac{f[x_1, x_2, \cdots, x_n] - f[x_0, x_1, \cdots, x_{n-1}]}{x_n - x_0}$$

***n*-Order Divided Difference**

Divided Differences Table

$\boldsymbol{x_i}$	$\boldsymbol{f_i}$	$\boldsymbol{f[x_i, x_{i+1}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}, x_{i+3}]}$
x_0	f_0			
x_1	f_1	$f[x_0, x_1] = \frac{f_1 - f_0}{x_1 - x_0}$		
x_2	f_2	$f[x_1, x_2] = \frac{f_2 - f_1}{x_2 - x_1}$	$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$	
x_3	f_3	$f[x_2, x_3] = \frac{f_3 - f_2}{x_3 - x_2}$	$f[x_1, x_2, x_3] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_3 - x_1}$	$f[x_0, x_1, x_2, x_3] = \frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0}$
x_4	f_4	$f[x_3, x_4] = \frac{f_4 - f_3}{x_4 - x_3}$	$f[x_2, x_3, x_4] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_4 - x_2}$	$f[x_1, x_2, x_3, x_4] = \frac{f[x_2, x_3, x_4] - f[x_1, x_2, x_3]}{x_4 - x_0}$

Write an **interpolating polynomial of degree 3** that fits data at all data points using **divided differences**

x	$f(x)$
3.2	22.0
2.7	17.8
1.0	14.2
4.8	38.3
5.6	51.7

$$P_3(x) = \boldsymbol{f_0^{[0]}} + (x - x_0)\boldsymbol{f_0^{[1]}} + (x - x_0)(x - x_1)\boldsymbol{f_0^{[2]}} + (x - x_0)(x - x_1)(x - x_2)\boldsymbol{f_0^{[3]}}$$

$\boldsymbol{x_i}$	$\boldsymbol{f_i}$	$\boldsymbol{f[x_i, x_{i+1}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}, x_{i+3}]}$
x_0	f_0			
x_1	f_1	$f[x_0, x_1] = \dfrac{f_1 - f_0}{x_1 - x_0}$		
x_2	f_2	$f[x_1, x_2] = \dfrac{f_2 - f_1}{x_2 - x_1}$	$f[x_0, x_1, x_2] = \dfrac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$	
x_3	f_3	$f[x_2, x_3] = \dfrac{f_3 - f_2}{x_3 - x_2}$	$f[x_1, x_2, x_3] = \dfrac{f[x_1, x_2] - f[x_0, x_1]}{x_3 - x_1}$	$f[x_0, x_1, x_2, x_3] = \dfrac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0}$

$\boldsymbol{x_i}$	$\boldsymbol{f_i}$	$\boldsymbol{f[x_i, x_{i+1}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}]}$	$\boldsymbol{f[x_i, x_{i+1}, x_{i+2}, x_{i+3}]}$
3.2	22.0			
2.7	17.8	8.400		
1.0	14.2	2.118	2.856	
4.8	38.3	6.342	2.012	−0.528

$$P_3(x) = \mathbf{22.0} + (x - 3.2)\mathbf{8.400} + (x - 3.2)(x - 2.7)\mathbf{2.856} + (x - 3.2)(x - 2.7)(x - 1.0)(\mathbf{-0.528})$$

Write an **interpolating polynomial of degree 4** that fits data at all points from $x_0 = 3.2$ to $x_3 = 4.8$ using **divided differences**

x	$f(x)$
3.2	22.0
2.7	17.8
1.0	14.2
4.8	38.3
5.6	51.7

$$P_3(x) = \boldsymbol{f_0^{[0]}} + (x - x_0)\boldsymbol{f_0^{[1]}} + (x - x_0)(x - x_1)\boldsymbol{f_0^{[2]}} + (x - x_0)(x - x_1)(x - x_2)\boldsymbol{f_0^{[3]}}$$

$$P_4(x) = P_3(x) + (x - x_0)(x - x_1)(x - x_2)(x - x_3)\boldsymbol{f_0^{[4]}}$$

"We only have to add one more term to $P_3(x)$"

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

$$P_4(x) = \mathbf{22.0} + (x - 3.2)\mathbf{8.400} + (x - 3.2)(x - 2.7)\mathbf{2.856} + (x - 3.2)(x - 2.7)(x - 1.0)(\mathbf{-0.528})$$

$$+(x - 3.2)(x - 2.7)(x - 1.0)(x - 4.8)(\mathbf{0.256})$$

Divided Difference for $f(x)$ a Polynomial

If $f(x) = a_n x^n + \cdots + a_1 x + a_0$ is a polynomial of degree n, then the interpolating polynomial
$P_n(x) = \boldsymbol{f}_{\mathbf{0}}^{[0]} + (x - x_0)\boldsymbol{f}_{\mathbf{0}}^{[1]} + (x - x_0)(x - x_1)\boldsymbol{f}_{\mathbf{0}}^{[2]} + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})\boldsymbol{f}_{\mathbf{0}}^{[n]}$

Since the polynomial that fits $n + 1$ points $x_0, x_1, \cdots x_n$ is unique, we have

$$f(x) = P_n(x) \Longrightarrow a_n = \boldsymbol{f}_{\mathbf{0}}^{[\boldsymbol{n}]}$$

$$f(x) = \mathbf{2}x^3 - x^2 + x - 1$$

The divided-difference of order greater than n are all zero

$\boldsymbol{x_i}$	$\boldsymbol{f_i}$	$\boldsymbol{f_i^{[1]}}$	$\boldsymbol{f_i^{[2]}}$	$\boldsymbol{f_i^{[3]}}$	$\boldsymbol{f_i^{[4]}}$	$\boldsymbol{f_i^{[5]}}$
0.30	−0.7360					
1.00	1.0000	2.4800				
0.70	−0.1040	3.6800	3.0000			
0.60	−0.3280	2.2400	3.6000	**2.0000**		
1.90	11.0080	8.7200	5.4000	**2.0000**	0.0000	
2.10	15.2120	21.0200	8.2000	**2.0000**	0.0000	0.0000

Divided Difference for $f(x)$ a Polynomial

If $f(x) = a_n x^n + \cdots + a_1 x + a_0$ is a polynomial of degree n, then the interpolating polynomial
$P_n(x) = \boldsymbol{f_0^{[0]}} + (x - x_0)\boldsymbol{f_0^{[1]}} + (x - x_0)(x - x_1)\boldsymbol{f_0^{[2]}} + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})\boldsymbol{f_0^{[n]}}$

Since the polynomial that fits n + 1 points $x_0, x_1, \cdots x_n$ is unique, we have

$$f(x) = P_n(x) \Longrightarrow a_n = \boldsymbol{f_0^{[n]}}$$

$f(x) = 6.5x^5 - x^2 + x - 1$

$$\boldsymbol{f_0^{[5]} = 6.5}$$

$$\boldsymbol{f_0^{[6]} = 0}$$

$$\boldsymbol{f_0^{[20]} = 0}$$

$f(x) = -10.33x^8 - x^5 + x - 20$

$$\boldsymbol{f_0^{[5]}} = ?$$

$$\boldsymbol{f_0^{[8]} = -10.33}$$

$$\boldsymbol{f_0^{[20]} = 0}$$

Evenly Spaced Data

The problem of interpolation from tabulated data is considerably ***simplified*** *if the values of the function are given at* ***evenly spaced intervals of the independent variable***

A data $(x_i, f_i), i = 0,1,\cdots,n$ is evenly spaced or **equi-spaced** if there is a constant h such that $x_{i+1} - x_i = h$ for $i = 0,1,\cdots,n-1$

First Order Difference: $\Delta f_i = f_{i+1} - f_i$

Second Order Difference: $\Delta^2 f_i = \Delta(\Delta f_i) = f_{i+2} - 2f_{i+1} + f_i$

***n*-Order Difference:** $\Delta^n f_i = \Delta(\Delta^{n-1} f_i)$

Construct a **difference table** for $f(x) = x^3 + 2$ for the interval $[0, 4]$ with spacing of 1

It is **necessary** here to arrange the data in a table with *x*-values in **ascending order**

$\boldsymbol{x_i}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f(x)}$	$\boldsymbol{\Delta^2 f(x)}$	$\boldsymbol{\Delta^3 f(x)}$	$\boldsymbol{\Delta^4 f(x)}$
0.00	2.00				
1.00	3.00	1.00			
2.00	10.00	7.00	6.00		
3.00	29.00	19.00	12.00	6.00	
4.00	66.00	37.00	18.00	6.00	0.00

Construct a **difference table** for $f(x) = x^3 + 2$ for the interval $[0, 4]$ with spacing of 1

$\boldsymbol{x_i}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f(x)}$	$\boldsymbol{\Delta^2 f(x)}$	$\boldsymbol{\Delta^3 f(x)}$	$\boldsymbol{\Delta^4 f(x)}$
0.00	2.00				
1.00	3.00	1.00			
2.00	10.00	7.00	6.00		
3.00	29.00	19.00	12.00	6.00	
4.00	66.00	**37.00**	**18.00**	6.00	0.00
			$\sum = 36$	$\sum = 12$	

One of the best ways to check for mistakes is to **add the sum of the numbers in each column to the top entry in the column to its left**. *This sum should equal the bottom entry in the column to the left*

Relation between Differences and Divided Differences

Let $(x_i, f_i), i = 0,1,\cdots,n$ is evenly spaced data with $x_{i+1} - x_i = h$

$$f_i^{[1]} = f[x_i, x_{i+1}] = \frac{f_{i+1} - f_i}{x_{i+1} - x_i} = \frac{\Delta f_i}{h}$$

$$f_i^{[2]} = f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i} = \frac{\frac{\Delta f_{i+1}}{h} - \frac{\Delta f_i}{h}}{2h} = \frac{\Delta^2 f_i}{2h^2}$$

$$f_i^{[n]} = f[x_i, x_{i+1}, \cdots, x_{i+n}] = \frac{\Delta^n f_i}{n!\, h^n}$$

Construct a **difference table** for $f(x) = x^3 + 2$ for the interval $[0, 4]$ with spacing of 1

$\boldsymbol{x_i}$	$\boldsymbol{f(x)}$	$\Delta \boldsymbol{f(x)}$	$\Delta^2 \boldsymbol{f(x)}$	$\Delta^3 \boldsymbol{f(x)}$	$\Delta^4 \boldsymbol{f(x)}$
0.00	2.00				
1.00	3.00	1.00			
2.00	10.00	7.00	6.00		
3.00	29.00	19.00	12.00	6.00	
4.00	66.00	37.00	18.00	6.00	0.00

$$f_i^{[n]} = f[x_i, x_{i+1}, \cdots, x_{i+n}] = \frac{\Delta^n f_i}{n!\, h^n}$$

$$f_i^{[3]} = \frac{\Delta^3 f_i}{(3)!\,(1)^3} = \frac{6.00}{6.00} = 1$$

Newton-Gregory Forward Polynomial

One of the easiest ways to write a polynomial that passes through a group of equispaced points

Newton-Gregory Forward Polynomial

One of the easiest ways to write a polynomial that passes through a group of equispaced points

$$P_n(x) = \boldsymbol{f_0^{[0]}} + (x - x_0)\boldsymbol{f_0^{[1]}} + (x - x_0)(x - x_1)\boldsymbol{f_0^{[2]}} + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})\boldsymbol{f_0^{[n]}}$$

$$f_i^{[n]} = f[x_i, x_{i+1}, \cdots, x_{i+n}] = \frac{\Delta^n f_i}{n!\, h^n}$$

$$P_n(x) = f_0 + (x - x_0)\frac{\Delta f_0}{h} + (x - x_0)(x - x_1)\frac{\Delta^2 f_0}{2!\, h^2} + \cdots + (x - x_0)(x - x_1)\cdots(x - x_{n-1})\frac{\Delta^n f_i}{n!\, h^n}$$

$$P_n(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2!}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_i + \cdots + \frac{s(s-1)\cdots(s-n+1)}{n!}\Delta^n f_i \qquad s = \frac{x - x_0}{h}$$

$$P_n(x) = f_0 + \binom{s}{1}\Delta f_0 + \binom{s}{2}\Delta^2 f_0 + \binom{s}{3}\Delta^3 f_i + \cdots + \binom{s}{n}\Delta^n f_i \qquad \binom{s}{m} = \frac{s(s-1)\cdots(s-m+1)}{m!}$$

Write a **Newton-Gregory forward polynomial** of degree 3 that fits the four data points from $x = 0.4$ to $x = 1.0$ with spacing of 0.2. Then, use it to interpolate for $f(0.73)$

$\boldsymbol{x_i}$	$\boldsymbol{f(x)}$	$\Delta \boldsymbol{f(x)}$	$\Delta^2 \boldsymbol{f(x)}$	$\Delta^3 \boldsymbol{f(x)}$
0.4	0.423			
0.6	0.684	0.261		
0.8	1.030	0.346	0.085	
1.0	1.557	0.527	0.181	0.096

$$P_n(x) = f_0 + \binom{s}{1}\Delta f_0 + \binom{s}{2}\Delta^2 f_0 + \binom{s}{3}\Delta^3 f_i$$

$$\binom{s}{m} = \frac{s(s-1)\cdots(s-m+1)}{m!} \qquad s = \frac{x - x_0}{h}$$

$$P_n(x) = 0.423 + \binom{s}{1}0.261 + \binom{s}{2}0.085 + \binom{s}{3}0.096$$

$$P_n(0.73) = 0.423 + \binom{s}{1}0.261 + \binom{s}{2}0.085 + \binom{s}{3}0.096 \qquad s = \frac{0.73 - 0.4}{0.2} = 1.65$$

$$P_n(0.73) = 0.423 + \binom{1.65}{1}0.261 + \binom{1.65}{2}0.085 + \binom{1.65}{3}0.096 = 0.893$$

Differences Versus Divided Differences

$$f(x) = x^3 + 2$$

x_i	$f(x)$	$f^{[1]}$	$f^{[2]}$	$f^{[3]}$	$f^{[4]}$
0.00	2.00				
1.00	3.00	1.00			
2.00	10.00	7.00	3.00		
3.00	29.00	19.00	6.00	1.00	
4.00	66.00	37.00	9.00	1.00	0.00

$$a_n = f_0^{[n]}$$

a_n is the coefficient of x^n

x_i	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$
0.00	2.00				
1.00	3.00	1.00			
2.00	10.00	7.00	6.00		
3.00	29.00	19.00	12.00	6.00	
4.00	66.00	37.00	18.00	6.00	0.00

$$f_i^{[n]} = f[x_i, x_{i+1}, \cdots, x_{i+n}] = \frac{\Delta^n f_i}{n!\, h^n}$$

$$a_n = f_0^{[n]} = \frac{\Delta^n f_0}{n!\, h^n}$$

Least-Squares Approximations

*We look for an **approximation function** $P(x)$ from some particular class of functions such that the least-squares measure of the error is **minimized***

Instead of the interpolating condition $P(x_i) = f(x_i)$, we impose the condition:

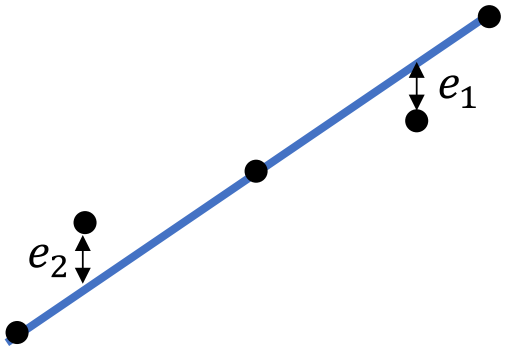
$$E = \sum_{i=0}^{n} e_i^2 = \sum_{i=0}^{n} [P(x_i) - f(x_i)]^2 \ \textbf{is minimum}$$

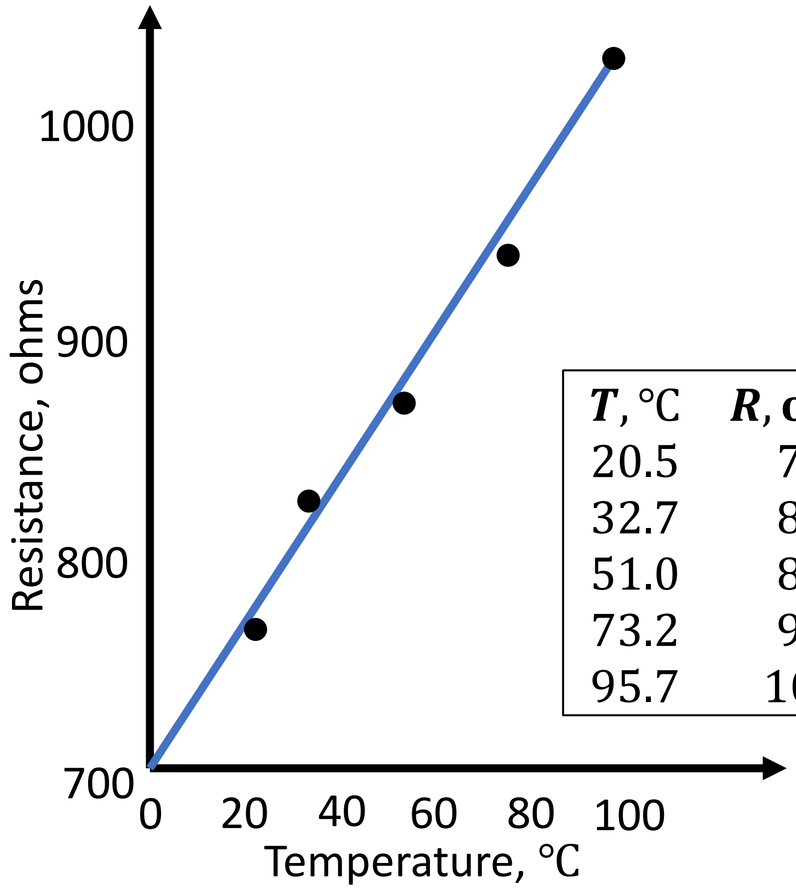
Least-Squares Approximations

Find a line that would make a **best fit**

"Least-squares" principle is to <u>minimize</u> the sum of the squares of the errors

$$R = aT + b$$





T, ℃	R, ohms
20.5	765
32.7	826
51.0	873
73.2	942
95.7	1032

Least-Squares Approximations

Let Y_i represent an experimental value, and let y_i be a value from the equation $y_i = a\,x_i + b$, where x_i is a particular value of the variable assumed to be **free of error**

We wish to determine the best values for *a* and *b* so that the *y's* predict the function values that correspond to *x*-values

*The least-squares criterion requires the following to be **minimum***

$$S = e_1^2 + e_2^2 + \cdots + e_N^2$$

$$= \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} (Y_i - a x_i - b)^2$$

where *N* is the number of (x, Y) pairs

$$e_i = Y_i - y_i$$

We reach the minimum by proper choice of the parameters *a* and *b*, so they are the "variables" of the problem

Least-Squares Approximations

$$S = e_1^2 + e_2^2 + \cdots + e_N^2$$
$$= \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} (Y_i - ax_i - b)^2$$

At a minimum for S, the two partial derivatives will both be zero

$$\frac{\partial S}{\partial a} = 0 = \sum_{i=1}^{N} 2(Y_i - ax_i - b)(-x_i)$$
$$\frac{\partial S}{\partial b} = 0 = \sum_{i=1}^{N} 2(Y_i - ax_i - b)(-1)$$

Dividing each of these equations by -2 and expanding the summation

$$a \sum x_i^2 + b \sum x_i = \sum x_i Y_i$$
$$a \sum x_i + bN = \sum Y_i$$

Normal Equations

Solving these equations simultaneously gives the values for slope and intercept *a* and *b*

$$a\sum x_i^2 + b\sum x_i = \sum x_i Y_i$$
$$a\sum x_i + bN = \sum Y_i$$

$N = 5,\quad \sum x_i = 273.1$

$\sum x_i^2 = 18{,}607.27 \quad \sum Y_i = 4438$

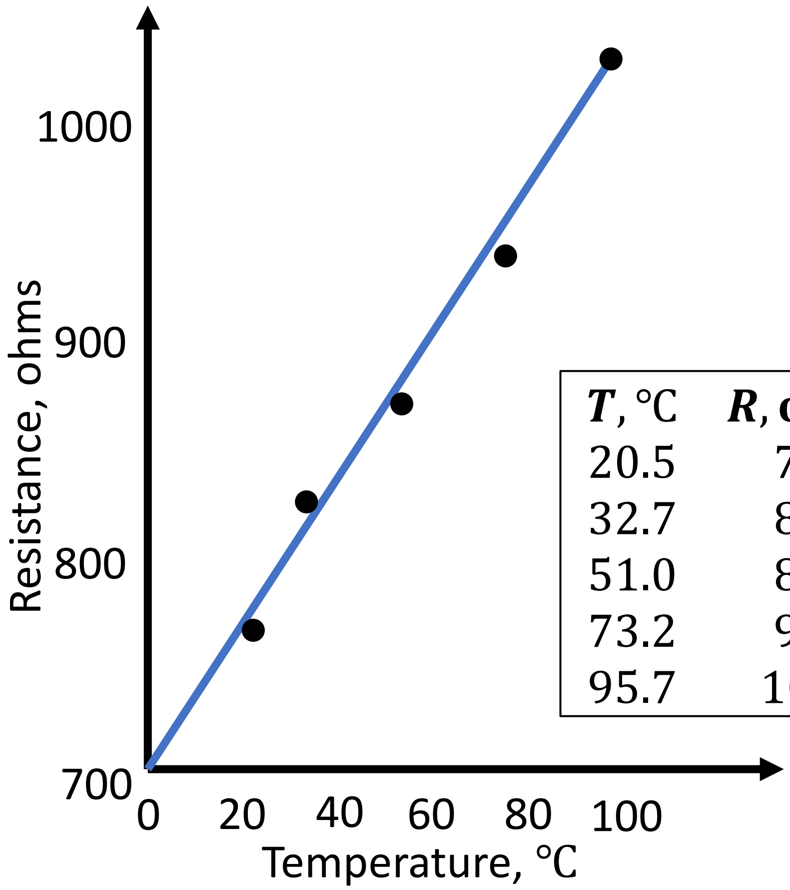
$\sum x_i Y_i = 254{,}932.5$

$$18{,}607.27a + 273.1b = 254{,}932.5$$
$$273.1a + 5b = 4438$$

$a = 3.395, b = 702.2$

$$R = 3.395T + 702.2$$

Find the **least-square line** for the data



T, °C	***R*, ohms**
20.5	765
32.7	826
51.0	873
73.2	942
95.7	1032

What if we have a non-linear data?

In many cases, data from experimental tests are not linear, so we need to fit to them some function other than a first-degree polynomial

Exponential forms

$y = ax^b, y = ae^{bx}$

n-Degree **Polynomial Forms:**

$y = a_0 + a_1x + a_2x^2 + \cdots + a_nx^n$

Non-Linear Data with Exponential Form Fitting

Popular forms that are tried are the **exponential forms:**

$y = ax^b$ OR $y = ae^{bx}$

We can develop normal equations for these analogously to the preceding development for a least-squares line by **setting the partial derivatives equal to zero**

Such nonlinear simultaneous equations are much **more difficult** to solve than linear equations

$y = ax^b$

$y = ae^{bx}$

Linearized by taking logarithms

$\ln y = \ln a + b \ln x$

$W = \ln y$
$A = \ln a$
$Z = \ln x$

$W = A + bZ$

$\ln y = \ln a + bx$

$W = \ln y$
$A = \ln a$

$W = A + bx$

Non-Linear Data with Exponential Form Fitting

$$Y_i = ax_i + b$$

$$a\sum x_i^2 + b\sum x_i = \sum x_i Y_i$$

$$a\sum x_i + bN = \sum Y_i$$

$$W = A + bZ$$

$$b\sum Z^2 + A\sum Z = \sum ZW$$

$$b\sum Z + AN = \sum W$$

$$y = ax^b$$

$$W = A + bx$$

$$b\sum x_i^2 + A\sum x_i = \sum x_i W$$

$$b\sum x_i + AN = \sum W$$

$$y = ae^{bx}$$

Find the **least-square exponential curve on the form** $y = ax^b$ for the given data points

x	y
1	2
2	16
3	54
4	128
5	250
6	432

$$W = A + bZ$$

$$b\sum Z^2 + A\sum Z = \sum ZW$$

$$b\sum Z + AN = \sum W$$

$$W = \ln y$$
$$A = \ln a$$
$$Z = \ln x$$

x	y	Z	Z^2	W	$Z*W$
1	2	0	0	0.693147	0
2	16	0.693147181	0.480453	2.772589	1.921812
3	54	1.098612289	1.206949	3.988984	4.382347
4	128	1.386294361	1.921812	4.85203	6.726342
5	250	1.609437912	2.59029	5.521461	8.886449
6	432	6.579251212	2.210402	6.068426	10.87316
	Σ	**6.579251212**	**9.409906**	**23.89664**	**32.79011**

$$9.409906b + 6.579251212A = 32.79011$$

$$6.579251212b + 6A = 12.89664$$

$$b = 3.0133, A = 0.6787, a = e^A = 1.97$$

$$y = 1.97x^{3.0133}$$

Non-Linear Data with Polynomial Form Fitting

n-Degree **Polynomial Forms:**

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

In the development of normal equations, we use *n* as the degree of the polynomial and *N* as the number of data pairs

if ***N* = *n* + 1**, the polynomial passes exactly through each point and the methods discussed earlier in this chapter apply, so we will always have ***N* > *n* + 1** in the following

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

$$e_i = Y_i - y_i = Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \cdots - a_n x_i^n$$

We want to **minimize the sum of squares**:

$$S = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} \left(Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \cdots - a_n x_i^n\right)^2$$

Non-Linear Data with Polynomial Form Fitting

We want to **minimize the sum of squares**:

$$S = \sum_{i=1}^{N} e_i^2 = \sum_{i=1}^{N} \left(Y_i - a_0 - a_1 x_i - a_2 x_i^2 - \cdots - a_n x_i^n\right)^2$$

At the minimum, all **the partial derivatives vanish** “Equal to Zero”:

$$\frac{\partial S}{\partial a_0} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - \cdots - a_i x_i^n)(-1)$$

$$\frac{\partial S}{\partial a_1} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - \cdots - a_i x_i^n)(-x_i)$$

$$\vdots$$

$$\frac{\partial S}{\partial a_n} = 0 = \sum_{i=1}^{N} 2(Y_i - a_0 - a_1 x_i - \cdots - a_n x_i^n)(-x_i^n)$$

Non-Linear Data with Polynomial Form Fitting

Dividing each by **-2** and rearranging gives the *n* + 1 **normal equations** to be solved simultaneously:

$$a_0 N + a_1 \sum x_i + a_2 \sum x_i^2 + \cdots + a_n \sum x_i^n = \sum Y_i$$

$$a_0 \sum x_i + a_1 \sum x_i^2 + a_2 \sum x_i^3 + \cdots + a_n \sum x_i^{n+1} = \sum x_i Y_i$$

$$a_0 \sum x_i^2 + a_1 \sum x_i^3 + a_2 \sum x_i^4 + \cdots + a_n \sum x_i^{n+2} = \sum x_i^2 Y_i$$

$$\vdots$$

$$a_0 \sum x_i^n + a_1 \sum x_i^{n+1} + a_2 \sum x_i^{n+2} + \cdots + a_n \sum x_i^{2n} = \sum x_i^n Y_i$$

All the summations run from 1 to N

Non-Linear Data with Polynomial Form Fitting

Putting these equations in matrix form shows an interesting pattern in the coefficient matrix

$$\begin{bmatrix} N & \sum x_i & \sum x_i^2 & \sum x_i^3 & \cdots & \sum x_i^n \\ \sum x_i & \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \cdots & \sum x_i^{n+1} \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 & \sum x_i^5 & \cdots & \sum x_i^{n+2} \\ \vdots & & & & & \vdots \\ \sum x_i^n & \sum x_i^{n+1} & \sum x_i^{n+2} & \sum x_i^{n+3} & \cdots & \sum x_i^{2n} \end{bmatrix} a = \begin{bmatrix} \sum Y_i \\ \sum x_i Y_i \\ \sum x_i^2 Y_i \\ \vdots \\ \sum x_i^n Y_i \end{bmatrix}$$

All the summations run from 1 to N

Solving large sets of linear equations is **not** a simple task

Round-off errors in solving them cause unusually **large errors** in the solutions

Up to n = 4 or 5, the problem is not too great, but beyond this point special methods are needed

Find the **least-square quadratic curve** $y = a_0 + a_1 x + a_2 x^2$ for the given data points

x_i	Y_i
0.05	0.956
0.11	0.890
0.15	0.832
0.31	0.717
0.46	0.571
0.52	0.539
0.70	0.378
0.74	0.370
0.82	0.306
0.98	0.242
1.17	0.104

$$\begin{bmatrix} N & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} a = \begin{bmatrix} \sum Y_i \\ \sum x_i Y_i \\ \sum x_i^2 Y_i \end{bmatrix}$$

$$\begin{bmatrix} 11 & 6.01 & 4.6545 \\ 6.01 & 4.6545 & 4.1150 \\ 4.6545 & 4.1150 & 3.9161 \end{bmatrix} a = \begin{bmatrix} 5.905 \\ 2.1839 \\ 1.3357 \end{bmatrix}$$

$$a = \begin{bmatrix} 0.998 \\ -1.018 \\ 0.225 \end{bmatrix}$$

$$y = 0.998 - 1.018x + 0.225x^2$$

Find the **least-square quadratic curve** $y = a_0 + a_1 x + a_2 x^2$ for the given data points

x_i	Y_i
0.05	0.956
0.11	0.890
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$$\begin{bmatrix} N & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} a = \begin{bmatrix} \sum Y_i \\ \sum x_i Y_i \\ \sum x_i^2 Y_i \end{bmatrix}$$

$$\begin{bmatrix} 11 & 6.01 & 4.6545 \\ 6.01 & 4.6545 & 4.1150 \\ 4.6545 & 4.1150 & 3.9161 \end{bmatrix} a = \begin{bmatrix} 5.905 \\ 2.1839 \\ 1.3357 \end{bmatrix}$$

$$a = \begin{bmatrix} 0.998 \\ -1.018 \\ 0.225 \end{bmatrix}$$

$$y = 0.998 - 1.018x + 0.225x^2$$

$\boldsymbol{y = 1 - x + 0.2x^2}$

We do **not** expect to reproduce the coefficients exactly because of the **errors in the data**

What Degree Polynomial Should be Used?

As we use **higher-degree polynomials**, we of course will reduce the deviations of the points from the curve until, when the degree of the polynomial, $n = N - 1$, there is an exact match and we have an *interpolating polynomial*

One can increase the **degree of approximating polynomial** as long as there is a statistically significant **decrease in the variance** which is computed by:

$$\sigma^2 = \frac{\sum e_i^2}{N - n - 1}$$

x_i	Y_i
0.05	0.956
0.11	0.890
0.15	0.832
0.31	0.717
0.46	0.571
0.52	0.539
0.70	0.378
0.74	0.370
0.82	0.306
0.98	0.242
1.17	0.104

Degree	Equation	σ^2	$\sum e^2$
1	$y = 0.952 - 0.760x$	0.0010	0.0092
2	$y = 0.998 - 1.018x + 0.225x^2$	0.0002	0.0018
3	$y = 1.004 - 1.079x + 0.351x^2 - 0.069x^3$	0.0003	0.0018
4	$y = 0.998 - 0.838x - 0.522x^2 + 1.040x^3 - 0.454x^4$	0.0003	0.0016
5	$y = 1.031 - 1.704x + 4.278x^2 - 9.477x^3 + 9.394x^4 - 3.290x^5$	0.0001	0.0007
6	$y = 1.038 - 1.910x + 5.952x^2 - 15.078x^3 + 18.277x^4 - 9.835x^5 + 1.836x^6$	0.0002	0.0007
7	$y = 1.032 - 1.742x + 4.694x^2 - 11.898x^3 + 16.645x^4 - 14.346x^5 + 8.141x^6 - 2.293x^7$	0.0002	0.0007