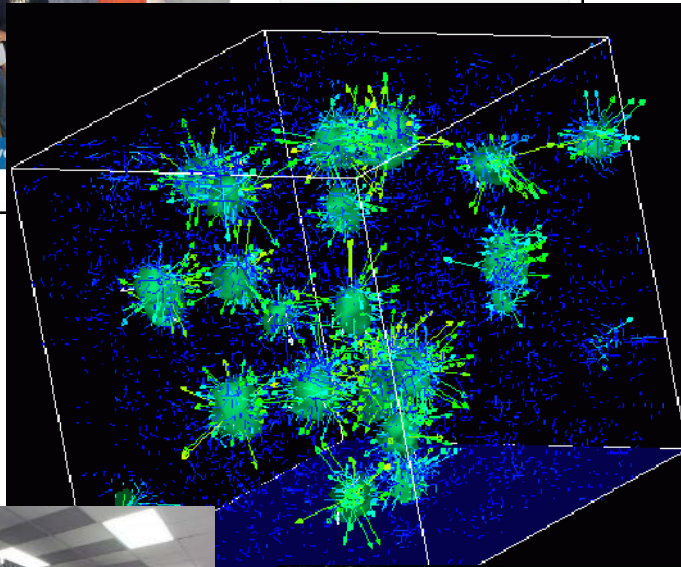




# Survey of Scientific Computing (SciComp 301)

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```
1 using System;
2 using System.Collections.Generic;
3 using System.ComponentModel;
4 using System.Data;
5 using System.Drawing;
6 using System.Linq;
7 using System.Text;
8 using System.Windows.Forms;
9
10 namespace SimpleEvents
11 {
12     public partial class Form1 : Form
13     {
14         Person person = new Person();
15
16         public Form1()
17         {
18             InitializeComponent();
19             person.FirstName = "Christian";
20             person.LastName = "Pano";
21         }
22
23         private void button1_Click(object sender, EventArgs e)
24         {
25             person.MainColor = textBox1.Text;
26         }
27     }
28 }
```

**Session 23**  
Difference Tables,  
Least Squares

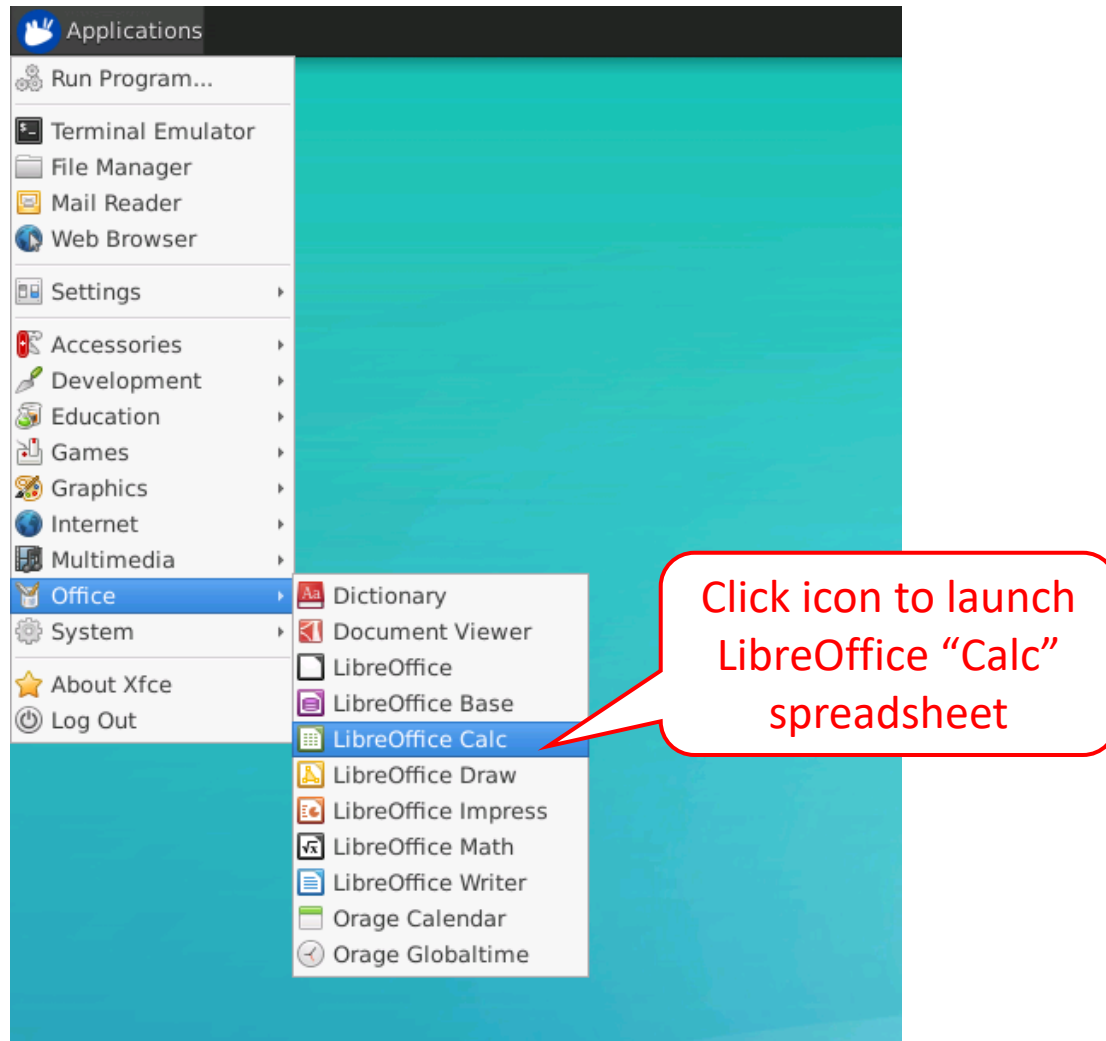
# Session Goals

- Determine the exact formula of the underlying **generator** for a sequence of integers (a ***functional equation***)
  - Fit a **quadratic** curve to a set of observations to **interpolate** resulting values that lie between the observations
  - Understand how to create difference tables in the open source (and free) LibreOffice **Calc** spreadsheet program
  - Appreciate **% relative error** as a measure of **goodness of fit** of a model to experimental data
- Fit a curve using the **Method of Least Squares**
  - Derive the least squares equations using the **partial derivatives** for each coefficient of the unknown quadratic

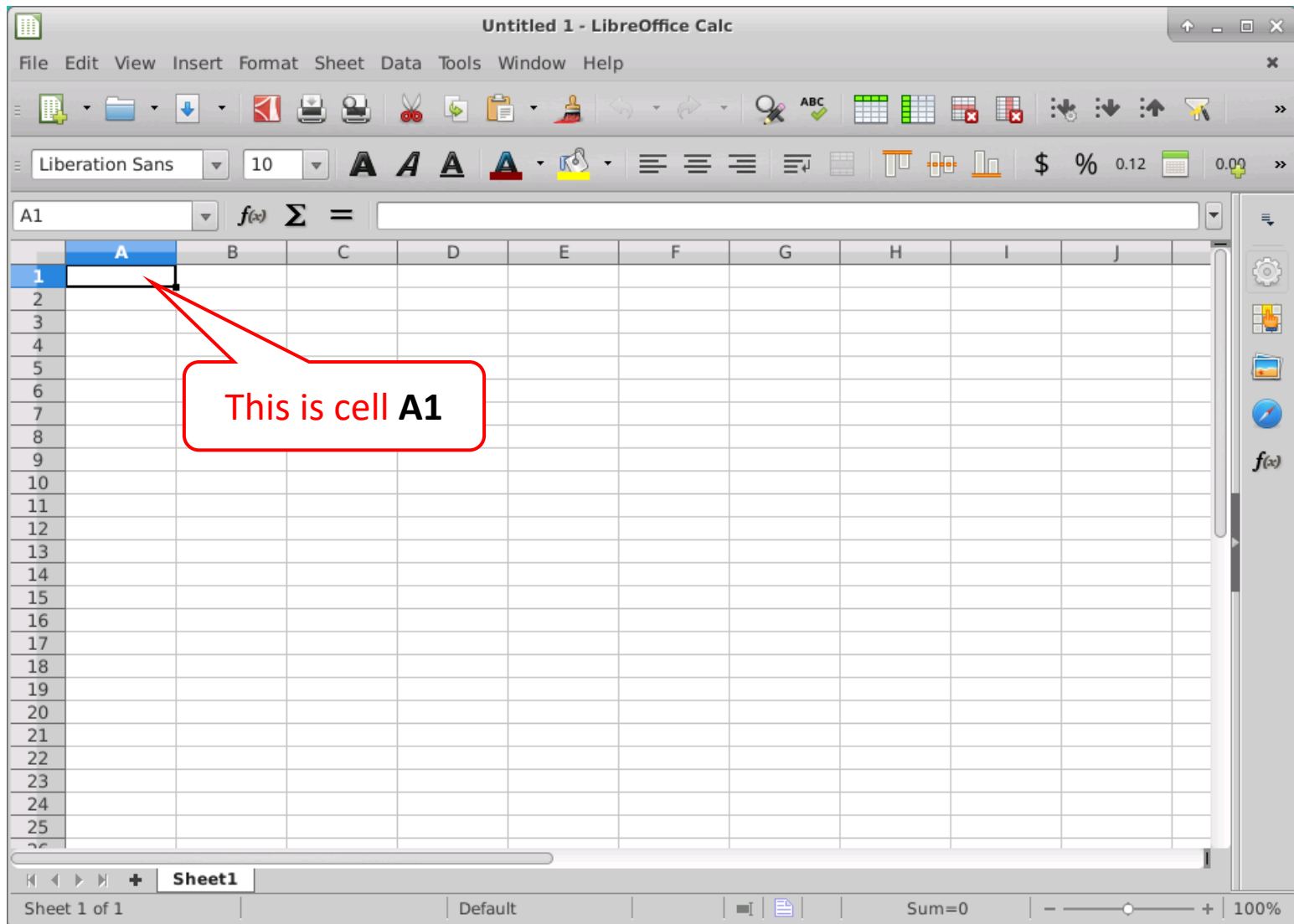
# Creating a Spreadsheet

- A **spreadsheet** is a flexible computing tool that allows you to enter data and write formulas to operate on that data
- Everything is based on the concept of a “**cell**” that has a unique **column** (letter) and **row** (number) address
- A formula entered in one cell can reference data in one or more other cells by using a cell addresses, or by using a **range of cell addresses**
- When source data cells are update, the spreadsheet *automatically recalculates all dependent formula cells*
- Graphs can be created to depict the values in cells

# Creating a Spreadsheet



# Lab 1 - Creating a Spreadsheet



# Lab 1 - Creating a Spreadsheet

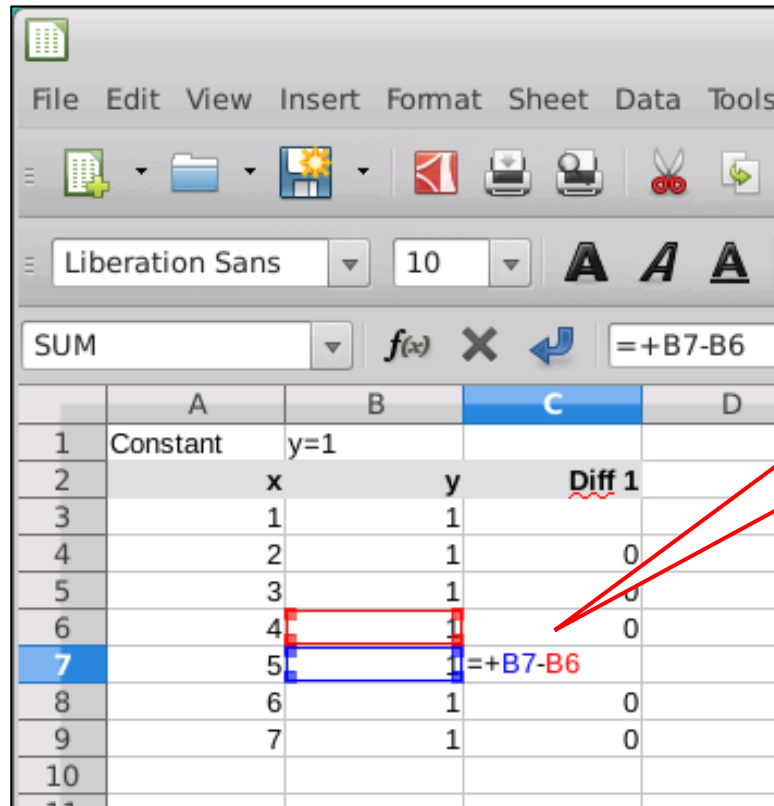
The screenshot shows a spreadsheet application window titled "Untitled 1 - Lib". The menu bar includes File, Edit, View, Insert, Format, Set, Data, Tools, Window, and Help. The toolbar contains icons for file operations and formatting. The font settings are Liberation Sans, size 10. The formula bar shows the formula  $=+B4-B3$  for cell C4. The spreadsheet data is as follows:

	A	B	C	D	E	F	G
1	Constant	y=1					
2	x	y	<u>Diff 1</u>				
3	1	1					
4	2	1	0				
5	3	1	0				
6	4	1	0				
7	5	1	0				
8	6	1	0				
9	7	1	0				
10							

Callouts:

- Bold, Italic, Underline a cell**: Points to the Bold, Italic, and Underline buttons in the formatting toolbar.
- Left, Center, Right Justify a cell**: Points to the Left, Center, and Right justify buttons in the formatting toolbar.
- Cell C4 is a formula using relative cell addresses**: Points to the formula bar showing  $=+B4-B3$  and the value 0 in cell C4.

# Lab 1 - Creating a Spreadsheet

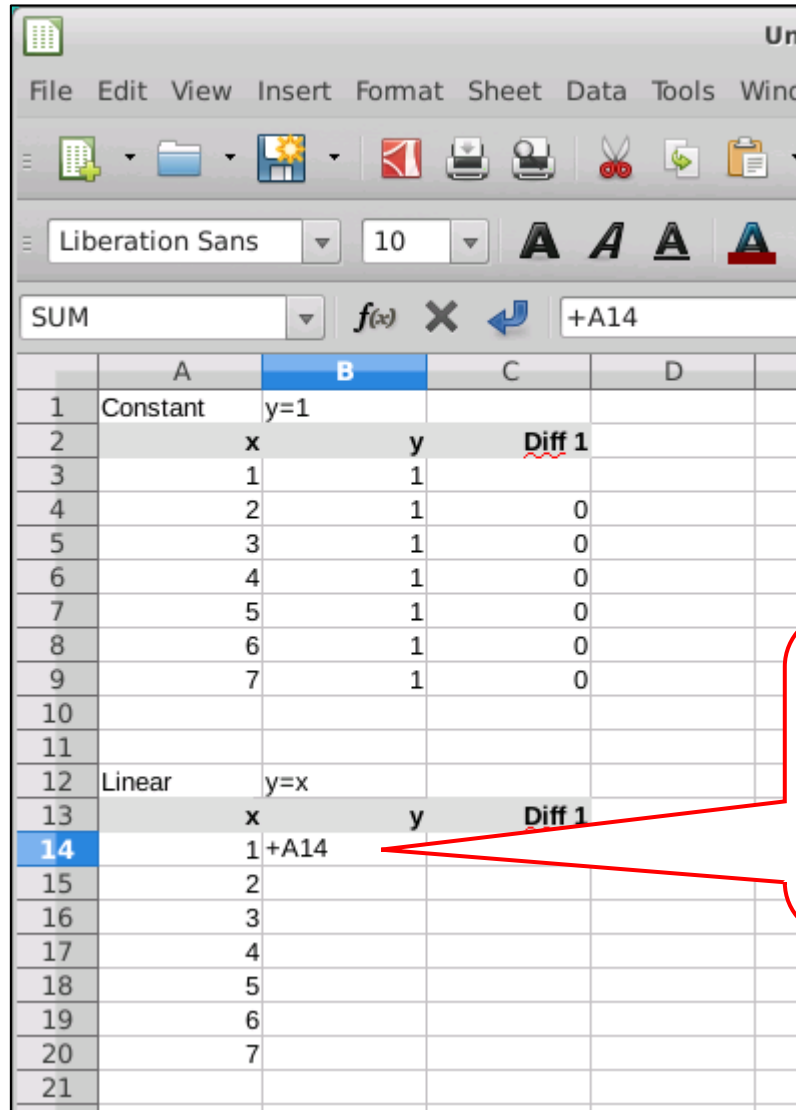


The screenshot shows a spreadsheet application with a menu bar (File, Edit, View, Insert, Format, Sheet, Data, Tools) and a toolbar. The font is Liberation Sans, size 10. The active cell is C7, and the formula bar shows =+B7-B6. The spreadsheet data is as follows:

	A	B	C	D
1	Constant	y=1		
2	x	y	Diff 1	
3	1	1		
4	2	1	0	
5	3	1	0	
6	4	1	0	
7	5	1	=+B7-B6	
8	6	1	0	
9	7	1	0	
10				
11				

To check a formula cell,  
hit **F2** to edit the  
formula – color coding  
identifies the cells

# Lab 1 – Creating a Spreadsheet



	A	B	C	D
1	Constant	y=1		
2	x	y	Diff 1	
3	1	1		
4	2	1	0	
5	3	1	0	
6	4	1	0	
7	5	1	0	
8	6	1	0	
9	7	1	0	
10				
11				
12	Linear	y=x		
13	x	y	Diff 1	
14	1	+A14		
15	2			
16	3			
17	4			
18	5			
19	6			
20	7			
21				

To enter a formula cell, press **+**, then use the arrow keys to select the source data cells. Press **ENTER** when done with the formula



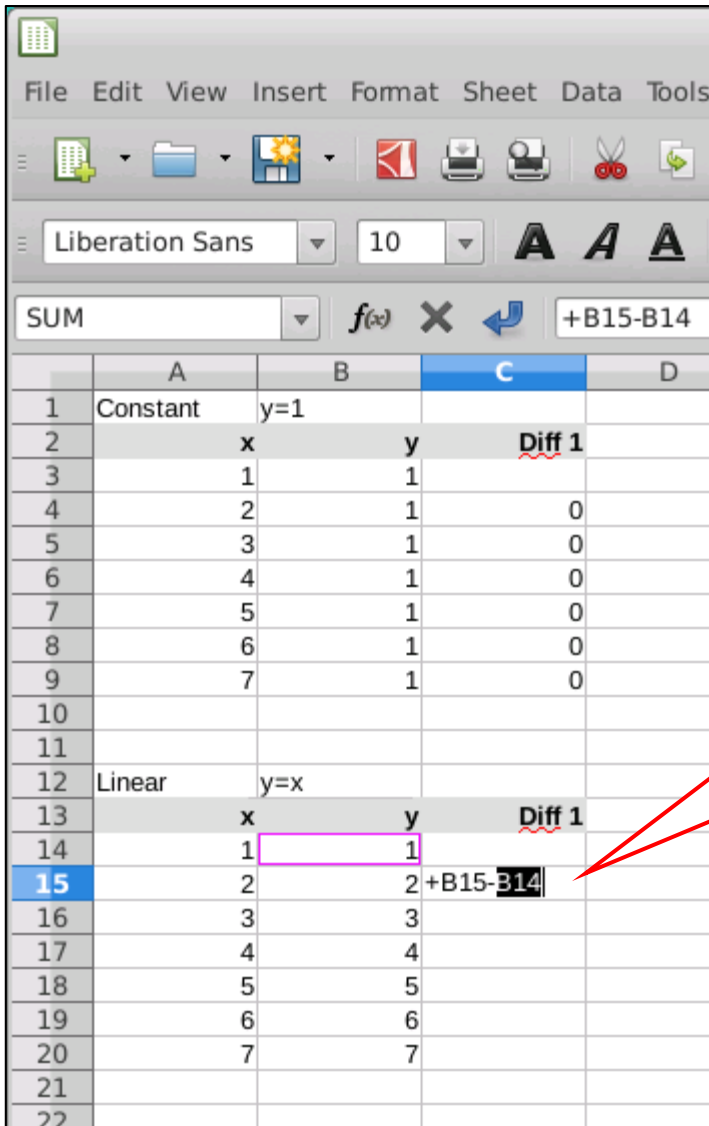
# Lab 1 - Creating a Spreadsheet

The screenshot shows a spreadsheet application with a menu bar (File, Edit, View, Insert, Format, Sheet, Data, Tools, Window) and a toolbar. The active sheet is named 'Un'. The selected range is B15:B20. The spreadsheet contains two tables:

	A	B	C	D
1	Constant	$y=1$		
2	x	y	Diff 1	
3	1	1		
4	2	1	0	
5	3	1	0	
6	4	1	0	
7	5	1	0	
8	6	1	0	
9	7	1	0	
10				
11				
12	Linear	$y=x$		
13	x	y	Diff 1	
14	1	1		
15	2			
16	3			
17	4			
18	5			
19	6			
20	7			
21				
22				

To copy a formula to other cells, highlight the source cell, press "Control + C" to copy, then use arrow keys + SHIFT to highlight a destination **range**, and press ENTER to paste

# Lab 1 - Creating a Spreadsheet



	A	B	C	D
1	Constant	y=1		
2	x	y	<u>Diff 1</u>	
3	1	1		
4	2	1	0	
5	3	1	0	
6	4	1	0	
7	5	1	0	
8	6	1	0	
9	7	1	0	
10				
11				
12	Linear	y=x		
13	x	y	<u>Diff 1</u>	
14	1	1		
15	2	2	+B15-B14	
16	3	3		
17	4	4		
18	5	5		
19	6	6		
20	7	7		
21				
22				

Create the **Diff 1** column using the difference between the left-adjacent cell and the cell above that one. Then copy that formula down the remaining cells in the **Diff 1** column.

# Lab 1 - Creating a Spreadsheet

22					
23	Quadratic	$y=x^2$			
24		<b>x</b>	<b>y</b>	<b>Diff 1</b>	<b>Diff 2</b>
25		1	$+A25^2$		
26		2			
27		3			
28		4			
29		5			
30		6			
31		7			
32					

Create the y column with the **exponent 2** and then copy down

23	Quadratic	$y=x^2$			
24		<b>x</b>	<b>y</b>	<b>Diff 1</b>	<b>Diff 2</b>
25		1	1		
26		2	4	3	
27		3	9	$5+C27-C26$	
28		4	16	7	
29		5	25	9	
30		6	36	11	
31		7	49	13	
32					

Add the **Diff 1** & **Diff 2** columns and formulas and then copy down

23	Quadratic	$y=x^2$			
24		<b>x</b>	<b>y</b>	<b>Diff 1</b>	<b>Diff 2</b>
25		1	1		
26		2	4	3	
27		3	9	5	2
28		4	16	7	2
29		5	25	9	2
30		6	36	11	2
31		7	49	13	2
32					

The completed **quadratic** difference table

# Lab 1 - Creating a Spreadsheet

34	Cubic	$y=x^3$					
35	x	y	Diff 1	Diff 2	Diff 3		
36	1	1					
37	2	8	7				
38	3	27	19	12			
39	4	64	37	18	6		
40	5	125	61	24	6		
41	6	216	91	30	6		
42	7	343	127	36	6		
43							
44							
45	Quadratic	$y=x^4$					
46	x	y	Diff 1	Diff 2	Diff 3	Diff 4	
47	1	1					
48	2	16	15				
49	3	81	65	50			
50	4	256	175	110	60		
51	5	625	369	194	84	24	
52	6	1296	671	302	108	24	
53	7	2401	1105	434	132	24	
54							

Finish the Cubic  
and Quartic  
Difference Tables

# Difference Tables

- A difference table calculates the gap between **successive** values of a given function
- For every higher power of the *independent* variable (the domain) we add **another** difference column
- Difference column #2 is the gap between successive values of difference column #1
- We keep adding difference columns until the row values achieve a **steady state**: they are the same for each row
- The **cubic** table needed **3** difference columns – the **quartic** table needed **4** difference columns to achieve **steady state**

# Difference Tables

34	Cubic	$y=x^3$					
35		<u>x</u>	<u>y</u>	<u>Diff 1</u>	<u>Diff 2</u>	<u>Diff 3</u>	
36		1	1				
37		2	8	7			
38		3	27	19	12		
39		4	64	37	18	6	
40		5	125	61	24	6	
41		6	216	91	30	6	
42		7	343	127	36	6	
43							
44							
45	Quadratic	$y=x^4$					
46		<u>x</u>	<u>y</u>	<u>Diff 1</u>	<u>Diff 2</u>	<u>Diff 3</u>	<u>Diff 4</u>
47		1	1				
48		2	16	15			
49		3	81	65	50		
50		4	256	175	110	60	
51		5	625	369	194	84	24
52		6	1296	671	302	108	24
53		7	2401	1105	434	132	24
54							

Keep adding difference columns until the **rightmost** column reaches a **steady** value

# Difference Tables – What They Reveal

		Steady Difference
Constant	$y = 1$	0
Linear	$y = x$	1
Quadratic	$y = x^2$	2
Cubic	$y = x^3$	6
Quartic	$y = x^4$	24

# Difference Tables – What They Reveal

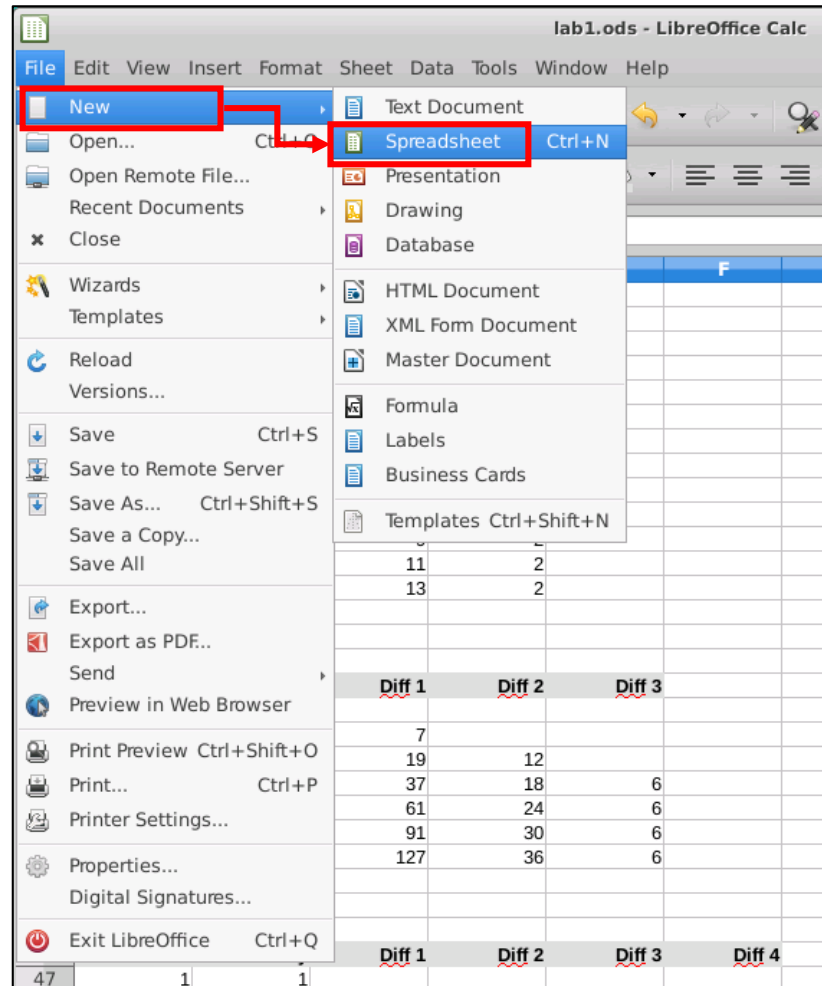
- If we believe a given a set of observations obeys a general underlying law but remains an unknown specific formula, we can use difference tables to systematically reveal the set's hidden functional equation (the generator)
- We start by “guessing” the highest power of  $x$  that would likely be in the underlying generator
- We compare the expected steady state values for each power of  $x$  with the our observed values
- As we determine the coefficient of each decreasing power of  $x$ , we begin to expose the underlying functional equation that originally generated the sequence



## Lab 2

- Find an equation to generate this sequence: **5, 14, 27, 44, 65, 90, 119, 152 ...**
- We will guess this data set is generated by a quadratic formula:  $y = ax^2 + bx + c$
- We have to figure out the values for  $a, b, c$
- We then create difference tables, working *backwards*, starting with a **quadratic**, then a linear table, and then a constant table (if necessary)
- We stop when our model produces **values that match our observations** to a reasonable level of *accuracy*

# Lab 2 – Create a new Spreadsheet



# Calculating the Mean Steady Difference

Untitled 1 - LibreOffice Calc

File Edit View Insert Format Sheet Data Tools Window Help

Liberation Sans 10

SUM  $f(x)$   $\times$   $\leftarrow$  `=average(D6:D11)`

	A	B	C	D	E
1					
2	Quadratic	$y=x^2$			
3	x	y	Diff 1	Diff 2	
4	1	5			
5	2	14	9		
6	3	27	13	4	
7	4	44	17	4	
8	5	65	21	4	
9	6	90	25	4	
10	7	119	29	4	
11	8	152	33	4	
12				=average(D6:D11)	
13					
14					

The **B** column holds your observations

Enter **=AVERAGE** then select the range of cells to include in the average – for every table always put the average cell at the **bottom** row under the **last** difference column

# Mean Difference = Term's Coefficient

2	Quadratic	$y=x^2$		
3	x	y	<u>Diff 1</u>	<u>Diff 2</u>
4	1	5		
5	2	14	9	
6	3	27	13	4
7	4	44	17	4
8	5	65	21	4
9	6	90	25	4
10	7	119	29	4
11	8	152	33	4
12			mean:	4
13				

- The  $y = x^2$  table had an expected steady difference of **2**
- In our sequence we have steady difference mean of **4**
- This means the coefficient for the  $x^2$  term is  $a = \frac{4}{2} = 2$
- So we know the est. generator so far is  $y = 2x^2 + bx + c$

# Delta = Observed - Expected

15	Linear	y=x				
16		x	y Obs	y Est	delta	Diff 1
17		1	5	=+2*A17^2		
18		2	14			
19		3	27			
20		4	44			
21		5	65			
22		6	90			
23		7	119			
24		8	152			
25						

- $y_{obs} = \text{given values}$
- $y_{est} = 2x^2$
- $\Delta = y_{obs} - y_{est}$

15	Linear	y=x				
16		x	y Obs	y Est	delta	Diff 1
17		1	5	2	=+B17-C17	
18		2	14			
19		3	27			
20		4	44			
21		5	65			
22		6	90			
23		7	119			
24		8	152			
25						

15	Linear	y=x				
16		x	y Obs	y Est	delta	Diff 1
17		1	5	2	3	
18		2	14	8	6	=+D18-D17
19		3	27	18	9	
20		4	44	32	12	
21		5	65	50	15	
22		6	90	72	18	
23		7	119	98	21	
24		8	152	128	24	
25						

Add the **Diff 1** column and formula, then copy down all rows

# Delta = Observed - Expected

15	Linear	y=x				
16	x	y Obs	y Est	delta	Diff 1	
17	1	5	2	3		
18	2	14	8	6	3	
19	3	27	18	9	3	
20	4	44	32	12	3	
21	5	65	50	15	3	
22	6	90	72	18	3	
23	7	119	98	21	3	
24	8	152	128	24	3	
25				mean: =+AVERAGE(E18:E24)		
26						

- $y_{obs} = \text{given values}$
- $y_{est} = 2x^2$
- $\Delta = y_{obs} - y_{est}$
- Observed mean steady value = **3**
- Expected linear steady value = **1**
- $b = \frac{\mathbf{3}}{\mathbf{1}} = \mathbf{3}$
- Est. generator is now  $y = 2x^2 + \mathbf{3}x$

# % Relative Error

28	Complete	y=2*x^2+3*x			
29		x	y Obs	y Est	% Err
30		1	5	=+2*A30^2+3*A30	
31		2	14	14	0.00%
32		3	27	27	0.00%
33		4	44	44	0.00%
34		5	65	65	0.00%
35		6	90	90	0.00%
36		7	119	119	0.00%
37		8	152	152	0.00%
38					

Remember to add any final constant term to the **estimated y** function

- ABS = Absolute Value
- $\%_{err} = \left| \frac{(y_{obs} - y_{est})}{y_{obs}} \right|$
- 0% error = perfect fit
- $y = 2x^2 + 3x$

28	Complete	y=2*x^2+3*x			
29		x	y Obs	y Est	% Err
30		1	5	=+(B30-C30)/B30	
31		2	14	14	0.00%
32		3	27	27	0.00%
33		4	44	44	0.00%
34		5	65	65	0.00%
35		6	90	90	0.00%
36		7	119	119	0.00%
37		8	152	152	0.00%
38					

# Changing Cell Number Format

The screenshot shows the LibreOffice Calc interface with the following details:

- Title Bar:** Untitled 1 - LibreOffice Calc
- Menu Bar:** File, Edit, View, Insert, Format, Tools, Data, Window, Help
- Toolbar:** Includes icons for file operations, editing, and formatting. The percentage format icon (a blue square with a white %) is highlighted, and the text "0.0" is visible next to it.
- Formula Bar:** Shows the formula  $=ABS(B29-C29)/B29$  for the selected range D29:D36.
- Spreadsheet Data:**

	A	B	C	D	E	F	G	H	I	J
25										
26										
27	Complete:	$y = 2x^2 + 3x$								
28	x	y Obs	y Est	% err						
29	1	5	5	0.00%						
30	2	14	14	0.00%						
31	3	27	27	0.00%						
32	4	44	44	0.00%						
33	5	65	65	0.00%						
34	6	90	90	0.00%						
35	7	119	119	0.00%						
36	8	152	152	0.00%						
37										
38										
39										
40										

A red callout box points to the percentage format icon in the toolbar with the text: "Highlight a range and click the % icon to format the numbers as percentages".



# Lab 3

- Create a new Lab 3 spreadsheet and generate the difference tables to find the underlying equation that generate this sequence: **36, 103, 244, 489, 868, 1411, 2148, 3109, 4324...**
- Hint: This data set is generated by a cubic formula:

$$y = ax^3 + bx^2 + cx + d$$

- You have to figure out the values for ***a, b, c, d***
- Create difference tables, starting with a **cubic**, then quadratic, then linear, then constant table (if necessary)
- Stop when your model produces **values that match our observations** with 0% relative error
- Create a new worksheet named **Lab 3.ods**

# Lab 3

	A	B	C	D	E
1	Cubic	$y=x^3$			
2	x	y Obs	Diff 1	Diff 2	Diff 3
3	1	36			
4	2	103	67		
5	3	244	141	74	
6	4	489	245	104	30
7	5	868	379	134	30
8	6	1411	543	164	30
9	7	2148	737	194	30
10	8	3109	961	224	30
11	9	4324	1215	254	30
12				mean:	30
13					

		Steady Difference
Constant	$y = 1$	0
Linear	$y = x$	1
Quadratic	$y = x^2$	2
Cubic	$y = x^3$	6
Quartic	$y = x^4$	24

Expected difference for a cubic = 6,  
while observed steady diff mean = 30,  
so coefficient of  $x^3$  must be

$$\frac{30}{6} = 5$$

So far ...  $y = 5x^3 + bx^2 + cx + d$

# Lab 3

	A	B	C	D	E	F
1	Cubic	$y=x^3$				
2		x	y Obs	Diff 1	Diff 2	Diff 3
3		1	36			
4		2	103	67		
5		3	244	141	74	
6		4	489	245	104	30
7		5	868	379	134	30
8		6	1411	543	164	30
9		7	2148	737	194	30
10		8	3109	961	224	30
11		9	4324	1215	254	30
12				mean:	30	
13						
14	Quadratic	$y=x^2$				
15		x	y Obs	y Est	delta	Diff 1
16		1	36	$+5*A16^3$	31	Diff 2
17		2	103	40	63	32
18		3	244	135	109	46
19		4	489	320	169	60
20		5	868	625	243	74
21		6	1411	1080	331	88
22		7	2148	1715	433	102
23		8	3109	2560	549	116
24		9	4324	3645	679	130
25					mean:	14
26						

		Steady Difference
Constant	$y = 1$	0
Linear	$y = x$	1
Quadratic	$y = x^2$	2
Cubic	$y = x^3$	
Quartic	$y = x^4$	

Expected difference for a quadratic = 2, while observed steady diff mean = 14, so coefficient of  $x^2$  must be

$$\frac{14}{2} = 7$$

Now so far ...  $y = 5x^3 + 7x^2 + cx + d$

# Lab 3

Remember to add the new quadratic term to the estimated y function

27	Linear	y=x				
28	x	y Obs	y Est	delta	Diff 1	
29	1	36	=+5*A29^3+7*A29^2			
30	2	103	68	35	11	
31	3	244	198	46	11	
32	4	489	432	57	11	
33	5	868	800	68	11	
34	6	1411	1332	79	11	
35	7	2148	2058	90	11	
36	8	3109	3008	101	11	
37	9	4324	4212	112	11	
38				mean:	11	
39						

		Steady Difference
Constant	y = 1	0
Linear	y = x	1
Quadratic	y = x <sup>2</sup>	
Cubic	y = x <sup>3</sup>	
Quartic	y = x <sup>4</sup>	

Steady difference for a linear = **1**, while observed steady diff mean = **11**, so coefficient of x<sup>2</sup> must be

$$\frac{11}{1} = 11$$

Now so far ...  $y = 5x^3 + 7x^2 + 11x + d$

# Lab 3

40	Constant	y=c			
41	x	y Obs	y Est	delta	
42	1	36	23	13	
43	2	103	90	13	
44	3	244	231	13	
45	4	489	476	13	
46	5	868	855	13	
47	6	1411	1398	13	
48	7	2148	2135	13	
49	8	3109	3096	13	
50	9	4324	4311	13	
51			mean:	13	
52					
53	Complete				
54	x	y Obs	y Est	% Error	
55	1	36	$5 \cdot A55^3 + 7 \cdot A55^2 + 11 \cdot A55 + 13$		
56	2	103	103	0.00%	
57	3	244	244	0.00%	
58	4	489	489	0.00%	
59	5	868	868	0.00%	
60	6	1411	1411	0.00%	
61	7	2148	2148	0.00%	
62	8	3109	3109	0.00%	
63	9	4324	4324	0.00%	
64					

If delta values are all the same, then that value is the final constant term

Functional Equation

$$y = 5x^3 + 7x^2 + 11x + 13$$

with  $x \in \mathbb{Z}^+$

Generates the sequence:

**36, 103, 244, 489, 868,  
1411, 2148, 3109, 4324...**

# Lab 4



Elapsed Time (10 mins each)	Observed Counter
1	205
2	430
3	677
4	945
5	1233
6	1542
7	1872
8	2224

- This case study will use data from an experiment that measured the **counter on a tape machine vs. the elapsed time** the tape had been played
- Ideally this would be a linear relationship – but due to the changing circumference of a tape reel as it is played, the drive motor does not maintain consistent timing, so it is **non-linear**

# Lab 4



Elapsed Time (10 mins each)	Observed Counter
1	205
2	430
3	677
4	945
5	1233
6	1542
7	1872
8	2224

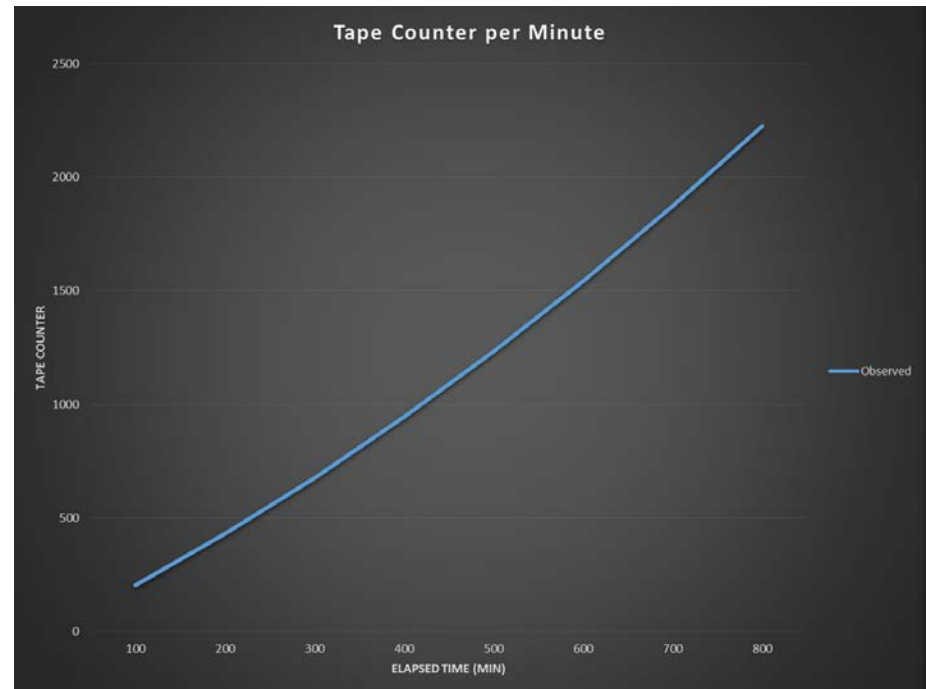
- Find an equation to model a tape counter as a function of playing time
  - X value is the number of 10 minute blocks the tape has been playing from the beginning
  - Y value is the counter on the tape player (linear feet)
- With a good fitting model we can answer questions like:  
Where should we stop the tape to be 65 minutes into the recording?

# Lab 4



Assume  
 $y = ax^2 + bx + c$

Elapsed Time (10 mins each)	Observed Counter
1	205
2	430
3	677
4	945
5	1233
6	1542
7	1872
8	2224





# Lab 4

1	Quadratic	y=x^2			
2		x	y Obs	<u>Diff 1</u>	<u>Diff 2</u>
3		1	205		
4		2	430	225	
5		3	677	247	22
6		4	945	268	21
7		5	1233	288	20
8		6	1542	309	21
9		7	1872	330	21
10		8	2224	352	22
11				mean:	21.1667

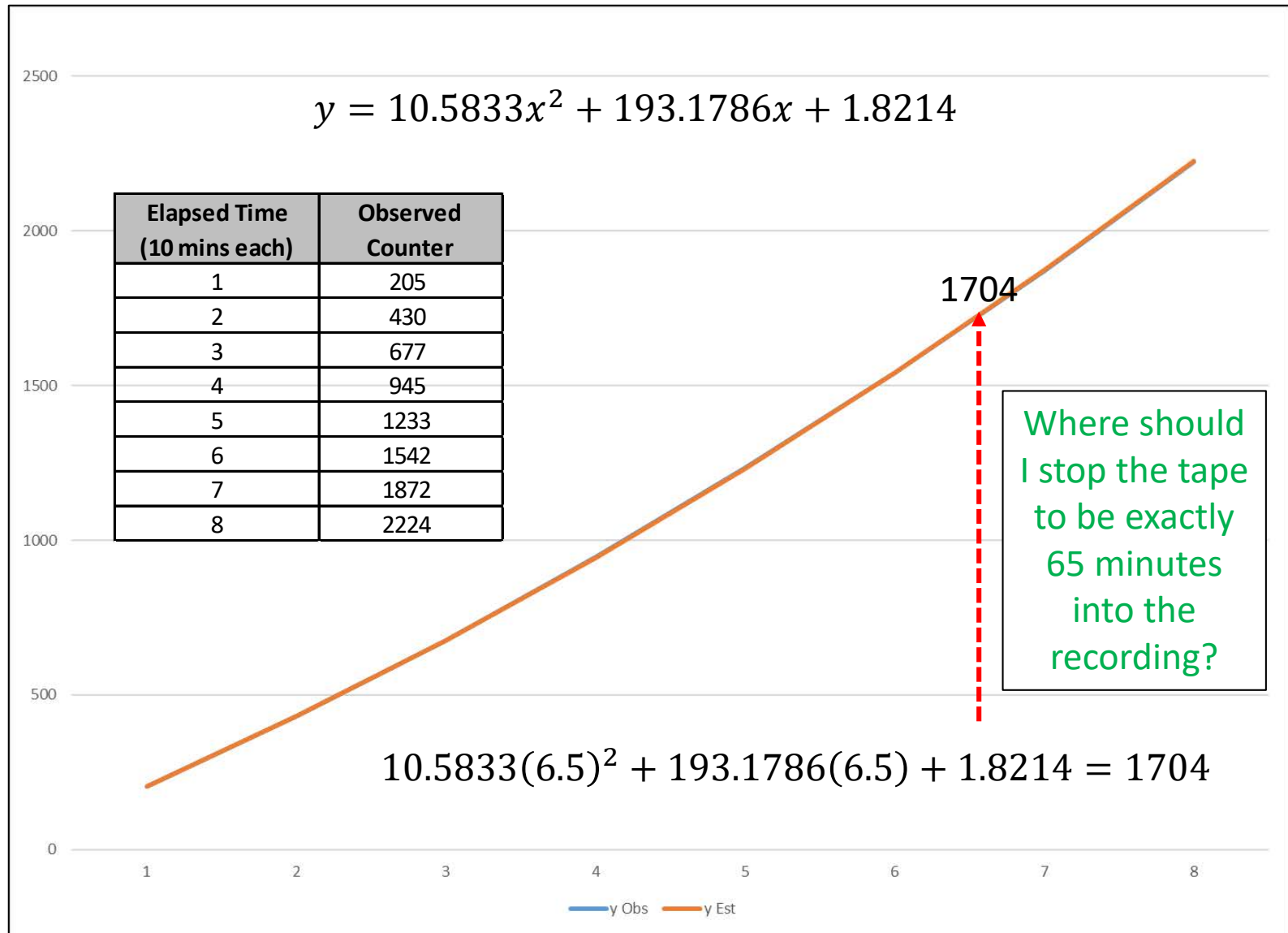
13	Linear	y=x			
14		x	y Obs	y Est	delta
15		1	205	10.5833	194.4167
16		2	430	42.3333	387.6667
17		3	677	95.2500	581.7500
18		4	945	169.3333	775.6667
19		5	1233	264.5833	968.4167
20		6	1542	381.0000	1,161.0000
21		7	1872	518.5833	1,353.4167
22		8	2224	677.3333	1,546.6667
23					mean:
24					193.1786

25	Constant	y=c			
26		x	y Obs	y Est	delta
27		1	205	203.7619	1.2381
28		2	430	428.6905	1.3095
29		3	677	674.7857	2.2143
30		4	945	942.0476	2.9524
31		5	1233	1,230.4762	2.5238
32		6	1542	1,540.0714	1.9286
33		7	1872	1,870.8333	1.1667
34		8	2224	2,222.7619	1.2381
35				mean:	1.8214

38	Complete				
39		x	y Obs	y Est	% Err
40		1	205	205.5833	-0.2846%
41		2	430	430.5119	-0.1190%
42		3	677	676.6071	0.0580%
43		4	945	943.8690	0.1197%
44		5	1233	1,232.2976	0.0570%
45		6	1542	1,541.8929	0.0069%
46		7	1872	1,872.6548	-0.0350%
47		8	2224	2,224.5833	-0.0262%

$$y_{est} = 10.5833x^2 + 193.1786x + 1.8214$$

# Lab 4



# Lab 5 - Method of Least Squares

- Developed by Gauss, least squares finds the coefficients of a polynomial of a given degree that **approximates** a set of observations with **minimal variance** from the data
- The modeler selects a curve whose **general shape** matches the trend of the data
- The **partial derivatives** of the chosen polynomial are then determined which leads to a system of linear equations that can be solved using matrices and **Cramer's Rule**
- The coefficients of each term of the model polynomial can then be determined to allow us to estimate the unknown function values

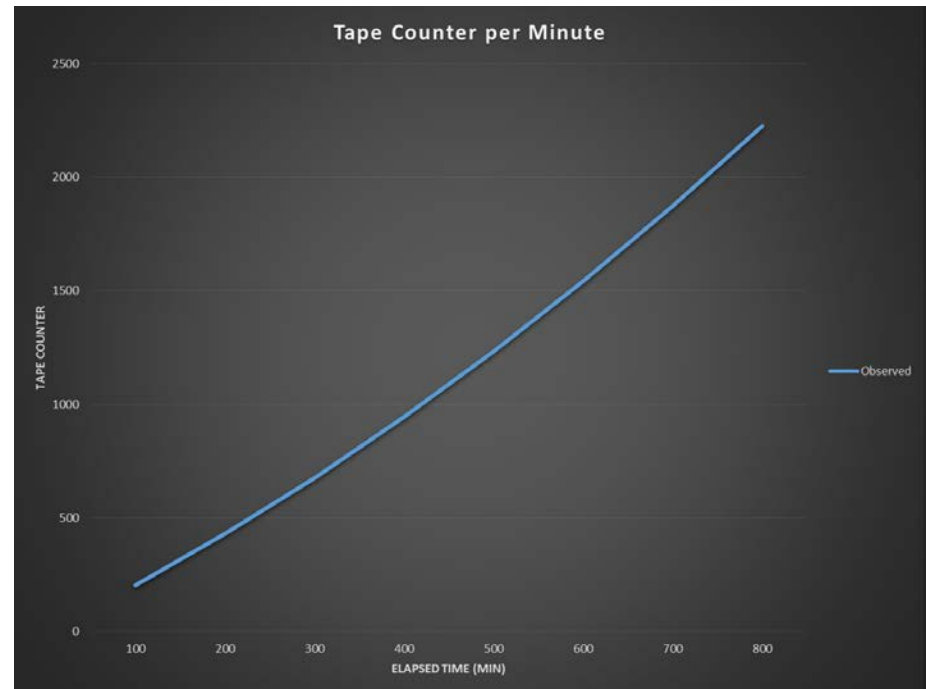
# Lab 5 - Method of Least Squares



Assume

$$y = ax^2 + bx + c$$

Elapsed Time (10 mins each)	Observed Counter
1	205
2	430
3	677
4	945
5	1233
6	1542
7	1872
8	2224



# Lab 5 - Method of Least Squares

$$\text{Minimize } S = \sum_{i=1}^n [y_i - (ax_i^2 + bx_i + c)]^2$$

$$(y - ax^2 - bx - c)(y - ax^2 - bx - c)$$

$$y^2 - ax^2y - bxy - cy$$

$$-ax^2y$$

$$-bxy$$

$$-cy$$

$$+ a^2x^4 + abx^3 + acx^2$$

$$+ abx^3$$

$$+ acx^2$$

$$+ b^2x^2 + bcx$$

$$+ bcx + c^2$$

$$S = y^2 - 2ax^2y - 2bxy - 2cy + a^2x^4 + 2abx^3 + 2acx^2 + b^2x^2 + 2bcx + c^2$$

## Lab 5 - Method of Least Squares

$$\text{Minimize } S = \sum_{i=1}^n [y_i - (ax_i^2 + bx_i + c)]^2$$

$$S = y^2 - 2ax^2y - 2bxy - 2cy + a^2x^4 + 2abx^3 + 2acx^2 + b^2x^2 + 2bcx + c^2$$

For S to have a minimum, these partial derivatives must exist:

$$\frac{\partial S}{\partial a} = 0, \frac{\partial S}{\partial b} = 0, \frac{\partial S}{\partial c} = 0$$

$$\frac{\partial S}{\partial a} = -2x^2y + 2ax^4 + 2bx^3 + 2cx^2 = 0$$

$$\frac{\partial S}{\partial b} = -2xy + 2ax^3 + 2bx^2 + 2cx = 0$$

$$\frac{\partial S}{\partial c} = -2y + 2ax^2 + 2bx + 2c = 0$$

## Lab 5 - Method of Least Squares

$$\text{Minimize } S = \sum_{i=1}^n [y_i - (ax_i^2 + bx_i + c)]^2$$

$$\begin{aligned}\frac{\partial S}{\partial a} &= -2x^2y + 2ax^4 + 2bx^3 + 2cx^2 = 0 \\ (x^4)a + (x^3)b + (x^2)c &= x^2y\end{aligned}$$

$$\begin{aligned}\frac{\partial S}{\partial b} &= -2xy + 2ax^3 + 2bx^2 + 2cx = 0 \\ (x^3)a + (x^2)b + (x)c &= xy\end{aligned}$$

$$\begin{aligned}\frac{\partial S}{\partial c} &= -2y + 2ax^2 + 2bx + 2c = 0 \\ (x^2)a + (x)b + c &= y\end{aligned}$$

## Lab 5 - Method of Least Squares

$$\text{Minimize } S = \sum_{i=1}^n [y_i - (ax_i^2 + bx_i + c)]^2$$

**This is a system of 3 linear equations and 3 unknowns!**

$$\begin{array}{lcl} \left( \sum x_i^4 \right) a + \left( \sum x_i^3 \right) b + \left( \sum x_i^2 \right) c & = & \left( \sum x_i^2 y_i \right) \\ \left( \sum x_i^3 \right) a + \left( \sum x_i^2 \right) b + \left( \sum x_i \right) c & = & \left( \sum x_i y_i \right) \\ \left( \sum x_i^2 \right) a + \left( \sum x_i \right) b + (n)c & = & \left( \sum y_i \right) \end{array}$$



## Open Lab 5 - Method of Least Squares

$$\text{Minimize } S = \sum_{i=1}^n [y_i - (ax_i^2 + bx_i + c)]^2$$

$$\left(\sum x_i^4\right)a + \left(\sum x_i^3\right)b + \left(\sum x_i^2\right)c = \left(\sum x_i^2 y_i\right)$$

$$\left(\sum x_i^3\right)a + \left(\sum x_i^2\right)b + \left(\sum x_i\right)c = \left(\sum x_i y_i\right)$$

$$\left(\sum x_i^2\right)a + \left(\sum x_i\right)b + (n)c = \left(\sum y_i\right)$$

```
double sumX = PowerSum(vecX, 1);
double sumX2 = PowerSum(vecX, 2);
double sumX3 = PowerSum(vecX, 3);
double sumX4 = PowerSum(vecX, 4);

double sumY = PowerSum(vecY, 1);

double sumXY = PowerSum(vecX, 1, vecY);
double sumX2Y = PowerSum(vecX, 2, vecY);

double coeffMatrix[3][3]{
    { sumX4, sumX3, sumX2},
    { sumX3, sumX2, sumX },
    { sumX2, sumX, 8 } };

double valueVector[3]{ sumX2Y, sumXY, sumY };
```

We have 8 sample points  
in the Lab 5 data set

## View Lab 5 - Method of Least Squares

```
double a = detA / detCoeff;  
double b = detB / detCoeff;  
double c = detC / detCoeff;
```

$$y = ax^2 + bx + c$$

```
cout << "a = " << setw(10) << setprecision(4) << fixed << a << endl;  
cout << "b = " << setw(10) << setprecision(4) << fixed << b << endl;  
cout << "c = " << setw(10) << setprecision(4) << fixed << c << endl;
```

```
cout << endl << "Actual vs. Estimate" << endl;  
cout << setw(6) << "X";  
cout << setw(12) << "Act";  
cout << setw(12) << "Est";  
cout << setw(10) << "Err" << endl;
```

```
for (int i{}; i < 8; ++i) {  
    double yp = a * pow(vecX[i], 2) + b * vecX[i] + c;  
    double err = abs(vecY[i] - yp) / vecY[i];  
    cout << setw(6) << i;  
    cout << setw(12) << vecY[i];  
    cout << setw(12) << yp;  
    cout << setw(10) << setprecision(4) << err << endl;
```

# Run Lab 5 - Method of Least Squares

```
quadratic-regression
File Edit View Terminal Tabs Help
DetCoeff = 56448

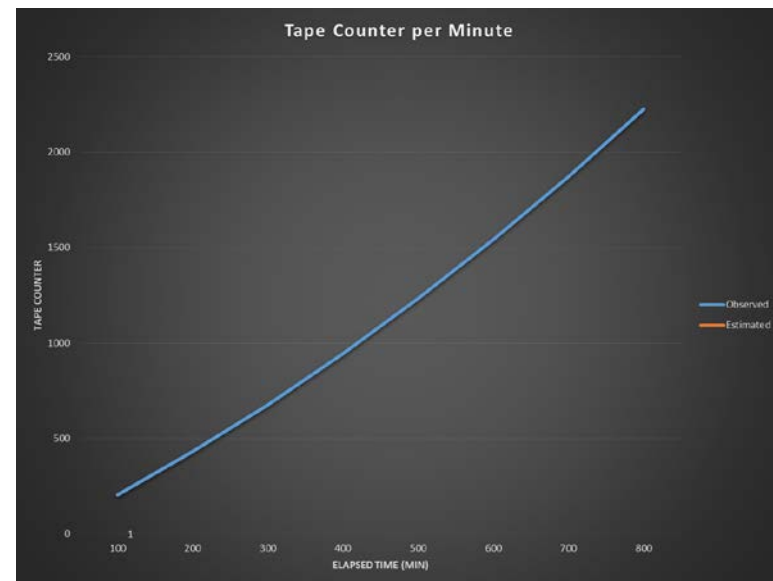
DetA = 590688.0000
DetB = 10963680.0000
DetC = 8064.0000

a = 10.4643
b = 194.2262
c = 0.1429

Actual vs. Estimate
X      Act      Est      % Err
0      205.0000  204.8333  0.0813 %
1      430.0000  430.4524  0.1052 %
2      677.0000  677.0000  0.0000 %
3      945.0000  944.4762  0.0554 %
4      1233.0000 1232.8810  0.0097 %
5      1542.0000 1542.2143  0.0139 %
6      1872.0000 1872.4762  0.0254 %
7      2224.0000 2223.6667  0.0150 %

Process returned 0 (0x0)  execution time : 0.012 s
Press ENTER to continue.
```

Elapsed Time (10 mins each)	Observed Counter	Estimated Counter
1	205	204.8333
2	430	430.4524
3	677	677.0000
4	945	944.4762
5	1233	1232.8810
6	1542	1542.2143
7	1872	1872.4762
8	2224	2223.6667



$$y = 10.4643x^2 + 194.2262x + 0.1429$$

# Verify Lab 5 - Method of Least Squares

via Difference Tables

$$y = 10.5833x^2 + 193.1786x + 1.8214$$

via Least Squares

$$y = 10.4643x^2 + 194.2262x + 0.1429$$

x	y Obs	y Est DT	% Err	y Est LS	% Err
1	205	205.5833	-0.2846%	204.8334	0.0813%
2	430	430.5119	-0.1190%	430.4525	-0.1052%
3	677	676.6071	0.0580%	677.0002	0.0000%
4	945	943.8690	0.1197%	944.4765	0.0554%
5	1233	1,232.2976	0.0570%	1232.8814	0.0096%
6	1542	1,541.8929	0.0069%	1542.2149	-0.0139%
7	1872	1,872.6548	-0.0350%	1872.477	-0.0255%
8	2224	2,224.5833	-0.0262%	2223.6677	0.0149%
		mean:	-0.0279%		0.0021%

The **method of least squares** guarantees the tightest possible fit between the observed data and the polynomial form chosen to model the data

## Now you know...

- Model fitting starts by assuming the degree of an appropriate curve that reasonably matches the data
- How to create **difference tables** for constant, linear, quadratic, cubic, and quartic terms along with their expected average
- Gauss's "**Method of Least Squares**" refers to shaping the approximating curve to *minimize the total deviations* between the observed data and points on that curve
  - The function to minimize must be expanded, and then **partial derivatives** must be found for each coefficient of the curve
- The **% relative error** measures the "goodness of fit" of a model to experimental observations