To Plot a Graph in Origin

Example: Number of Counts from a Geiger-Müller Tube as a Function of Supply Voltage

Digression on Error Bars

- What entity do you use for the magnitude of the error bars?
- Standard Deviation
 - Assumes data are "normally distributed"
 - A given measurement has a 68% probability of falling within σ of the mean of the measurements
 - It has a 95.5% probability of falling within $2x\sigma$.
 - Standard deviation only gives information about how close to the mean any given measurement can be expected to be.
 - Value of standard deviation depends little on number of measurements
 - Standard deviation is not useful for generating error bars.

Error Bars

- Standard Deviation of the Mean (SDoM)
 - Aka "Standard Error of the Mean"
 - Refers to the distribution of means (averages) of a series of measurements about the population mean.
 - Remember that the population mean is what you get by taking a census of all members of the population
 - There is a 68% probability that the mean of your measurements lies within one standard deviation of the mean of the true mean of the entire population. Get that?
- Good news: Mean of measurements approaches population mean with increasing number of measurements
- Bad news: Only approaches as $1/\sqrt{N}$
- SDoM approaches zero with increasing number of measurements

Error Bars

- The entity you want to plot as error bars is the Standard Deviation of the Mean ("Standard Error" for Origin).
 - Excel will calculate the Standard Deviation of a series of data/measurements
 - Excel will also determine the number of measurements
 - Rarely useful
 - How would you not know how many data you took?
 - Not equal to number of rows of data in Excel?

- SDoM = SD/SQRT(N)

Back to Plotting in Origin with Error Bars

- File:New or the New Project icon (next slide)
- Enter data (two slides down)
 - Manually (e.g. Pendulum)
 - Copy and paste
 - From Excel...
 - Data

Getting Started in Origin



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Plotting in Origin, cont'd

- Data to be plotted horizontally ("independent variable") must be in first column set as X or you may use another column set as Y and change it to X
- Data to be plotted vertically ("dependent variable", typically multiple measurements thereof) must be in columns to right of x-values
- If initial format is opposite (e.g. Geiger data)
 - Worksheet:Transpose: Open Dialog:Ok (two slides down)

Format for generating mean, SD and SDoM

- Block all (only) data for statistical analysis...click and drag...like blocking in any program?
- Statistics:Descriptive statistics:Statistics on rows (or "on columns" if your data are displayed in that way) :Open dialog
 - De-select everything, specifically including the "Optional Report" and "Quartiles", except Mean, SD and (add) Standard Error of Mean.
- Ok
- Mean, Standard Deviation and Standard Error of Mean will appear in columns to the right of data or in a new sheet

"Independent variable" values				Mul dep	tiple end	e val ent	lues varia	of able		N	lear	۱	SD	oM
Book1														
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4	480	671	688	735	702	715	715	692	721	714	718	707.1	18.81164	5.94876
5	500	742	739	725	719	725	709	701	693	716	737	720.6	16.35848	5.17301
6	520	723	744	739	736	746	750	736	764	724	757	741.9	13.16097	4.16186
7	540	773	745	714	725	736	742	745	752	717	658	730.7	30.89786	9.77076
8	560	789	719	741	797	775	774	770	776	753	725	761.9	26.38792	8.34459
9	580	734	712	761	736	785	751	750	756	807	730	752.2	27.64778	8.743
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- Block the first column [A(x)], [CTRL: click above column] the third from last [Mean] and last [SE of Mean] columns
- Plot:Line:Scatter
- If you double click on the plot (line or point) a menu appears allowing you to choose line and line+symbol curve, line or symbol shape, size and color, etc.
 - If your data are any good you will have to choose much smaller symbols to see your error bars!

Voilà! A plot!



Changing Plotting Parameters

- Double click on axes to change parameters therein
- Click on "T" on the left bar to add text (like the title of your graph!)
- If you entered text for "Long name" and "Units" in the headers of the "Sheet" in the "Book" they will appear as axis labels.

Adjust Axis Parameters



Adjust Plot Details



Adding a Legend





Column Manipulations

Select column where results are to appear, here B. Click the icon to "Set column values" Syntax: You are telling the program to generate in the new column rows whose values are the result of operating on the adjacent values in the named column [in this case col(A)] in the specified manner [in this case squared

Linear Least Squares Fitting

- Plot data!
- Analysis: Fitting: Linear Fit: Open Dialog
 - "Residual sum of squares" is another name for chi squared
 - Check "R-value" or "R-square" (this is the correlation coefficient)
 - Assure that it is checked!
 - Also check "Reduced chi Sqr" (for G-M experiment)
 - Also assure that Residual Analysis: Regular is checked
 - Uncheck the "Adj. R-Square" and "Pearson's r" (their formulas are not the typical ones for the correlation coefficient R or r)

- Alternatively
 - Enter all data into Excel
 - Calculate mean, Standard Deviation and Standard Deviation of the Mean
 - Transfer relevant rows to empty Book in Origin
 - Worksheet/Transpose/Dialog/OK
- Plot:Line:scatter
- Select columns to plot
 - A(X) for X
 - B(Y) for Y
 - C2(Y) for YEr
- Adjust symbols, line, axes and labels as appropriate
- Use "T" icon on left to generate plot label

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Histogram of the Residual Plot

Residual vs. Predicted Values Plot

Residual vs. the Order of the Data Plot

Residual Lag Plot

Parameters for Linear Fit: lower

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Plotted Data with Fit and Error Bars

Example: pendulum experiment



- Info about the linear fit (from previous slide graph):

Equation	y = A + Bx			
Weight	Instrumental			Considering error bars
Residual Sum of Squares	0.35095			Chi-squared ($\chi 2$) considering error bars
R-value	0.99951			Correlation coefficient (<i>r</i> or <i>R</i>)
		Value	Standard Error	Value and Absolute error
А	Intercept	0.05004	0.01975	
В	Slope	0.03962	5.18244E-4	

Residual Plot with Error Bars

- Residual values will appear as a new column in the sheet "FitLinearCurve1"
- Retrieve error bar magnitudes from original calculations [column SEM(yEr)]
- Plot residual values with error bars as a function of y-data as usual

A3(X2) 🔒	A4(Y2)	A(Y2)	
Independent Variable	Regular Residual of Sheet1 C"Y"	Error bars	
1	0.01/74	0.34	
2	-0.30879	0.68	
3	0.55795	1.02	
4	0.52993	1.36	
5	-0.27298	1.7	
6	1.20008		ta for
7	-3.66752		
8	0.78302		
9	2.06146	l Ke	esidual Plot:
10	3.06399		
11	-5.2316	🗌 Fit	linearCurve1
12	0.91976		
13	-4.87794	Ch	oot
14	-7.84186		eel
15	5.47137	5.1	
16	0.73543	5.44	
17	0.65829	5.78	
18	4.92268	6.12	
19	5.60616	6.46	
20	-2.40591	6.8	27

Test Fit Residuals with Error Bars



Residual plot for the example on slide 24 (pendulum experiment)

Plotting $Re = T^2 - T^2_{fit}$ vs. / with error bars for δT^2 :



Generating and Fitting a Histogram

- Import data to be plotted into a Y-column of a new book/worksheet.
 - The x-column doesn't work, even if you have only one set of data to generate a histogram. Don't ask.
- Block those data (CTRL click above column)

To Plot a Histogram

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Initial Histogram



Example of axis labels for the Geiger-Müller experiment



Histogram with Gaussian Overlay



34

Histogram Fit Sheet

	BinCenters(X	Counts(Y	CumulativeSum(Y	CumulativeProbab(Y	A(X2)	B(Y2) 健
Long Name	Bin Centers	Counts	Cumulative Sum	Cumulative Probability	Distri	bution	Normal
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Comments	Bins	Bins	Bins	Bins			Mean= 103.66, SD=9.2705899695671
1	81.5	0	0	0			
2	84.5	3	3	3	80.	Mea	n and Standard
3	87.5	1	4	4	80	Devi	ation: You have
4	90.5	5	9	9	80.	tho f	it Gaussian
5	93.5	7	16	16	80	the	
6	96.5	8	24	24	80.	25025	0.53247
7	99.5	13	37	37	80	.3003	0.53977
8	102.5	15	52	52	80.	35035	0.54716
9	105.5	11	63	63	80	0.4004	0.55463
10	108.5	12	75	75	80.	45045	0.56218
11	111.5	13	88	88	80	.5005	0.56982
12	114.5	1	<mark>8</mark> 9	89	80.	55055	0.57755
13	117.5	6	95	95	80	0.6006	0.58537
14	120.5	1	96	96	80.	65065	0.59328
15	123.5	1	97	97	80	0.7007	0.60127
16	126.5			97	80.	75075	0.60935
17	129.5	New she	eet with fit data	a 100	80	8008.	0.61753
18					80.	85085	0.6258
19					80	.9009	0.63415

Generating a Function

Sometimes you want to plot a function over some interval

- Enter the first few values of the independent variable (next slide)
- Block those values
- Set the cursor at the bottom right of the column until the cursor becomes a plus sign (next slide)
- Drag the cursor down for the number of rows corresponding to the range of x that you want to plot
 - To increase the number of rows, click on the bottom cell and hit Enter
- Block column to be used for dependent values
- Set column values: enter expression for function to be plotted
- Plot!
- Adjust axes, titles and legend to suit taste.

Example: $Y = X^3$ for -10 < X < 10

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	1	-10		
	2	-9.5		
	3	-9	1	
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	5			
	6			

Enter 2-3 values and block Move cursor to bottom right corner of cell (+)

20	-0.5				
21	0				
22	0.5				
23	1				
24	1.5				
25	2				
26	2.5				
27	3				
28	3.5				
29	4				
30	4.5				
31	5				
32	5.5				
33	6				
34	6.5				
35	7				
36	7.5				
37	8				
38	8.5				
39	9				
40	9.5				
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5	-91.125	Recalculate Manual 👻
4	-64	
5	-42.875	

A(X)

-7

Enter the cube of the value in col(A) in the blocked column

Voilà!



Integrating with Origin

- Useful analyzing optical data
 - Integrated intensity of an emission peak
- Chemical analysis: finding the total amount of material from an absorption curve
 - Beer's Law
 - Concentration is proportional to absorbance
- Easier and more accurate than olden times when Professor Lüty plotted data an paper, cut out curve with scissors and weighed paper!

Mercury Emission Spectrum

<u> 150 -</u>

Model: Integrated emission intensity is proportional to spectrometer slit width To test model we need to be able to calculate the integrated intensity!

Hg Emission Spectrum Nominal 2 micron slits FWHMA = 0.18 A







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Multiple Plots on a Graph

- Most common: several values of y with a common x
 - Import data
 - Simply block copy and import from Excel
 - File:Import:Multiple ASCII
 - Assumes data are in ASCII format!
 - Requires manipulation of columns after importing
 - You will have multiple columns with one headed by X and the others Y1, Y2...
 - Label each column and give units
 - Block contents of each column to be plotted (click above)
 - Plot: Line and symbol: Line and symbol



Multiple Plots, Continued

- If multiple plots have different x values
 - Obviously now you have at least four columns of data
 - Double click on the header cell of your second set of x-values
 - Designate second column as x

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Miscellany and Minutiae

- Huge amounts of stuff can be accessed by right clicking
 - The menu you get depends on where the cursor is pointed when you right click
- If your graph fills the screen you can reduce it and access the book/worksheet by clicking the expand/contract icon in the upper right
- What else belongs here? Lots!

- To add Greek or other special characters to a text box
 - CTRL M
 - Note that there is only one page of options