

Linear Regression

Standard error of a slope

From RLS to Trumpets

RLS = Robust Least Squares

Trumpets = Calculate Upper and Lower 95% Confidence Limits

There are two regression
worksheets: RLS and Trumpets

CH 452 (001) FALL 2021

- Participants
- Grades
- Week 1 - Introductory Material and Course Logistics
- Week 2 - Practice Lab & Distributions Computer Lab
- Week 3 - Lab Experiment 1
- Week 4 - Computer lab 3
- Week 5 - Lab Experiment 2
- Week 6 - Lab

Week 1 - Introductory Material and Course Logistics

- CH452 Zoom meetings link
- CH452- Syllabus Fall 2021
- Excel Macros sheets**
- Data Recording AND Reporting
 - Find in this book detailed instructions about writing a lab report as well as links to oral presentation and written lab report RUBRICS.
- Homework#1- Data Recording AND Reporting- UPLOAD
UPLOAD here your annotated graded sample lab report
- Introduction to Statistics, Rounding - the Rule of 2 and 15- AND Propagation of Error
- Homework#2 - Rounding - the Rule of 2 and 15 AND Propagation of Error - UPLOAD
- 8/20 CH452 - Pre-assessment
- Introduction to Statistics - (Intro, Error types, Physical measurements and

Calendar

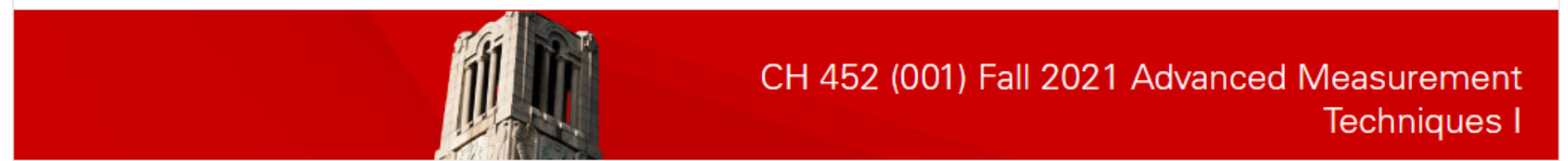
August 2021

Mon	Tue	Wed	Thu	Fri	Sat	Sun
						1
2	3	4	5	6	7	8
9	10	11	12	13	14	15
16	17	18	19	20	21	22
23	24	25	26	27	28	29
30	31					

- Hide site events
- Hide category events
- Hide course events
- Hide group events
- Hide user events
- Hide other events

- ### Activities
- Assignments
 - Forums
 - Quizzes

- CH 452 (001) FALL 2021
- Participants
- Grades
- Week 1 - Introductory Material and Course Logistics**
- Week 2 - Practice Lab & Distributions Computer Lab
- Week 3 - Lab Experiment 1
- Week 4 - Computer lab 3
- Week 5 - Lab Experiment 2
- Week 6 - Lab



WolfWare / Dashboard / My courses / CH 452 (001) FALL 2021 / Week 1 - Introductory Material and Course Logistics / Excel Macros sheets

Excel Macros sheets

- RLSmacro.xls ←
- SolvStat.xls
- trumpetExcel.xls ←

Downloads of the Excel Spreadsheets

Download folder Edit

◀ CH452- Syllabus Fall 2021

Jump to...

Data Recording AND Reporting ▶

Let's follow the download of the trumpets

Airplane mode off

- CH 452 (001) FALL 2021
- Participants
- Grades
- Week 1 - Introductory Material and Course Logistics**
- Week 2 - Practice Lab & Distributions Computer Lab
- Week 3 - Lab Experiment 1
- Week 4 - Computer lab 3
- Week 5 - Lab Experiment 2
- Week 6 - Lab



CH 452 (0

WolfWare / Dashboard / My courses / CH 452 (001) FALL 2021 / Week 1 - Introducto

Excel Macros sheets

- RLSmacro.xls
- SolvStat.xls
- trumpetExcel.xls

Download folder Edit

◀ CH452- Syllabus Fall 2021

Jump to... ▾

Data Recording AND Reporting ▶

Opening trumpetExcel.xls

You have chosen to open:

trumpetExcel.xls
 which is: Microsoft Excel 97-2003 Worksheet (52.5 KB)
 from: https://moodle-courses2122.wolfware.ncsu.edu

What should Firefox do with this file?

Open with Excel 2016 (default) ▾

Save File

Do this automatically for files like this from now on.

OK Cancel

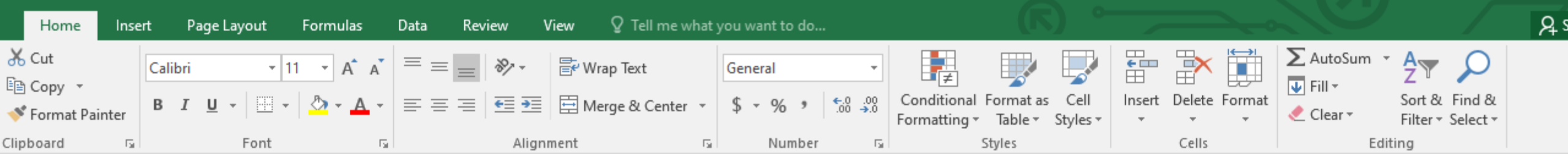
Download Trumpet Excel

Trumpets: the confidence limits of a line

The calibration error can statistically be represented by drawing the 95% **confidence** limits around the calibration line. These limits form the two branches of a hyperbolic function. The two sets of hyperbolic branches are given by:

$$Y_{confidence} = sX + b \pm t RMSE \sqrt{\frac{1}{N} + \frac{N(X - \bar{X})^2}{N \sum X^2 - (\sum X)^2}}$$

These are the trumpets. The t is determined using the t-test.



= $\$L\$11+\$K\$11*B11$

A B C D E F G H I J K L M N O P Q R S T U V
 standard addition you take an unknown as *spike it*
 th the chemical you want to analyse

Trumpets

Decent ones
(first graph'em)

formula for approximate
confidence limits

$a = t * RMSE / slop_m * Sqrt((X*X* n +$
 Where X is the calibrated value you re
 $DD = n * sum(x^2) - (sum(x))^2$
 n=number of calibration samples =df+2
 summations are over the x-calibration
 (Notice the difference with last page?)

We are using the standard data
 We can ignore the Pred limits for
 our purposes.

added	meas	fit	Conf95%+	Conf95%-	Pred95%+	Pred95%-
0	0.12266	0.13713	0.16402	0.11023	0.1875	0.08675
0.1	0.25097					
0.2	0.31211					
0.5	0.57296					
0.7	0.76219					
1	1.03219					

Fill by defining the area

slope	0.89213	0.13713
intercept	0.01773	0.00969
se slope	0.99842	0.01534
se intc	2530.83	4
R-square	0.59559	0.00094
RMSE (sy)	avg(x)	0.41667
df	sum(x)	2.5
	sum(x ²)	1.79
	t-value	2.77645
	n*sum(x ²)	4.49

File Home Insert Page Layout Formulas Data Review View Tell me what you want to do...

Clipboard: Paste, Cut, Copy, Format Painter

Font: Calibri, 11, Bold, Italic, Underline, Text Color, Background Color

Alignment: Wrap Text, Merge & Center

Number: General, Currency, Percentage, Decimals

Styles: Conditional Formatting, Format as Table, Cell Styles

Cells: Insert, Delete, Format

Editing: AutoSum, Fill, Clear, Sort & Filter, Find & Select

B11: 0

In standard addition you take an unknown as *spike it* with the chemical you want to analyse

It is convenient to graph the x, y, y_calc and y_upper and y_lower to plot on a clean sheet

Trumpets

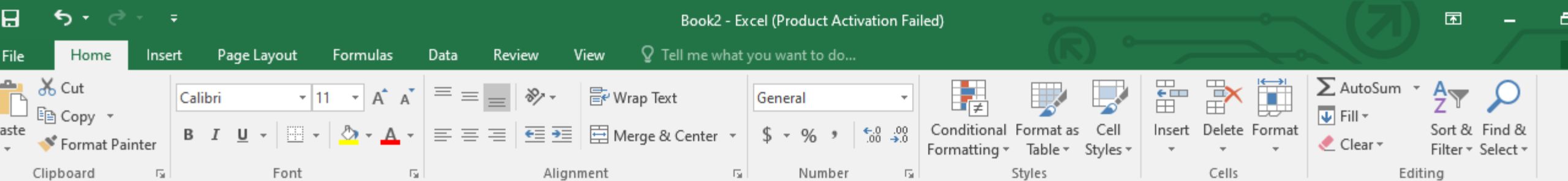
Decent ones (first graph'em)

formula for approximate confidence limits

$a = t^* \text{RMSE} / \text{slop}_m * \text{Sqrt}(\text{DD} = n * \text{sum}(x^2) - (\text{sum}(x))^2)$

Where X is the calibrated value
 $n = \text{number of calibration sam}$
 summations are over the x-co
 (Notice the difference with la

added	meas	fit	Conf95%+	Conf95%-	Pred95%+	Pred95%-	slope	intercept		
0	0.12266	0.13713	0.16402	0.11023	0.1875	0.08675	0.89213	0.13713		
0.1	0.25097	0.22634	0.24969	0.20298	0.27491	0.17776	se slope	0.01773	0.00969	se intc
0.2	0.31211	0.31555	0.33595	0.29515	0.36278	0.26833	R-square	0.99842	0.01534	RMSE (sy)
0.5	0.57296	0.58319	0.60106	0.56532	0.62938	0.537	2530.83	4	df	
0.7	0.76219	0.76162	0.78391	0.73932	0.80969	0.71354	0.59559	0.00094		
1	1.03219	1.02925	1.06283	0.99568	1.08349	0.97502	avg(x)	0.41667		
							sum(x)	2.5		
							sum(x ²)	1.79		
							t-value	2.77645		
							n*sum(x ²)	4.49		



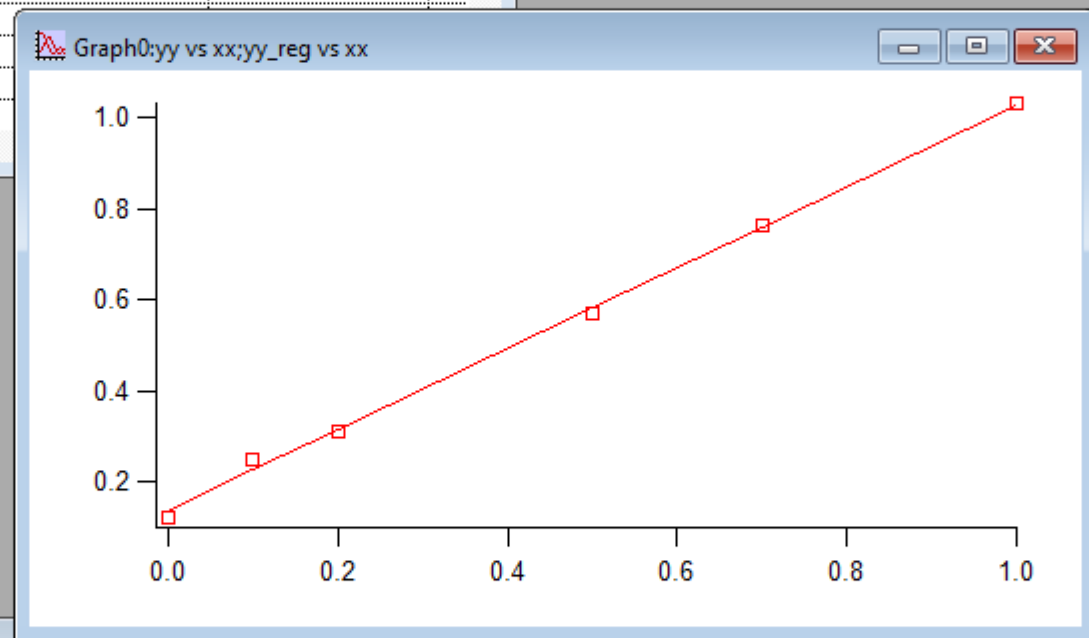
0

A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
0	0.12266	0.137126	0.164019	0.110233															
0.1	0.250966	0.226339	0.249694	0.202984															
0.2	0.31211	0.315552	0.335952	0.295152															
0.5	0.572956	0.58319	0.601056	0.565324															
0.7	0.76219	0.761616	0.783908	0.739323															
1	1.032195	1.029254	1.062829	0.99568															

Paste the data. I do not like Excel scatterplot for more than two columns. I will show you this in Igor. Igor is downloadable under tools. We have a group license. Ask me or Yuan.

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Paste the data. I do not like Excel scatterplot with more than two columns. I will show you this in Igor. Igor is downloadable under tools. We have a group license. Ask me or Yuan.



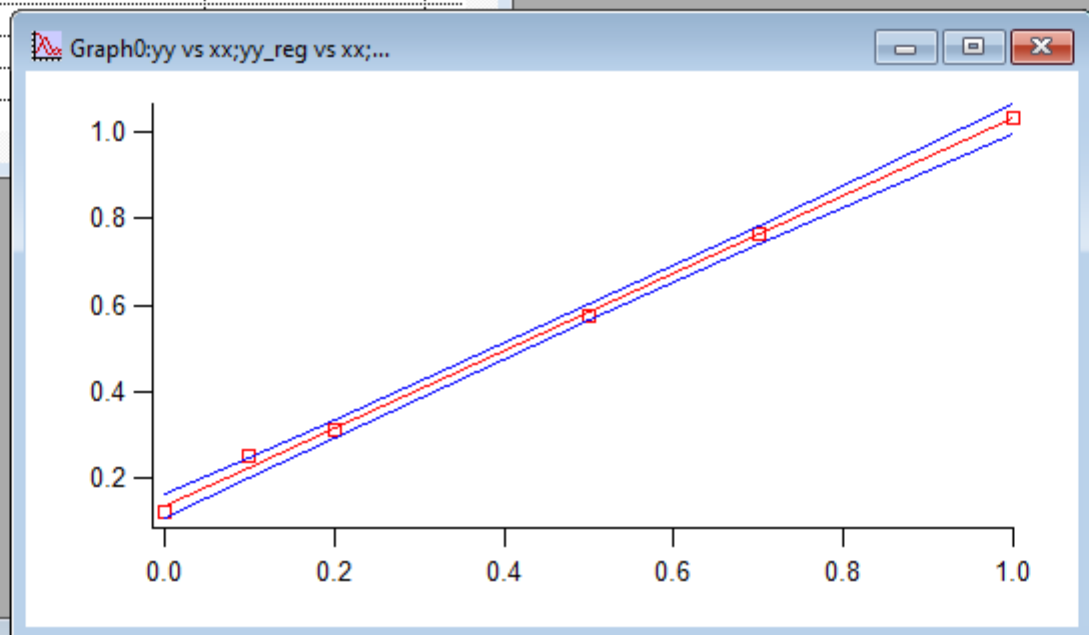
```

Untitled
•rename wave2 yy_reg
•rename wave3 yy_upp
•rename wave4 yy_low
•display yy vs xx
•ModifyGraph mode=3,marker=5
•appendtograph yy_reg vs xx

```

ble0:xx,yy,yy_reg,yy_upp,yy_low

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					



Untitled

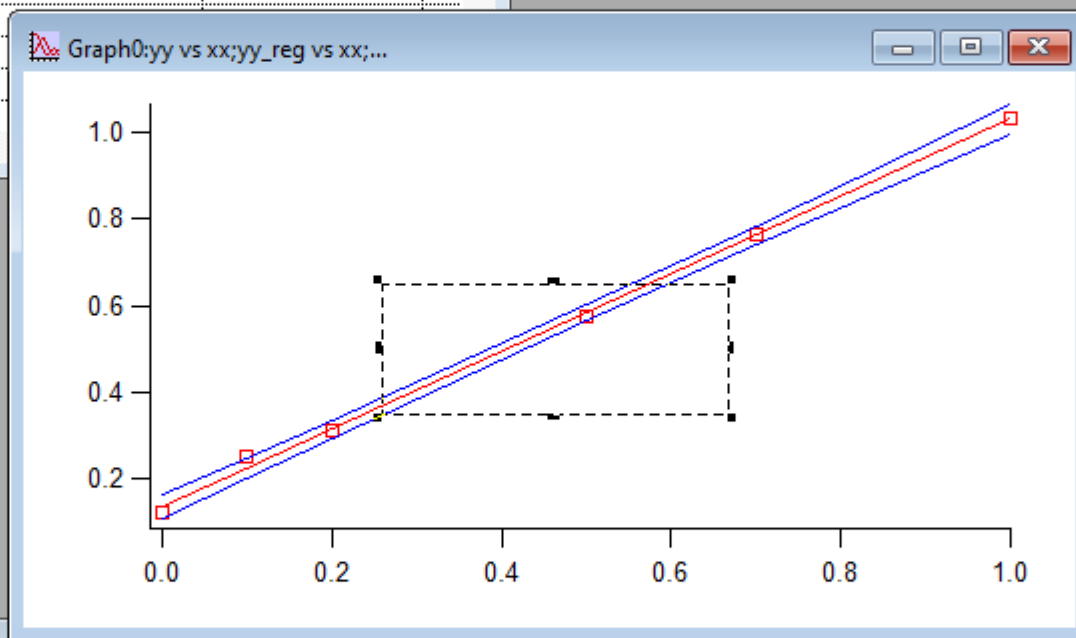
```

play yy vs xx
difyGraph mode=3,marker=5
pendtograph yy_reg vs xx
pendtograph yy_upp vs xx
pendtograph yy_low vs xx
difyGraph rgb(yy_upp)=(0,0,65280),rgb(yy_low)=(0,0,65280)
    
```

Table0:xx,yy,yy_reg,yy_upp,yy_low

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Expand a selection.



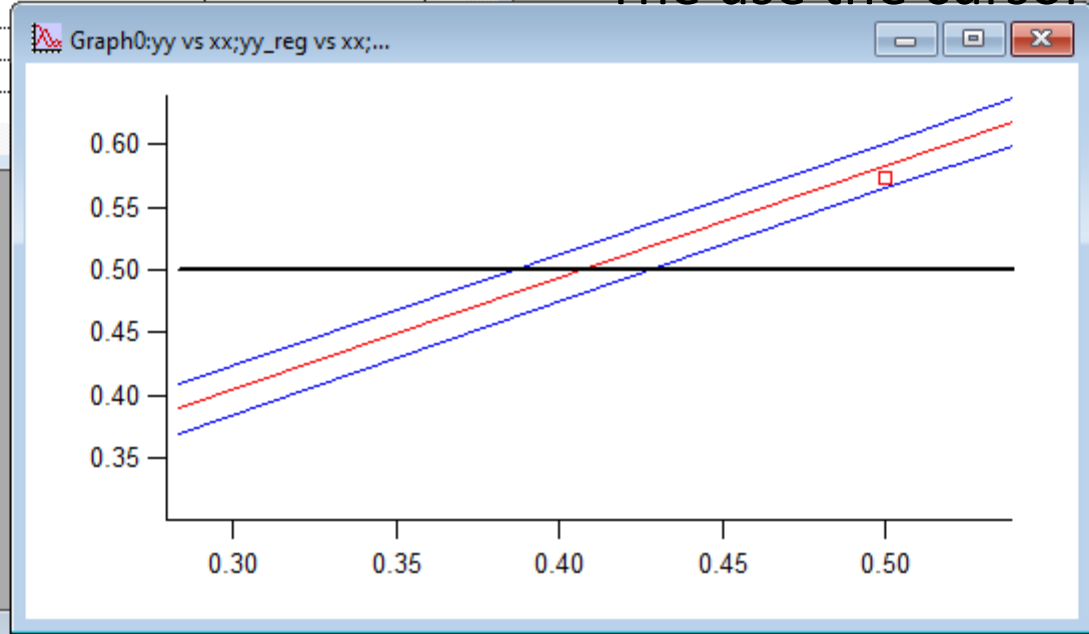
Untitled

- display yy vs xx
- ModifyGraph mode=3,marker=5
- appendtograph yy_reg vs xx
- appendtograph yy_upp vs xx
- appendtograph yy_low vs xx
- ModifyGraph rgb(yy_upp)=(0,0,65280),rgb(yy_low)=(0,0,65280)

ble0:xx,yy,yy_reg,yy_upp,yy_low

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Draw a horizontal line.
 Use 10000 points or so.
 Make /n=10000 yy_cal,xx_cal
 xx_cal=x/10000 (so the range is 0 to 1)
 The use the cursor (<ctrl>I).



ntitled

```

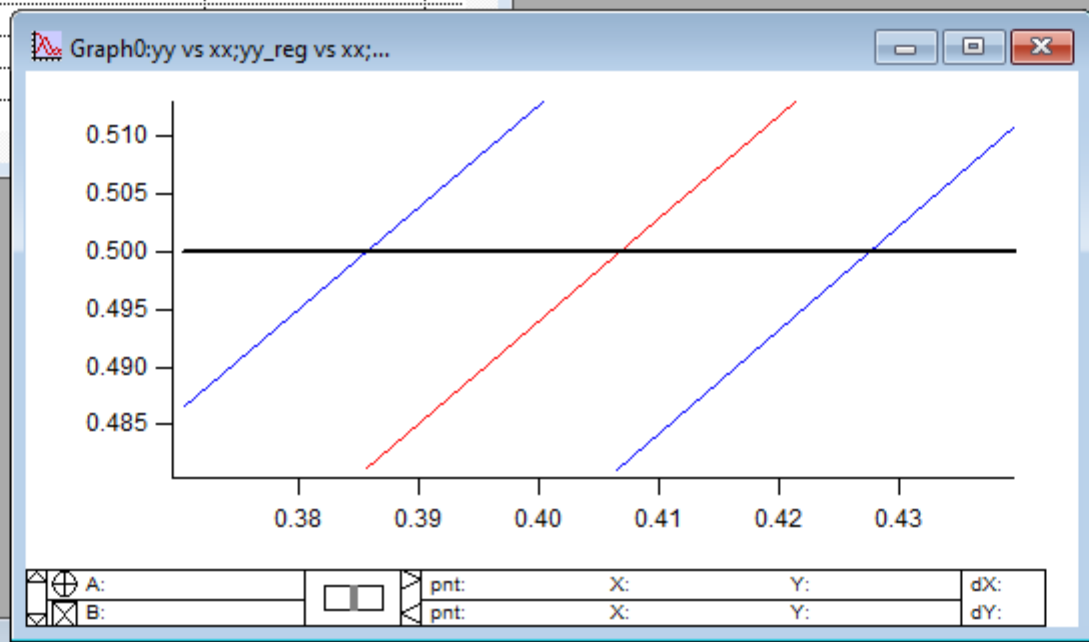
difyGraph rgb(yy_upp)=(0,0,65280),rgb(yy_low)=(0,0,65280)
uplicate yy yy_cal
_cal=0.5
endtograph yy_cal vs xx
difyGraph rgb(yy_cal)=(0,0,0)
difyGraph lsize(yy_cal)=2

```

Graph window title: Graph0:xx,yy,yy_reg,yy_upp,yy_low

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Expand a little further to see the intersections. You can also draw vertical lines down to the X-axis, but this is easier

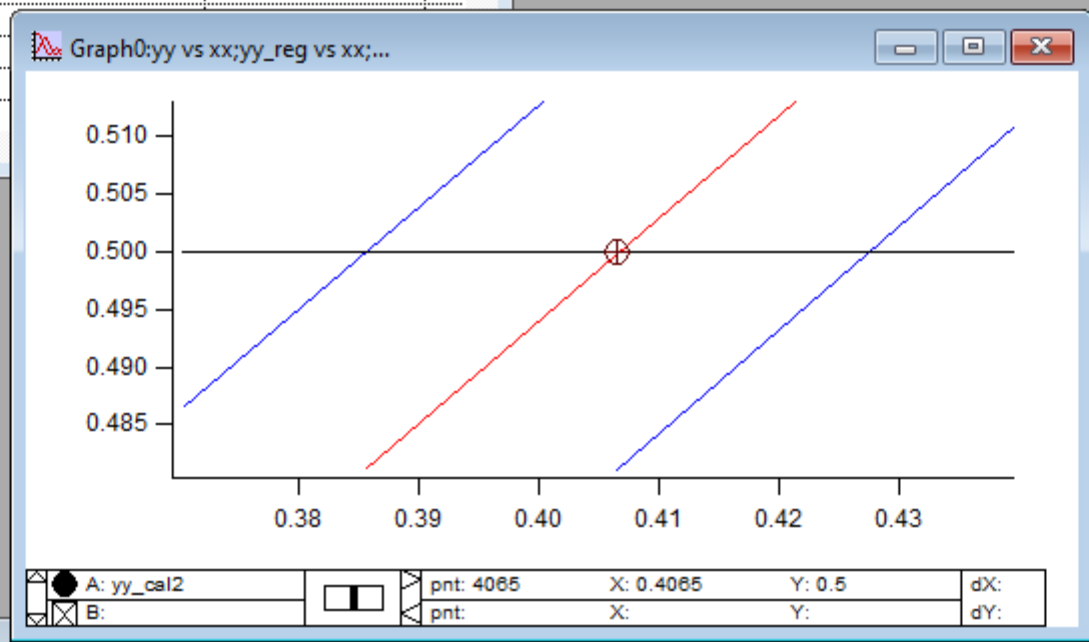


```
untitled
duplicate yy yy_cal
yy_cal=0.5
pendtograph yy_cal vs xx
difyGraph rgb(yy_cal)=(0,0,0)
difyGraph lsize(yy_cal)=2
showInfo
```


Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Read off the mean to 4 sig figs.

Mean: 0.4065

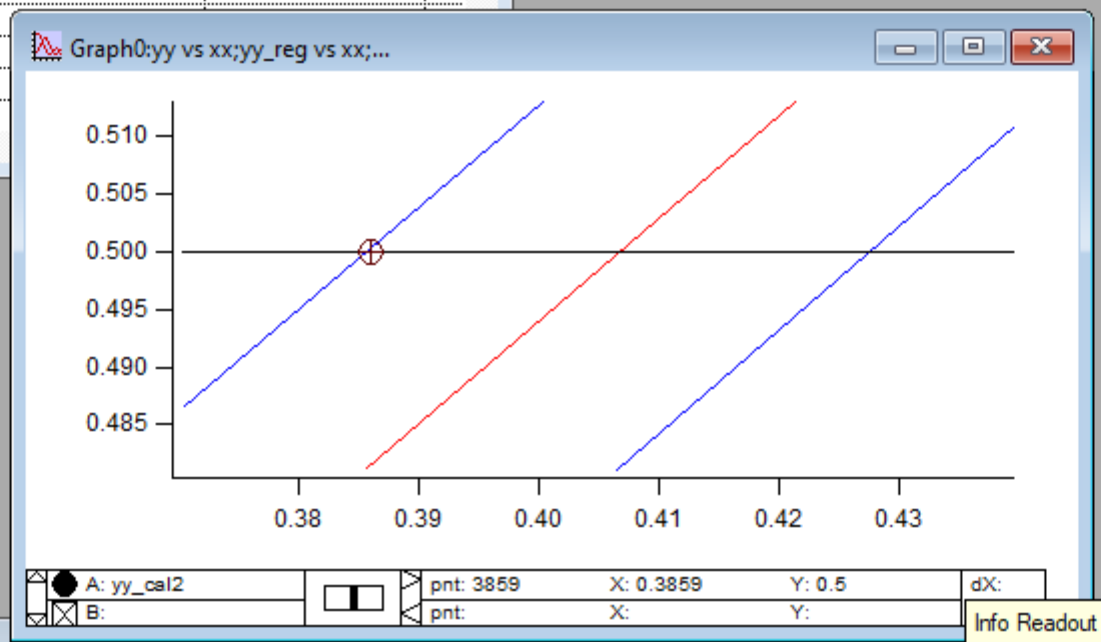


```
ntitled  
pendtograph yy_cal2 vs xx2  
moveFromGraph yy_cal  
_cal2=0.5  
difyGraph rgb(yy_cal2)=(0,0,0)  
lelInfo  
owInfo
```

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Read off the upper 95% to 4 sig figs.

Upper 95%: 0.3895

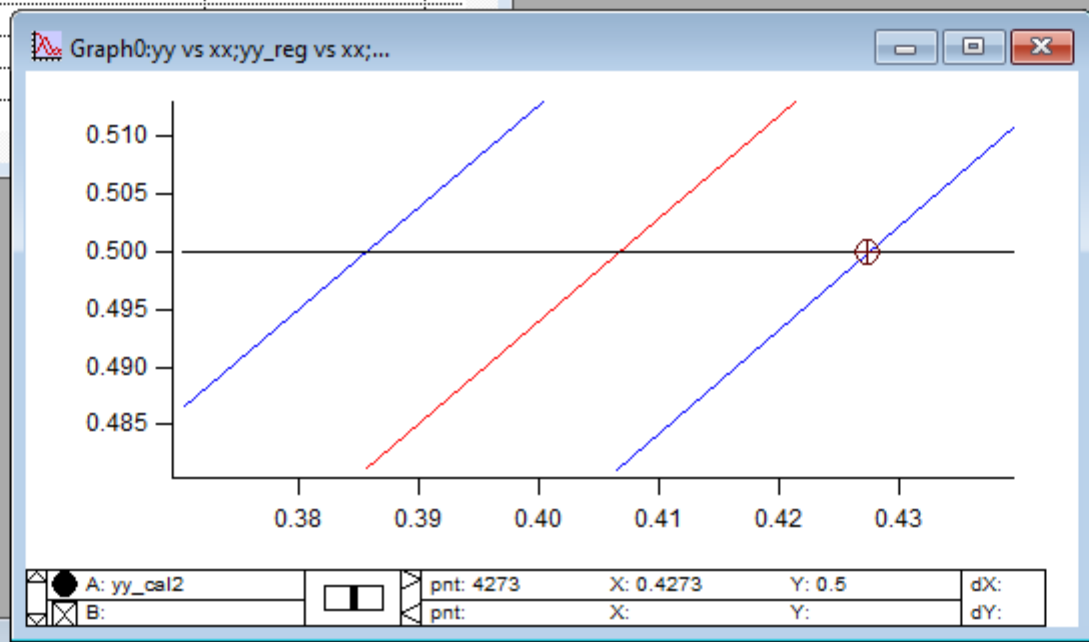


```

entitled
pendtograph yy_cal2 vs xx2
moveFromGraph yy_cal
_cal2=0.5
difyGraph rgb(yy_cal2)=(0,0,0)
leInfo
owInfo
  
```

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					

Read off the lower 95% to 4 sig figs.
Upper 95%: 0.4273



```
ntitled  
pendtograph yy_cal2 vs xx2  
moveFromGraph yy_cal  
_cal2=0.5  
difyGraph rgb(yy_cal2)=(0,0,0)  
lelInfo  
owInfo
```

The mean is the value of interest and upper – lower = 95% Confidence Limit

In the previous example it was 0.0208.

If you can plot this more easily on Excel, then please use it. I use Igor and make it Available under tools.

It is normally the case that the limit of detection (LOD) is larger than the error in the mid-regression. The errors in the ends are not as well determined since there are fewer data points.

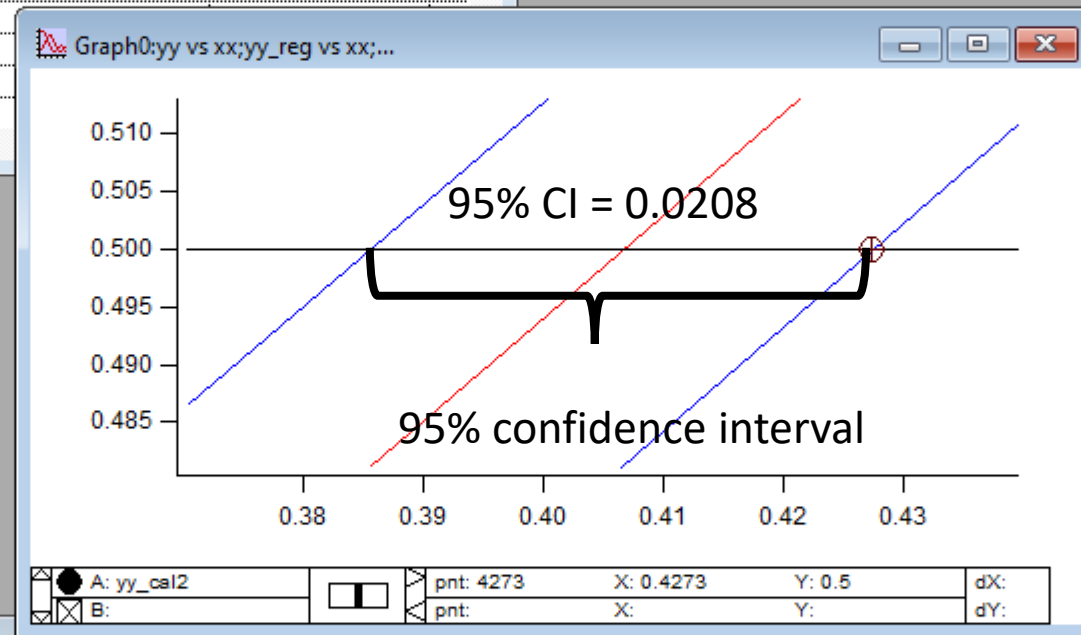
Read off the upper and lower 95% to 4 sig figs.
Calculate the difference and this is the 95% Confidence interval
for the calibration at this value.

Igor Pro 5.00

File Edit Data Analysis Macros Windows Graph Misc Help

Table0:xx,yy,yy_reg,yy_upp,yy_low

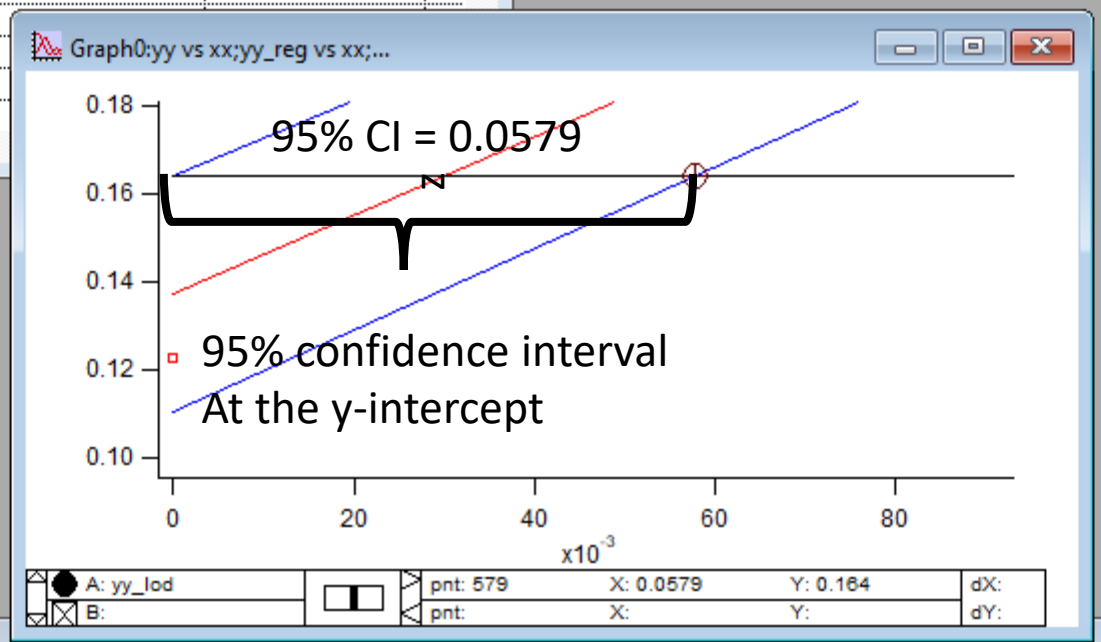
Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					



Untitled

- appendtograph yy_cal2 vs xx2
- RemoveFromGraph yy_cal
- yy_cal2=0.5
- ModifyGraph rgb(yy_cal2)=(0,0,0)

Point	xx	yy	yy_reg	yy_upp	yy_low
0	0	0.12266	0.137126	0.164019	0.110233
1	0.1	0.250966	0.226339	0.249694	0.202984
2	0.2	0.31211	0.315552	0.335952	0.295152
3	0.5	0.572956	0.58319	0.601056	0.565324
4	0.7	0.76219	0.761616	0.783908	0.739323
5	1	1.03219	1.02925	1.06283	0.99568
6					



```
untitled  
leInfo  
owInfo  
t yy_lod  
pendtograph yy_lod vs xx2  
difyGraph rgb(yy_lod#1)=(0,0,0)  
moveFromGraph yy_lod
```

Igor is available under Tools.