

Part I, Chapters 4 & 5

Data Tables and Data Analysis
Statistics and Figures

Descriptive Statistics, Simple Graphs
and Histograms

Descriptive Statistics 1

Are data points clumped?

(order variable / exp. variable)

- Concentrated around one value?
- Concentrated in several areas?

*This is the first
decision you need
to make!*

Do data point pairs show a pattern?

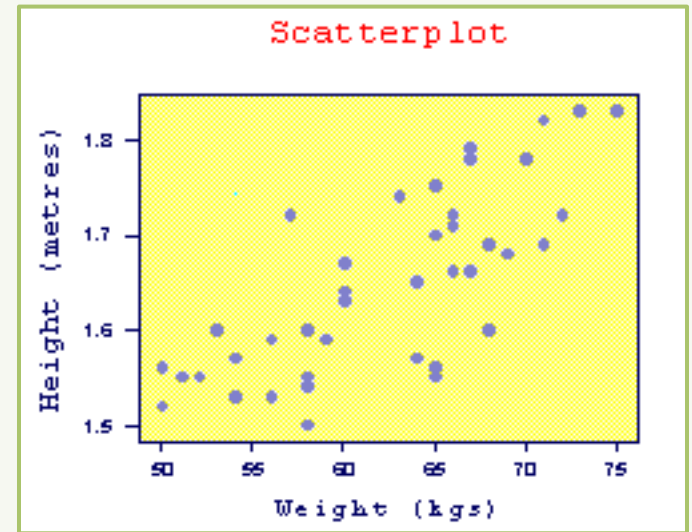
(exp. variable #1 / exp. variable #2)

- Straight line?
- Parabola?
- Sin function?

Scatter Graphs

A scatterplot is a useful summary of a set of bivariate data (two variables), usually drawn *before* working out a linear correlation coefficient or fitting a regression line. Each unit contributes one point to the scatterplot, on which points are plotted but not joined. The resulting pattern indicates the type and strength of the relationship between the two variables.

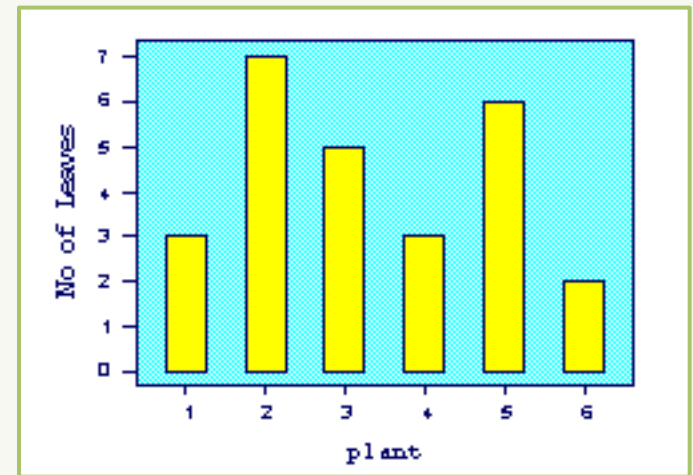
- Gives a good visual picture of the relationship between the variables
- Aids the interpretation of the correlation coefficient or regression model



Bar and Column Graphs

A bar / column graph is a way of summarising a set of categorical data. It is often used in exploratory data analysis to illustrate the major features of the distribution of the data in a convenient form. It displays the data using a number of rectangles, of the same width, each of which represents a particular category. The length (and hence area) of each rectangle is proportional to the number of cases in the category it represents, for example, age group, religious affiliation.

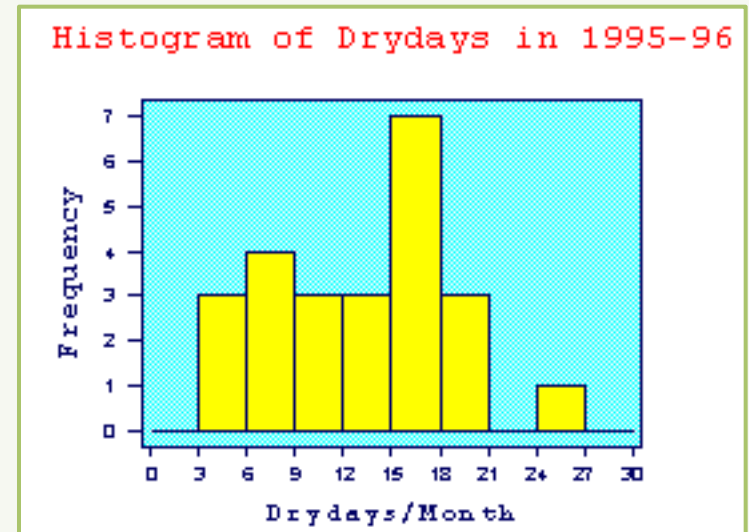
- Summarize nominal or ordinal data
- Displayed horizontally (bars) or vertically (column)
- Drawn with a gap between the bars (rectangles)



Frequency Analysis: Histograms

A histogram is a way of summarizing data that are measured on an interval scale (either discrete or continuous). It is often used in exploratory data analysis to illustrate the major features of the distribution of the data in a convenient form. It divides up the range of possible values in a data set into classes or groups. For each group, a rectangle is constructed with a base length equal to the range of values in that specific group, and an area proportional to the number of observations falling into that group. This means that the rectangles might be drawn of non-uniform height.

- Variables are numerical
- Variables are measured on an interval scale
- Used with large data sets (>100 observations)
- Detect unusual observations (outliers, gaps)



Descriptive Statistics 2

*Does the Study
Matter?*

Size – Total number of Data Points, N

- Number of reactions performed
- Numbers of points measured (i.e., for a spectrum)

*Does the Parameter
Matter?*

Range – Distance between smallest and largest data value

- Min., Max., and Range = Max. – Min.
- Average $\pm$ Difference/2

*How Does the
Parameter Matter?*

Middle – There are many types of averages

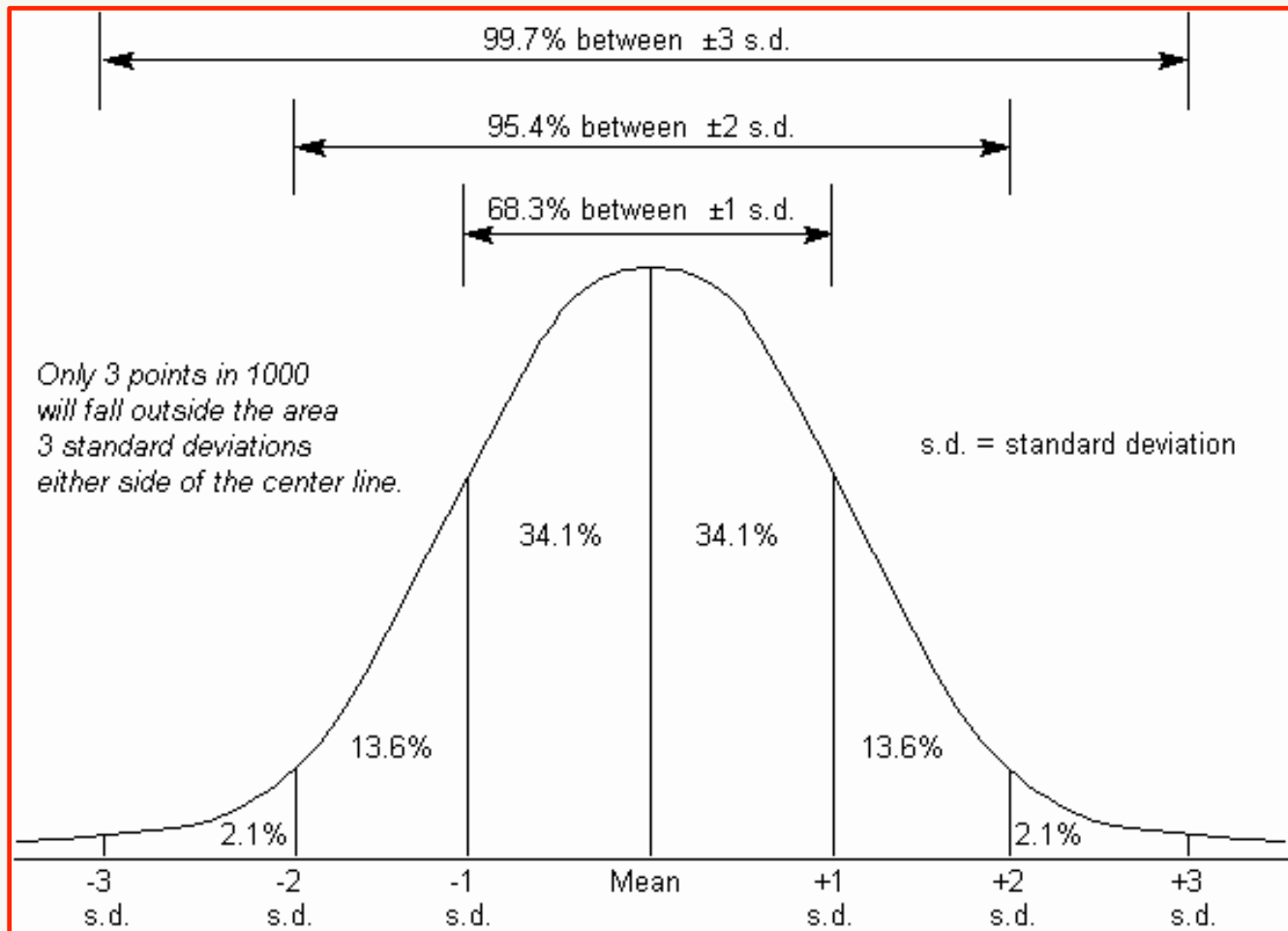
- Average = Mean = Arithmetic Mean: $\text{Sum}(\text{Data}) / N$
- Geometric Mean: $[\text{Product}(\text{Data})]^{1/N}$
- Mode: Most frequent data value
- Median: $N/2$ data are below and above.

*How Frequent
Are Deviations?*

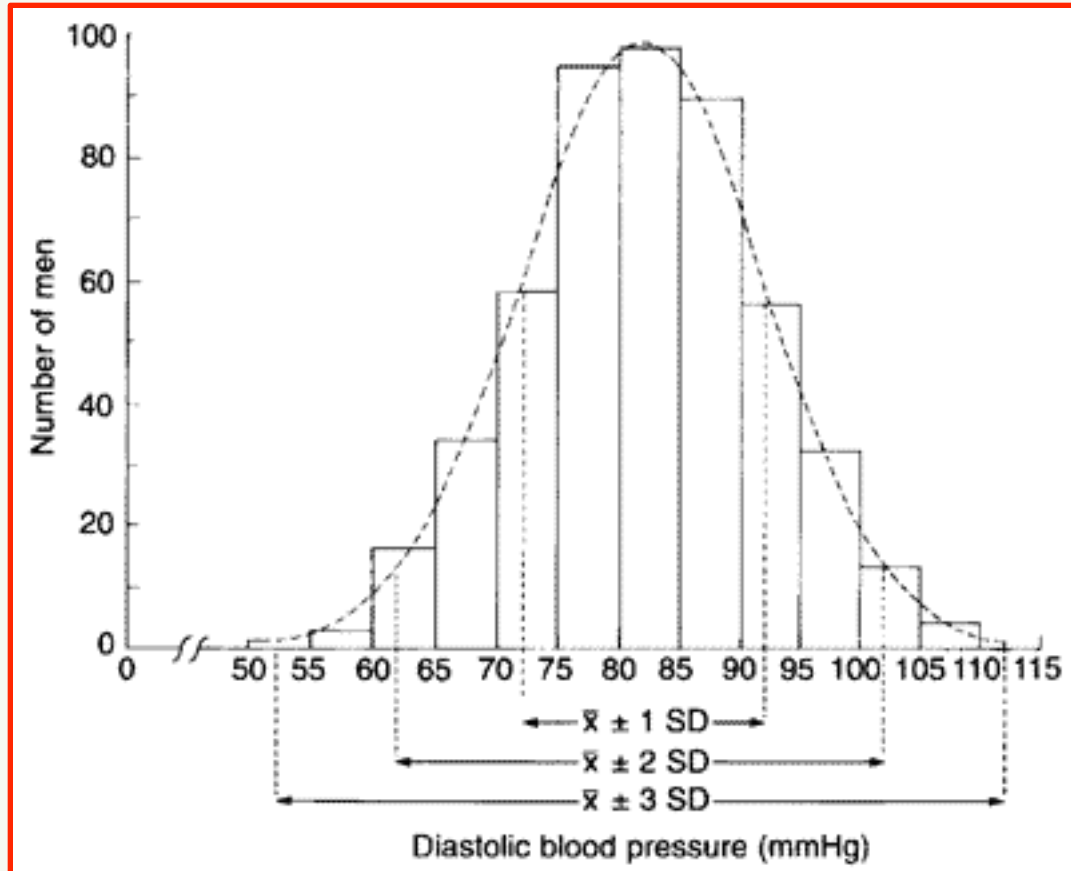
Spread – Frequency of Significant Deviation

- Standard Deviation
- Central 50%

Standard Deviation



Standard Deviation



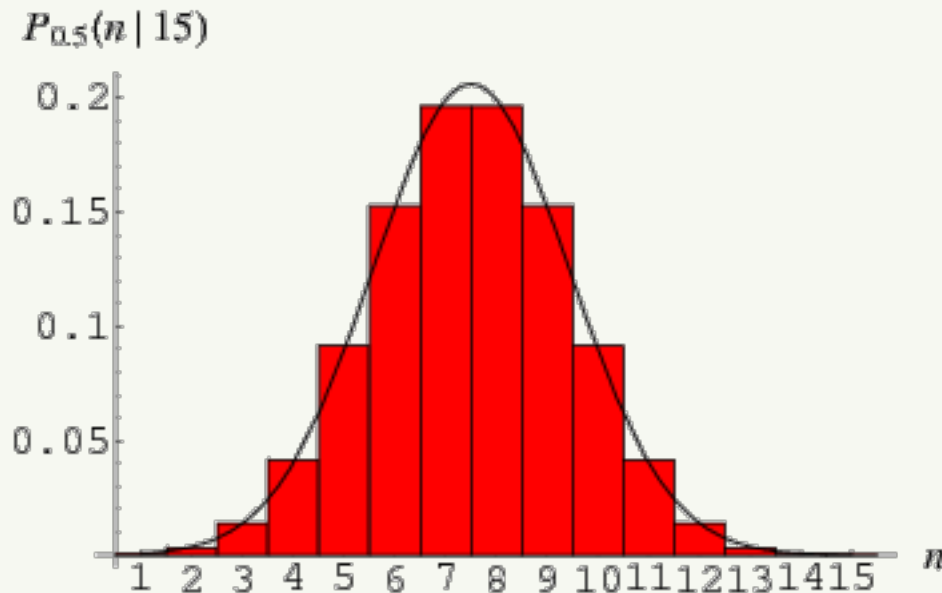
Real Work Sample:

Data Histogram

Mathematical World:

Inferential statistics maps the data by a formula that describes the population.

Normal or Gaussian Distribution Bell Curve



A normal distribution in a **variante x** with **mean μ** and **variance σ^2** is a statistic distribution with probability density function

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x - \mu)^2}{2\sigma^2}\right\}$$

If Gaussian, then: Mean = Median = Mode

Mean and Standard Deviation determine the distribution

Significance Test & p-Value

p-value = alpha level = significance level

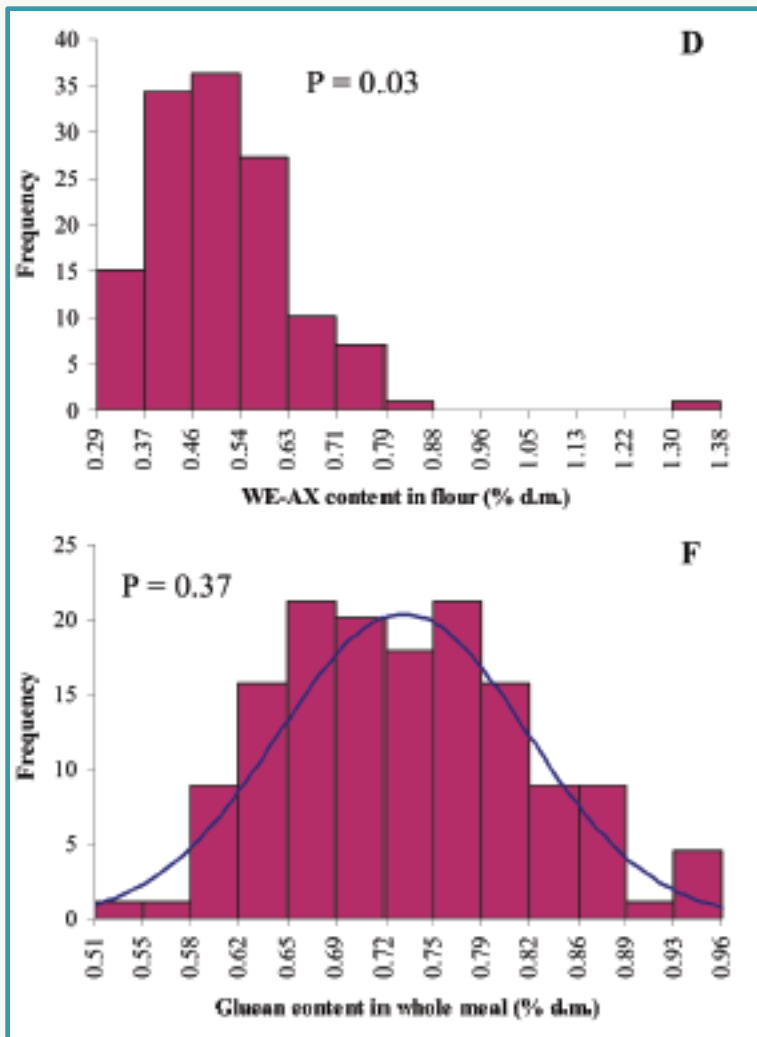
For significance tests there is a hypothesized condition (called null hypothesis, H_0) that one is testing to see if it is true. For a test of fit the hypothesized condition is that the selected distribution (i.e., a normal distribution) generated the data.

The p-value is the probability that the data have been generated under the hypothesized condition. A p-value of 0.05 indicates that the chance of the observed data is low, 1 in 20, due to variation alone. This is good evidence that the data was not generated under the hypothesized condition. The hypothesized condition is rejected if the p-value is 0.05 or below.

A p-value of 0.05 provides 95% confidence the hypothesized condition is not true (i.e., no normal distribution). The confidence level is calculated from the p-value as $100*(1 - p)$.

Cramer von Mises Test

Andersen-Darling Test



A “quadratic EDF statistics”
EDF = empirical dist. function

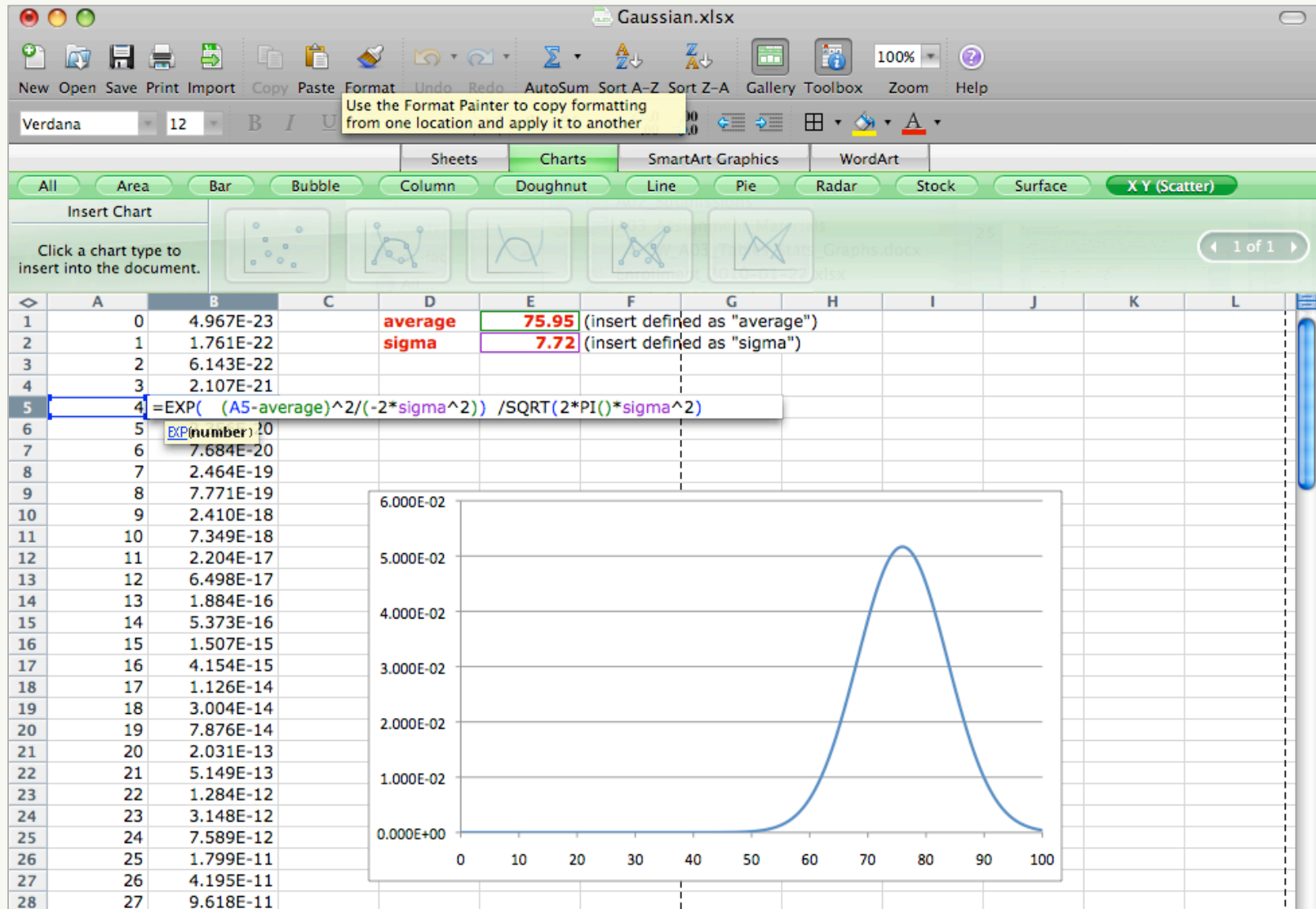
$$n \int_{-\infty}^{\infty} [F_n(x) - F(x)]^2 w(x) dF(x)$$

$$CvM: w(x) = 1$$

$$AD: w(x) = \frac{1}{F(x) - F(x)^2}$$

AD value → {Statistics} → p-value

Normal Distribution, 1D-Gaussian



Scatter Graph In Electronics Research

Electron Transport through CO Studied by Gold Break-Junctions in Nonpolar Liquids

D. den Boer,^{*,†} M. J. J. Coenen,[†] M. van der Maas,[†] T. P. J. Peters,[†] O. I. Shklyarevskii,^{†,‡}
J. A. A. W. Elemans,[†] A. E. Rowan,[†] and S. Speller[†]

Electron Transport through CO

J. Phys. Chem. C, Vol. 113, No. 34, 2009 15415

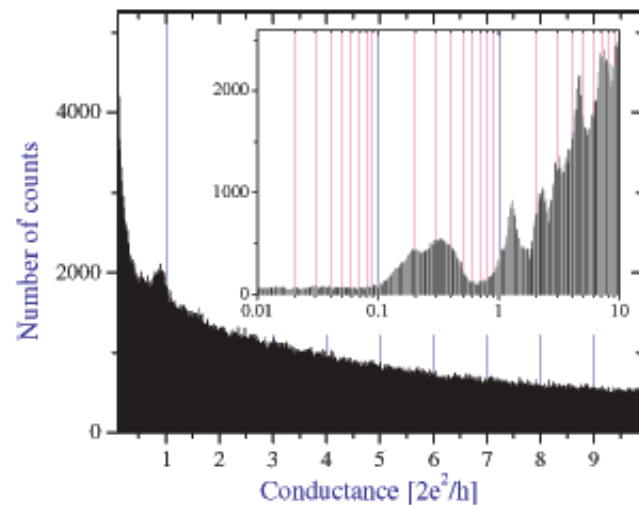


Figure 7. Conductance histogram for gold in toluene saturated with carbon monoxide. Inset: conductance histogram measured in diluted solution for the traces with steps in the range 0.1–0.4 G_0 (about 20% of data set).

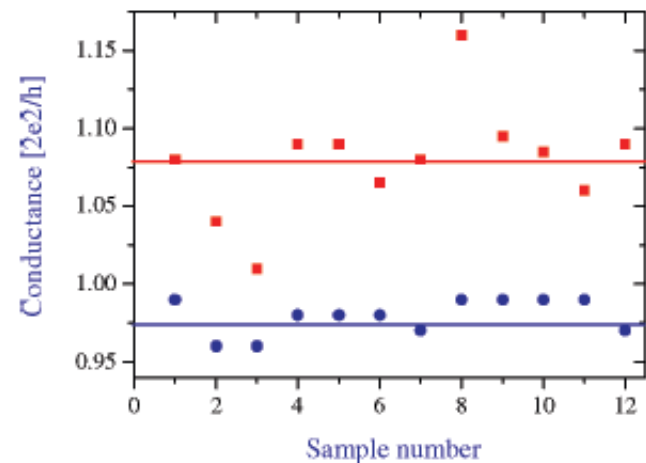


Figure 8. Position of the peak related to the single-atom contact between gold electrodes in the original conductance histograms (circles) and in the histograms constructed from selected traces with the steps in the range 0.2–0.4 G_0 (squares). The first six points are related to the measurements in toluene, while the last six are related to the measurements in cyclohexane.

Gaussian Dist. In Polymer Research

Positron/Positronium Annihilation as a Probe for the Chemical Environment of Free Volume Holes in Polymers

G. Dlubek,^{*,†,‡} H. M. Fretwell,^{†,§} and M. A. Alam[†]

Macromolecules, Vol. 33, No. 1, 2000

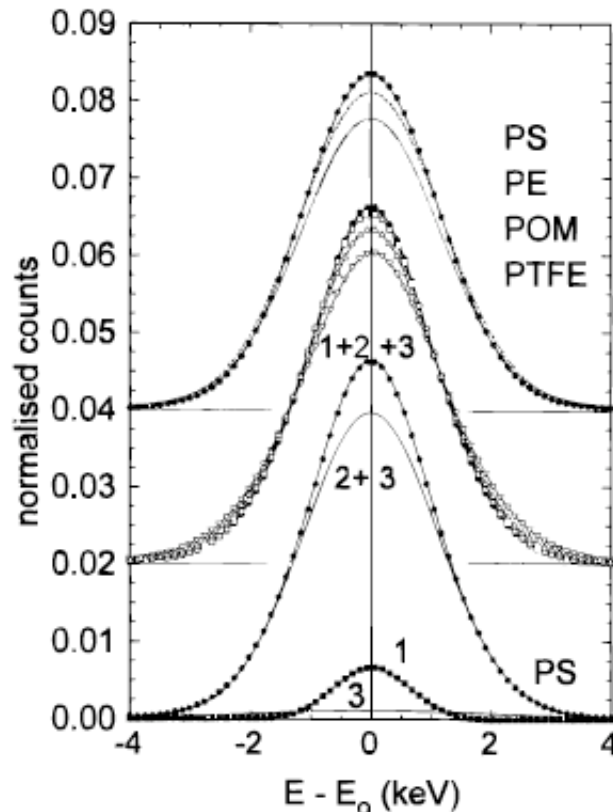


Figure 1. DB spectra in polymers corrected for nonconstant background. Middle: as-measured distributions for two hydrocarbon-based polymers (PS and PE) and for two polymers containing hydrocarbons plus oxygen (POM) and fluorine (PTFE). All curves are normalized to the same area. Bottom: fitting of the distributions with one narrow (1) (p-Ps self-annihilation) and two broad components (3, 2). Top: the broader components for the four polymers (after subtraction of the narrow component and normalization to the same area).

Gaussian Dist. In Food Chemistry

JOURNAL OF
AGRICULTURAL AND
FOOD CHEMISTRY

Variation in the Content of Dietary Fiber and Components Thereof in Wheats in the HEALTHGRAIN Diversity Screen

KURT GEBRUERS,^{*,†} EMMIE DORNEZ,[†] DANUTA BOROS,[§] ANNA FRAS,[§]
WIOLETTA DYNKOWSKA,[§] ZOLTAN BEDŐ,[#] MARIANN RAKSZEGI,[#]
JAN A. DELCOUR,[†] AND CHRISTOPHE M. COURTIN[†]

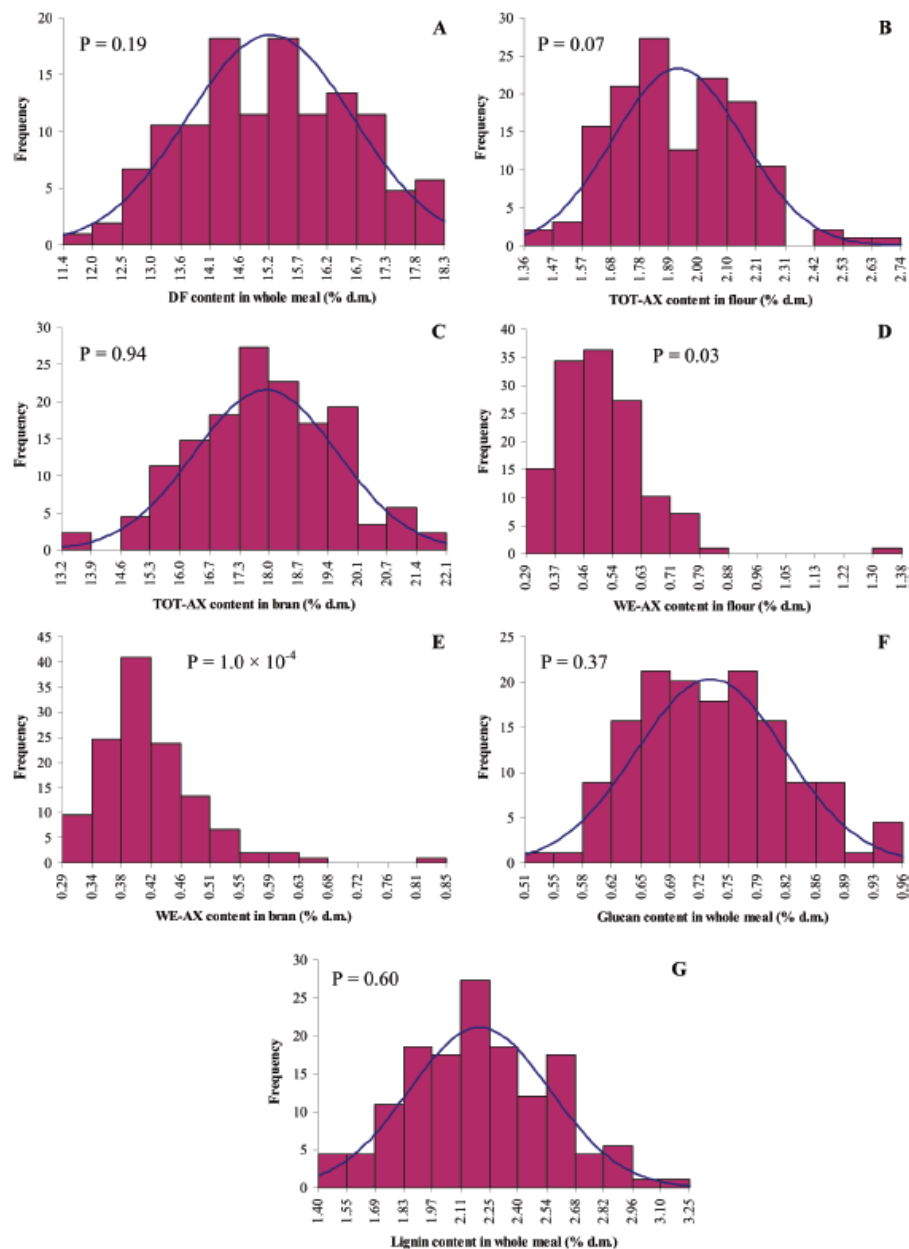


Figure 1. Frequency histograms (bars) for contents of DF in whole meal (A), TOT-AX in flour (B), and bran (C), WE-AX in flour (D) and bran (E), β -glucan in whole meal (F), and lignin in whole meal (G) from winter wheats. For the normally distributed data (Anderson–Darling P value > 0.05) also the corresponding normal distribution curves are shown.

Histogram In Food Chemistry

Analysis, Occurrence, and Potential Sensory Significance of Five Polyfunctional Mercaptans in White Wines

LAURA MATEO-VIVARACHO, JULIÁN ZAPATA, JUAN CACHO, AND VICENTE FERREIRA*

Laboratory for Flavor Analysis and Enology, Analytical Chemistry, Faculty of Sciences, University of Zaragoza, 50009 Zaragoza, Spain

10190 *J. Agric. Food Chem.*, Vol. 58, No. 18, 2010

Mateo-Vivaracho et al.

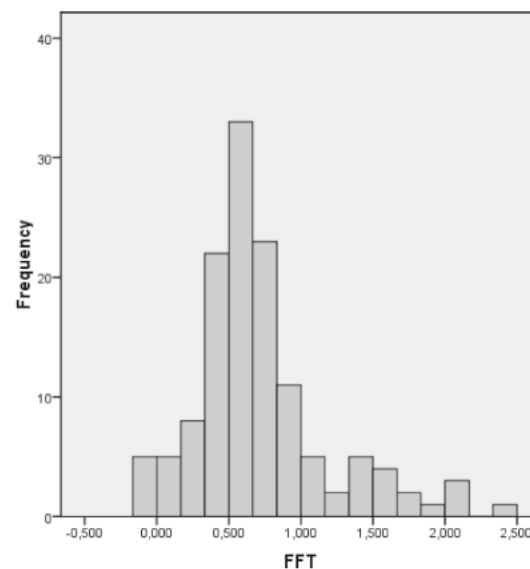
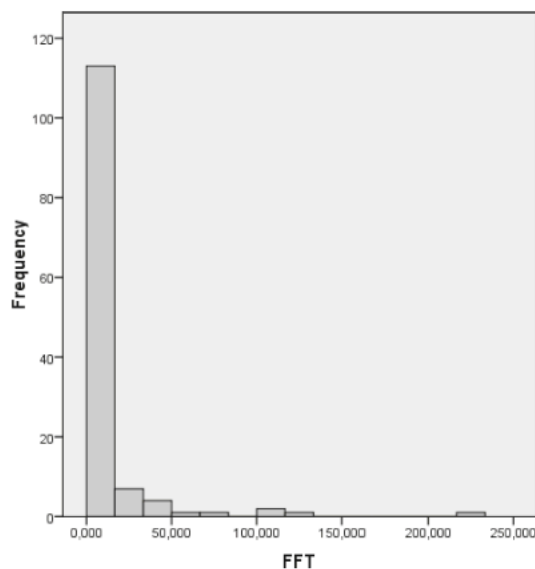
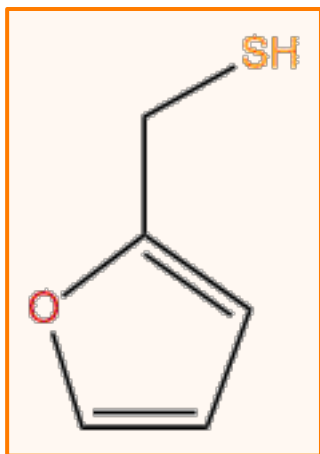


Figure 1. Histogram representing the distribution of FFT in the whole data set of samples in normal (left) or in logarithmic scales (right).

A log-normal distribution: variable whose logarithm is normally distributed.

Histogram In Nano Chemistry

J. Phys. Chem. C 2010, 114, 5773–5785

PRD = Particle Radius Distribution

*A log-normal distribution:
variable whose logarithm is
normally distributed.*

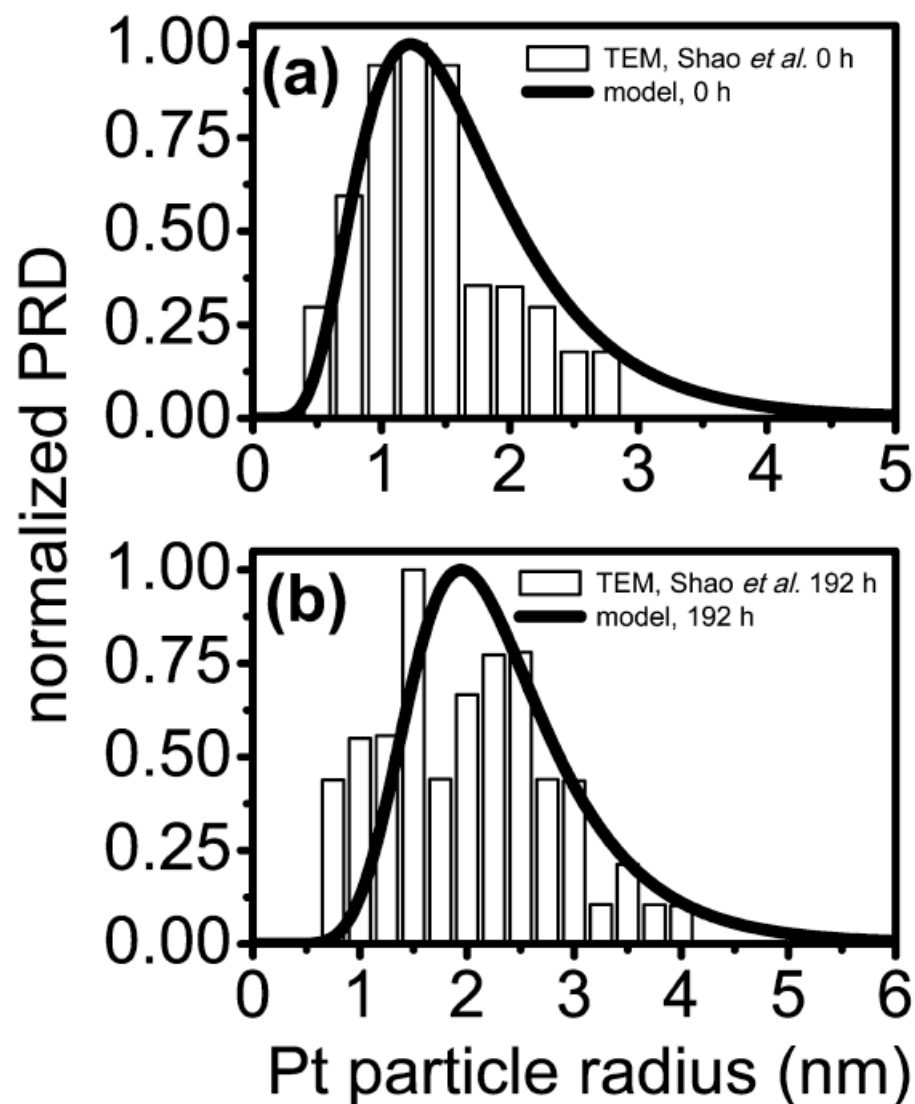
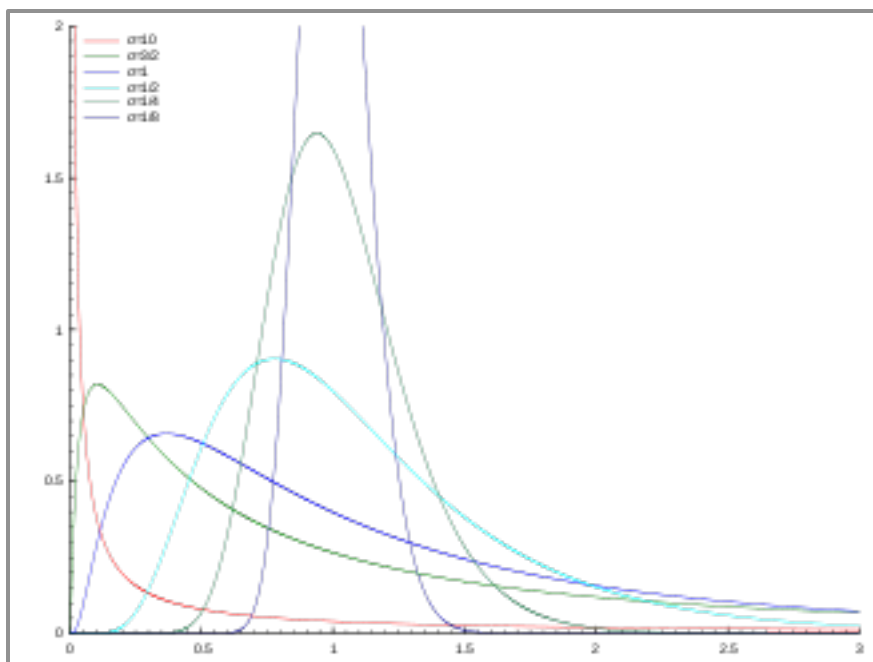


Figure 8. Comparison of initial (a) and final (b) particle radius distributions obtained from TEM micrographs in Shao *et al.*²⁶ Input parameters and experimental conditions are given in Table 1. An initial log-normal distribution with $r_0 = 1.5$ nm and $\sigma_{SD} = 0.45$ was used.

Histogram In Polymer Research

4874 Esselink et al.

Macromolecules, Vol. 31, No. 15, 1998

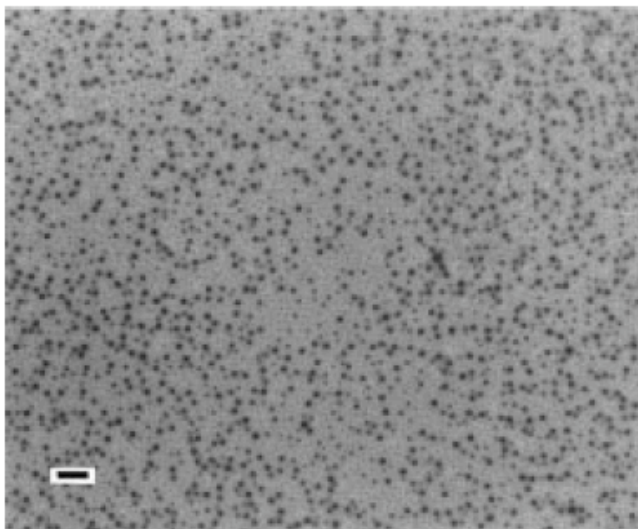


Figure 1. Electron micrograph of a mixture of two PVP-PS diblock copolymers (M_w 18k-75k and 102k-75k) after 1 h of aging. Scale bar represents 200 nm.

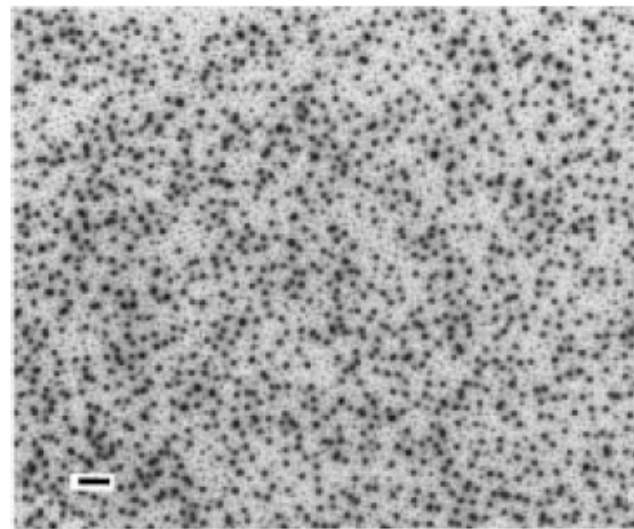


Figure 3. Electron micrograph of a mixture of two PVP-PS diblock copolymers (M_w 18k-75k and 102k-75k) after 38 days of aging. Scale bar represents 200 nm.

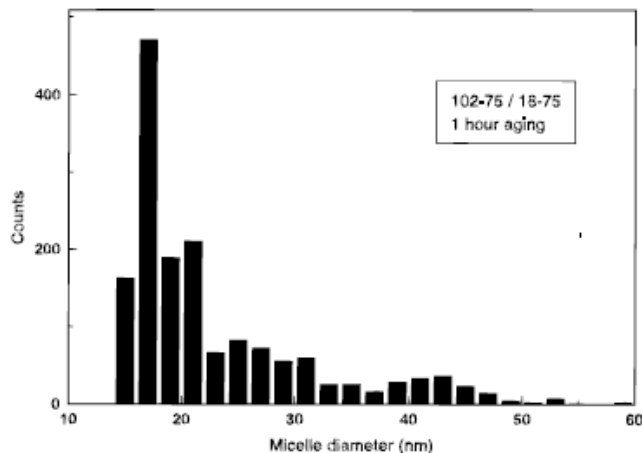


Figure 2. Histogram showing the size distribution belonging to Figure 1.

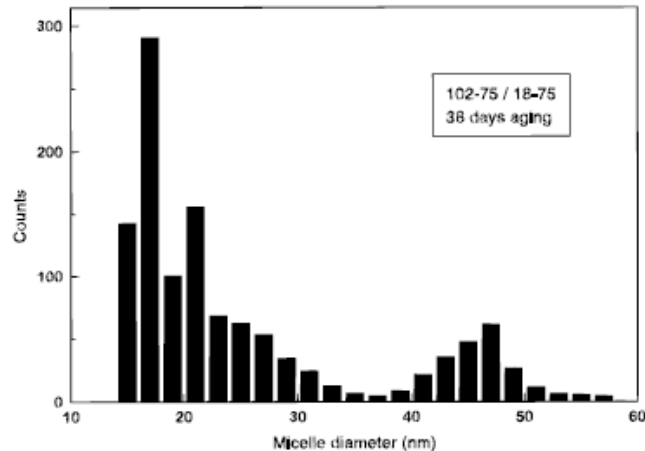


Figure 4. Histogram showing the size distribution belonging to Figure 3.

Histogram In Solid State Research

7384

J. Phys. Chem. 1996, 100, 7384–7391

Intermolecular Nonbonded Contact Distances in Organic Crystal Structures: Comparison with Distances Expected from van der Waals Radii

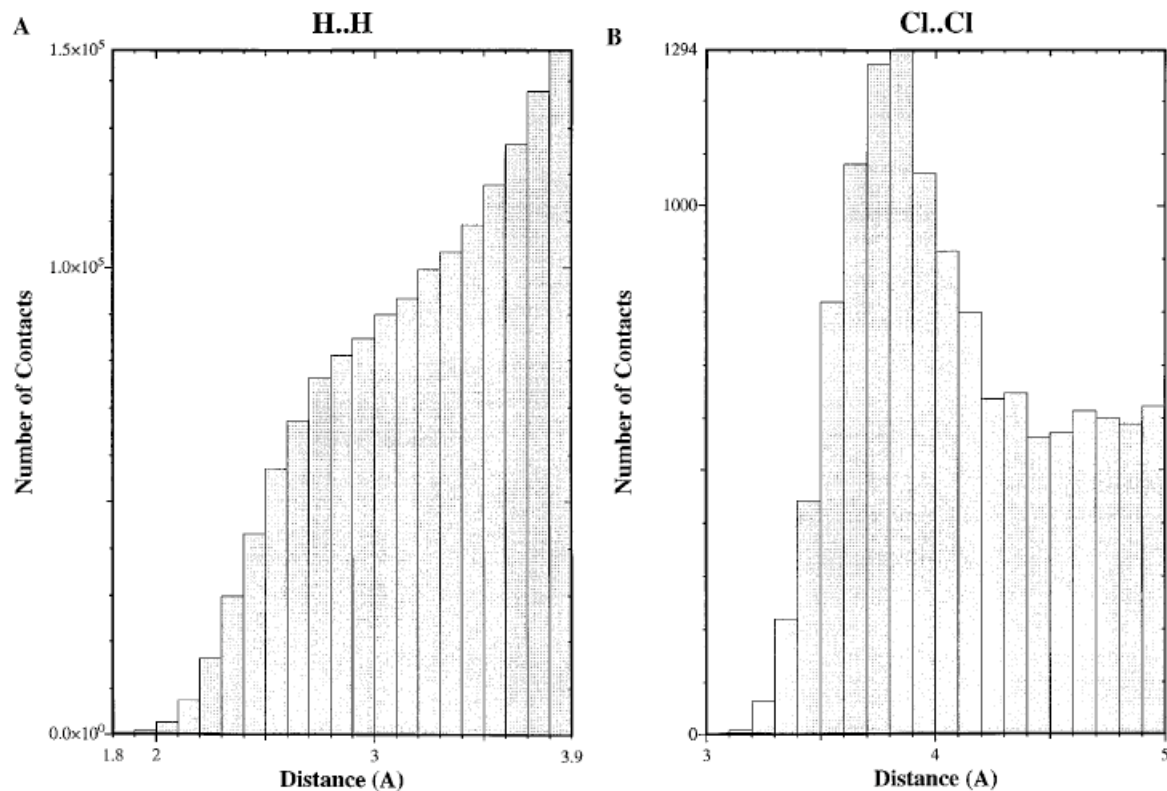
R. Scott Rowland* and Robin Taylor*

Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, U.K.

Received: October 24, 1995; In Final Form: January 28, 1996

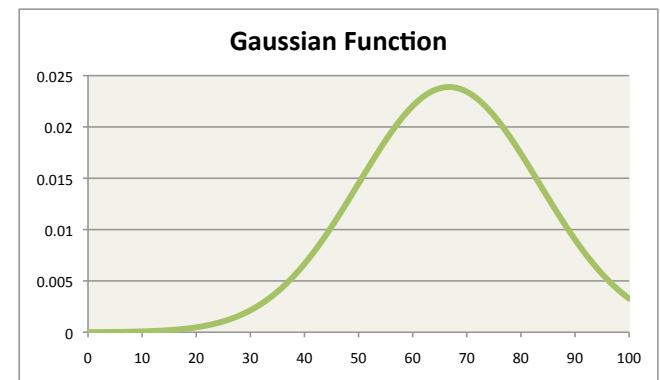
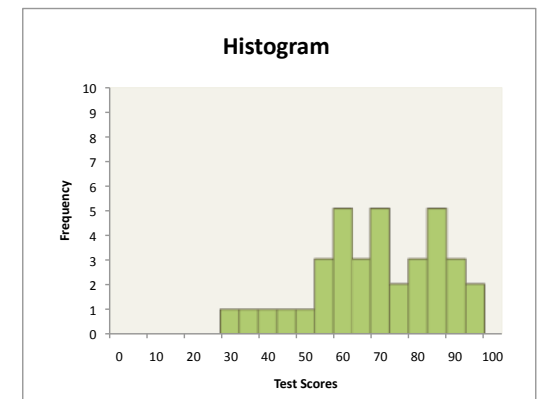
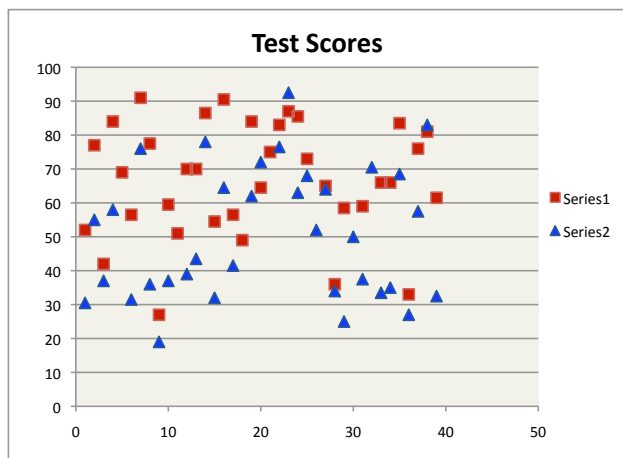
Contact Distances in Organic Crystal Structures

J. Phys. Chem., Vol. 100, No. 18, 1996 7385



How to Compute Descriptive Statistics, Present Scatter Graphs & Histograms, and Plot Functions using Excel

Example in Lecture: **Test Scores**
Assign. #3: Handout & online.



Microsoft Excel

Home Insert Page Layout Formulas Data Review View Acrobat

Clipboard Font Alignment Number Styles Cells Editing

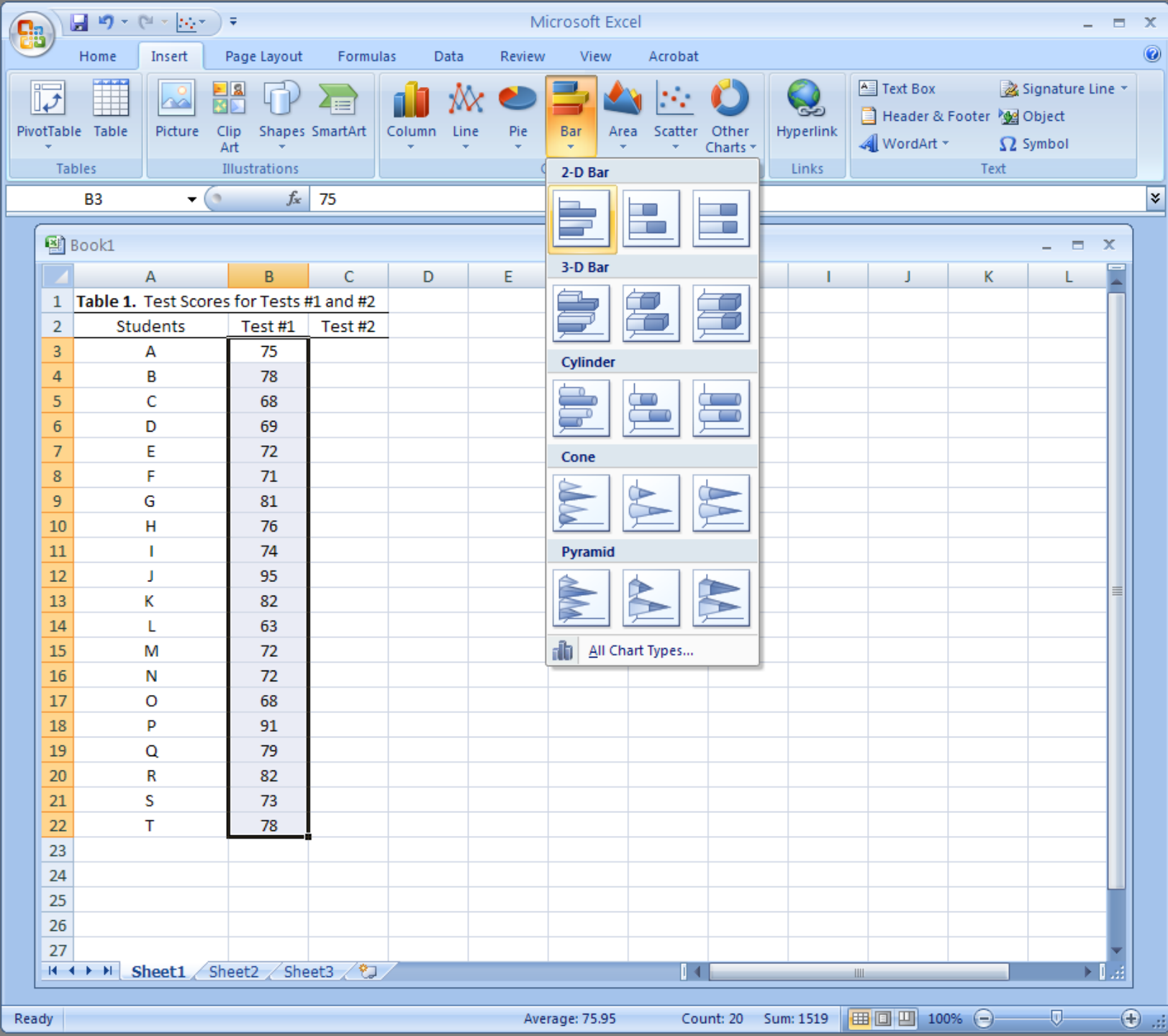
Calibri 11 A A

B 75

Book1

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2	Students	Test #1	Test #2									
3	A	75										
4	B	78										
5	C	68										
6	D	69										
7	E	72										
8	F	71										
9	G	81										
10	H	76										
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Sheet1 Sheet2 Sheet3



Microsoft Excel

Picture Tools

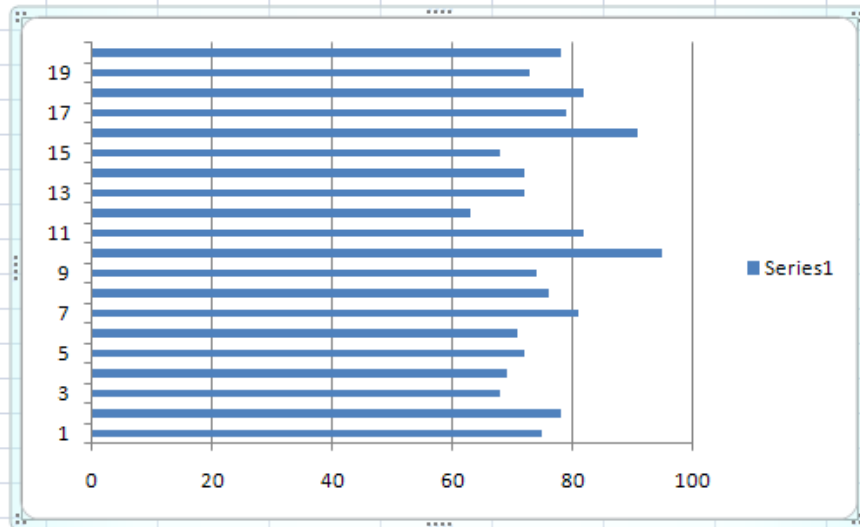
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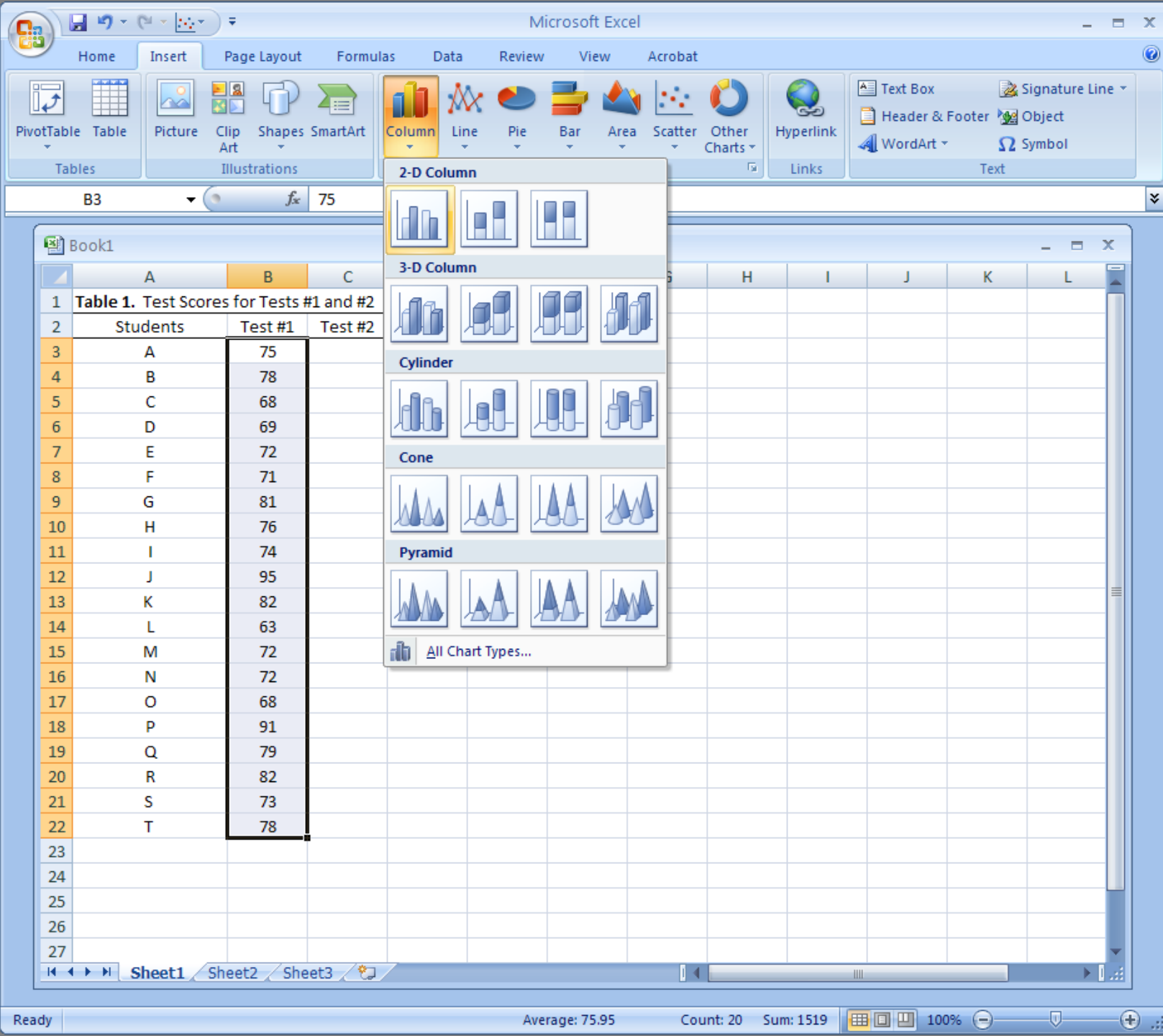
Clipboard Font Alignment Number Styles Cells Editing

Chart 1

Book1

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Microsoft Excel

Chart Tools

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Change Chart Type Save As Template Type Data

Switch Row/Column Select Data Data

Chart Layouts

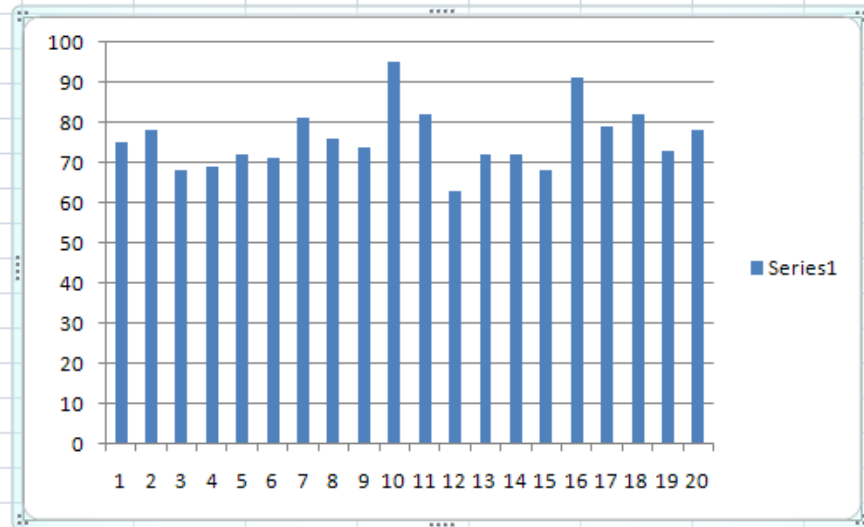
Chart Styles

Move Chart Location

Chart 3

Book1

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Sheet1 Sheet2 Sheet3

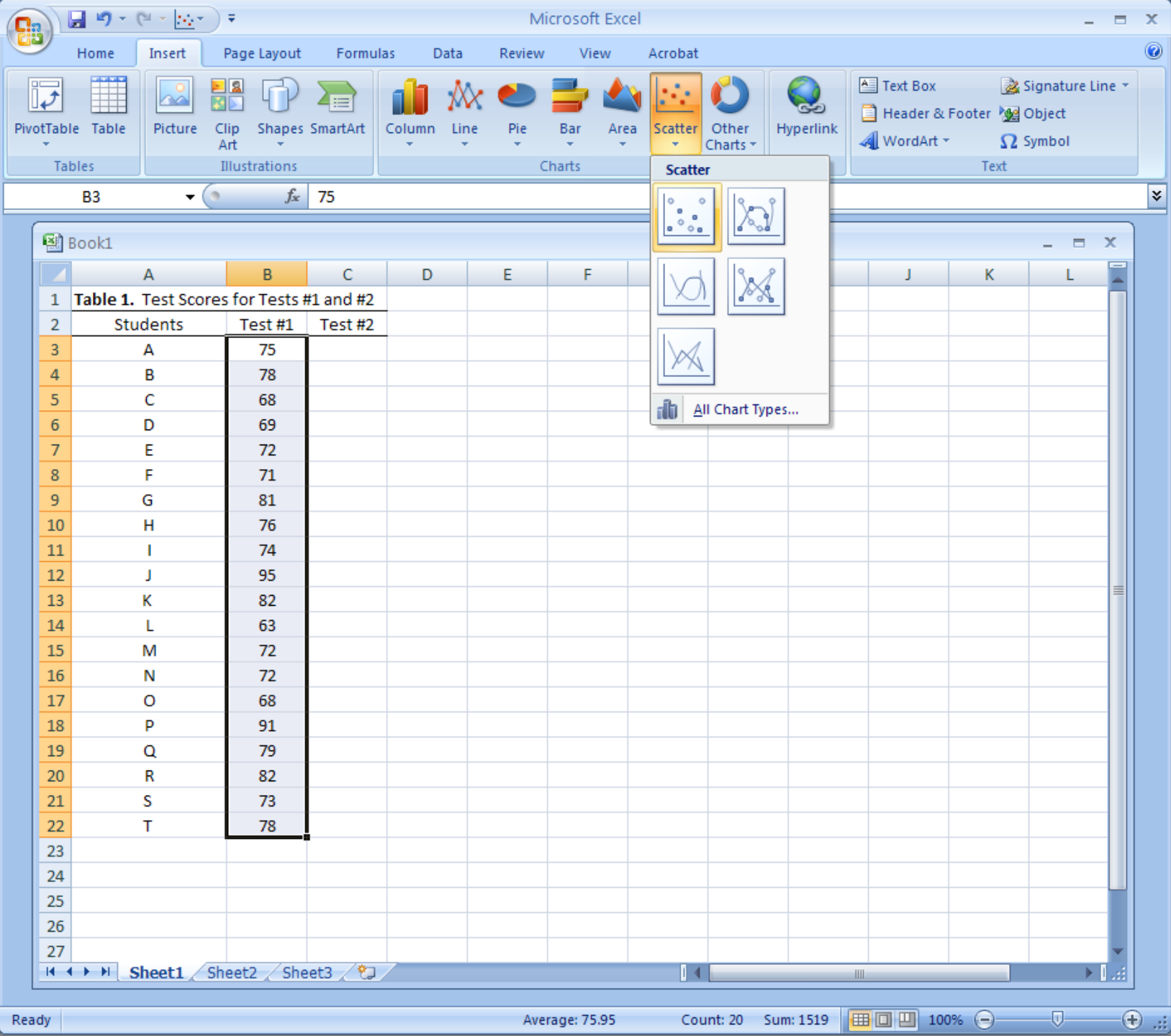
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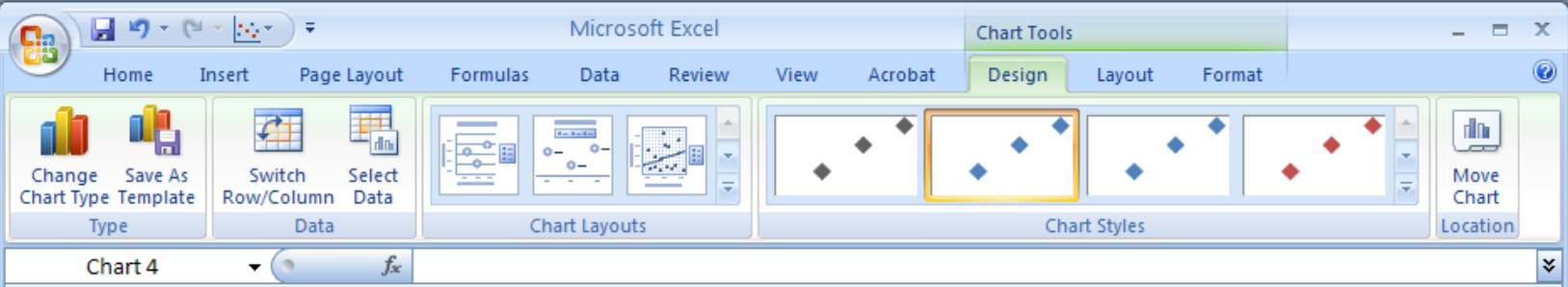
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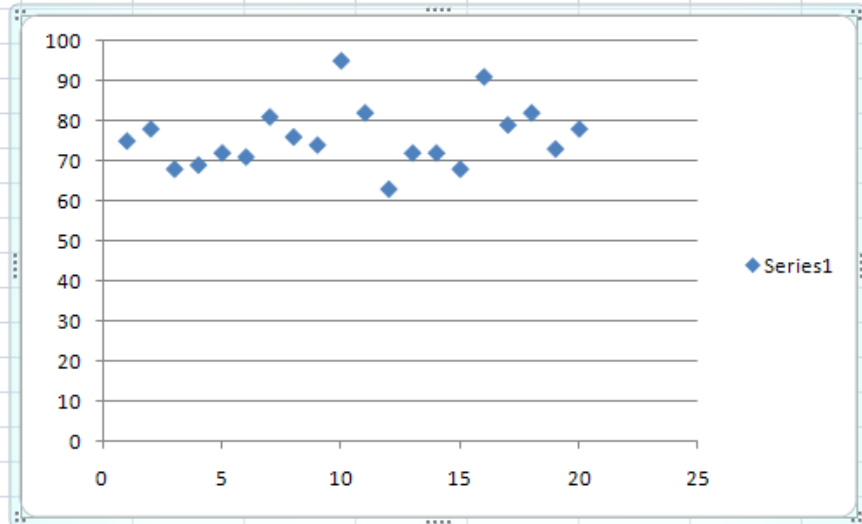
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Book1

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Sheet1 Sheet2 Sheet3

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Average: 75.95

Count: 20

Sum: 1519

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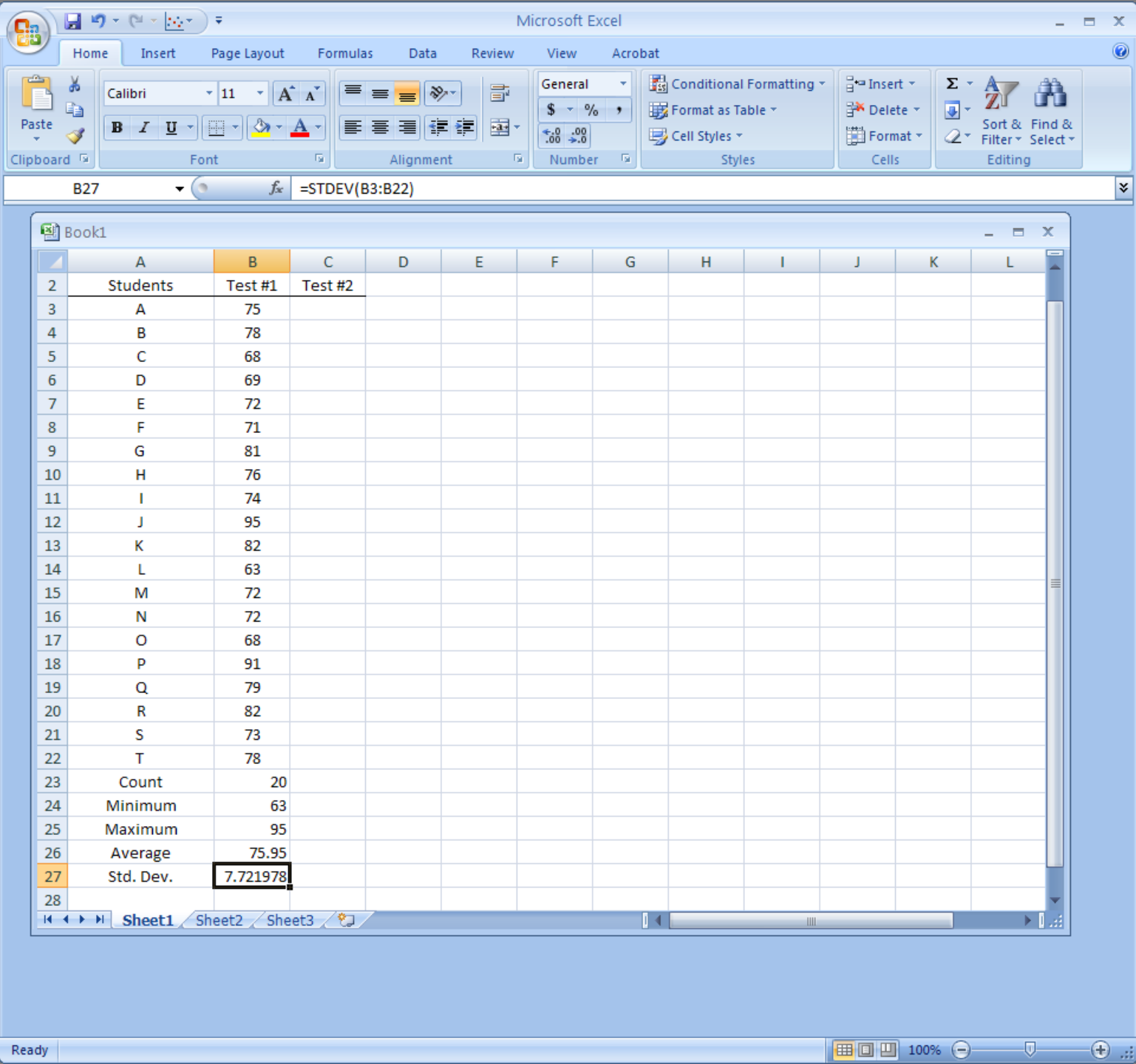
Paste Font Alignment Number Styles Cells Editing

RADIANS =Count(B3:B22)

Book1

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20	R	82										
21	S	73										
22	T	78										
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24	Minimum											
25	Maximum											
26	Average											
27	Std. Dev.											

Sheet1 Sheet2 Sheet3



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From Access From Web From Text From Other Sources Existing Connections Refresh All Properties Edit Links Connections Sort Filter Text to Columns Remove Duplicates Data Validation Consolidate What-If Analysis Group Ungroup Subtotal Show Detail Hide Detail Outline

A1 fx

Book1

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Sheet1 Sheet2 Sheet3

Excel Help

histogram Search

Load the Analysis ToolPak

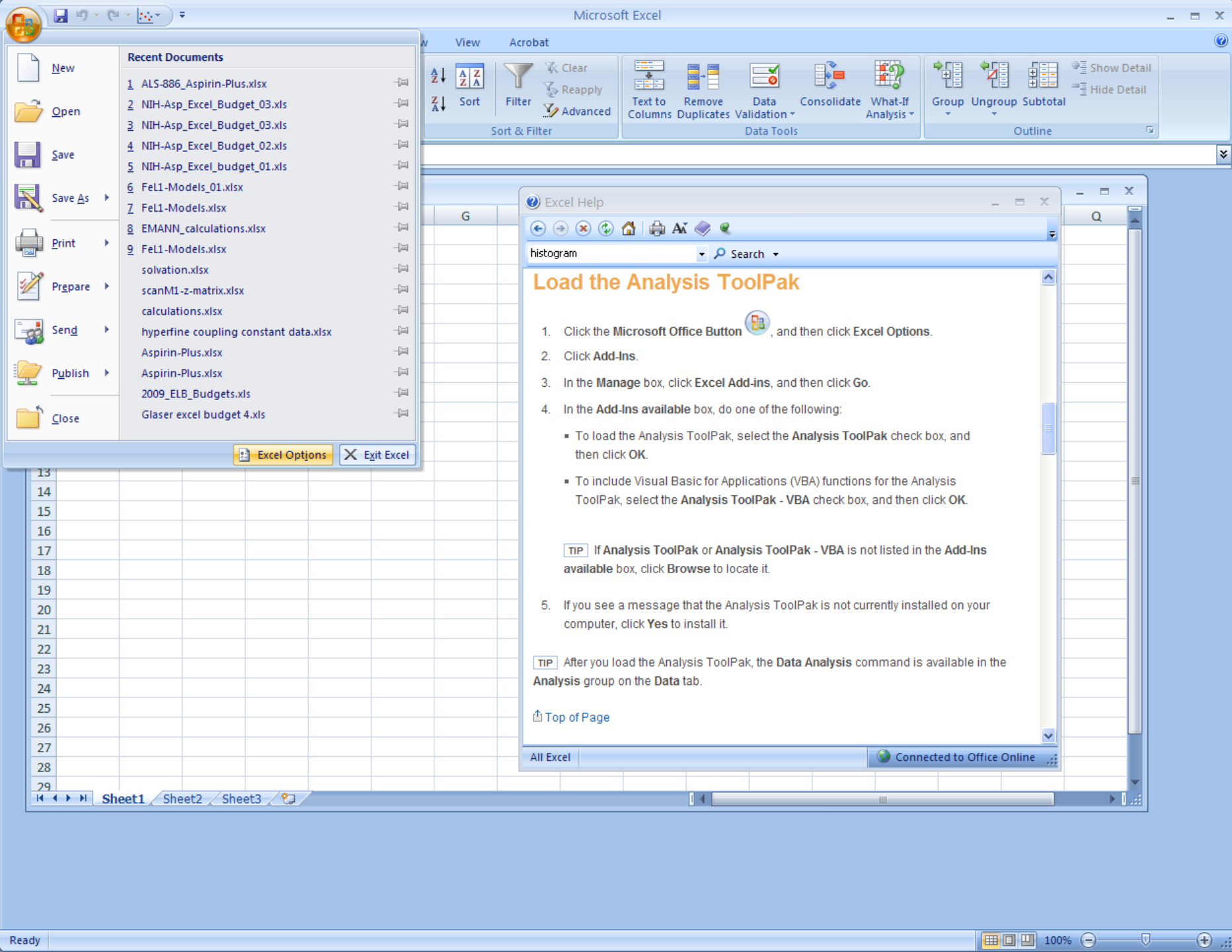
1. Click the **Microsoft Office Button** , and then click **Excel Options**.
2. Click **Add-Ins**.
3. In the **Manage** box, click **Excel Add-ins**, and then click **Go**.
4. In the **Add-Ins available** box, do one of the following:
 - To load the Analysis ToolPak, select the **Analysis ToolPak** check box, and then click **OK**.
 - To include Visual Basic for Applications (VBA) functions for the Analysis ToolPak, select the **Analysis ToolPak - VBA** check box, and then click **OK**.
5. If you see a message that the Analysis ToolPak is not currently installed on your computer, click **Yes** to install it.

TIP If **Analysis ToolPak** or **Analysis ToolPak - VBA** is not listed in the **Add-Ins available** box, click **Browse** to locate it.

TIP After you load the Analysis ToolPak, the **Data Analysis** command is available in the **Analysis** group on the **Data** tab.

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NIH-Asp_Excel_Budget_03.xls

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NIH-Asp_Excel_Budget_02.xls

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Fel1-Models_01.xlsx

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EMANN_calculations.xlsx

9

Fel1-Models.xlsx

solvation.xlsx

scanM1-z-matrix.xlsx

calculations.xlsx

hyperfine coupling constant data.xlsx

Aspirin-Plus.xlsx

Aspirin-Plus.xlsx

2009_ELB_Budgets.xls

Glaser excel budget 4.xls

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Consolidate

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Group

Ungroup

Subtotal

Show Detail

Hide Detail

Outline

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histogram

Load the Analysis ToolPak

1.

Click the **Microsoft Office Button** , and then click **Excel Options**.

2.

Click **Add-Ins**.

3.

In the **Manage** box, click **Excel Add-Ins**, and then click **Go**.

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 If **Analysis ToolPak** or **Analysis ToolPak - VBA** is not listed in the **Add-Ins available** box, click **Browse** to locate it.

5.

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TIP

 After you load the Analysis ToolPak, the **Data Analysis** command is available in the **Analysis** group on the **Data** tab.

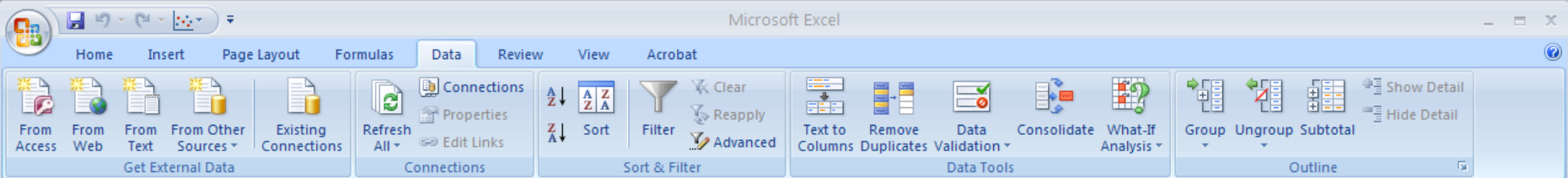
Top of Page

All Excel

Connected to Office Online

Ready

100%



A1

Book1

Excel Options

Popular

Formulas

Proofing

Save

Advanced

Customize

Add-Ins

Trust Center

Resources

Change the most popular options in Excel.

Top options for working with Excel

- ☒ Show **M**ini Toolbar on selection
- ☒ Enable **L**ive Preview
- ☐ Show **D**eveloper tab in the Ribbon
- ☒ Always use ClearType

Color scheme: Blue

ScreenTip style: Show feature descriptions in ScreenTips

Create lists for use in sorts and fill sequences: [Edit Custom Lists...](#)

When creating new workbooks

Use this font: Body Font

Font size: 11

Default view for new sheets: Normal View

Include this many sheets: 3

Personalize your copy of Microsoft Office

User name: glaser

Choose the languages you want to use with Microsoft Office: [Language Set...](#)

Excel Help

histogram

Search

Load the Analysis ToolPak

1. Click the **Microsoft Office Button**, and then click **Excel Options**.
2. Click **Add-Ins**.
3. In the **Manage** box, click **Excel Add-ins**, and then click **Go**.
4. In the **Add-Ins available** box, do one of the following:
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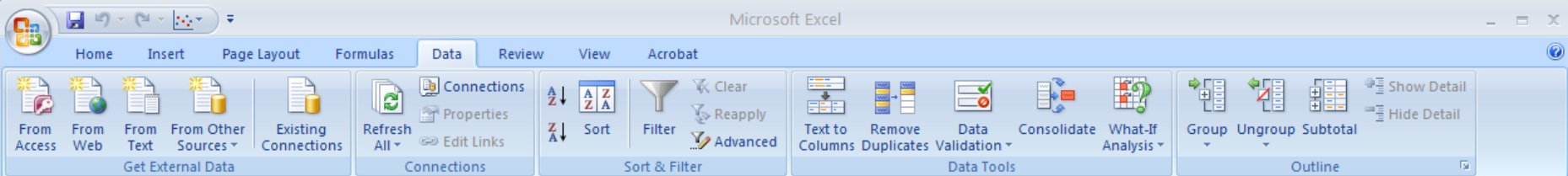
[Top of Page](#)

All Excel

Connected to Office Online

OK

Cancel



Excel Options

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Add-Ins

Trust Center

Resources

View and manage Microsoft Office add-ins.

Add-ins

Name	Location
Active Application Add-ins	
Acrobat PDFMaker Office COM Addin	C:\... 8.0\PDFMaker\Office\PMO...
Inactive Application Add-ins	
Analysis ToolPak	C:\...ice\Office12\Library\An...
Analysis ToolPak - VBA	C:\...Office12\Library\Analys...
ChemOffice/Excel 11	C:\...s\Microsoft Office\Offic...
Conditional Sum Wizard	sumif.xlam
Custom XML Data	C:\...iles\Microsoft Office\Of...
Date (Smart tag lists)	C:\...iles\Microsoft Shared\St...
Euro Currency Tools	eurotool.xlam
Financial Symbol (Smart tag lists)	C:\...iles\Microsoft Shared\St...
Headers and Footers	C:\...iles\Microsoft Office\Of...
Hidden Rows and Columns	C:\...iles\Microsoft Office\Of...
Hidden Worksheets	C:\...iles\Microsoft Office\Of...
Internet Assistant VBA	C:\...icrosoft Office\Office12\...
Invisible Content	C:\...iles\Microsoft Office\Of...
Lookup Wizard	lookup.xlam
Person Name (Outlook e-mail recipients)	C:\...es\Microsoft Shared\Sm...
Solver Add-in	solver.xlam
Document Related Add-ins	
No Document Related Add-ins	
Add-in:	Acrobat PDFMaker Office COM Addin
Publisher:	Adobe Systems, Incorporated
Location:	C:\Program Files\Adobe\Acrobat 8.0\PDFMaker\Office\PMO...
Description: Acrobat PDFMaker Office COM Addin	
Manage:	Excel Add-ins
Go...	

Excel Help

histogram

Search

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All Excel

Connected to Office Online

OK

Cancel

Microsoft Excel

Home Insert Page Layout Formulas Data Review View Acrobat

From Access From Web From Text From Other Sources Existing Connections Refresh All Connections Sort Filter Text to Columns Remove Duplicates Data Validation Consolidate What-If Analysis Group Ungroup Subtotal Show Detail Hide Detail Outline

A1

Book1

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

A B C D E F G H

Add-Ins

Add-Ins available:

- ☒ Analysis ToolPak
- ☒ Analysis ToolPak - VBA
- ☐ ChemOffice/Excel 11
- ☐ Conditional Sum Wizard
- ☐ Euro Currency Tools
- ☐ Internet Assistant VBA
- ☐ Lookup Wizard
- ☐ Solver Add-in

OK Cancel Browse... Automation...

Analysis ToolPak - VBA

VBA functions for Analysis ToolPak

Excel Help

histogram Search

Load the Analysis ToolPak

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All Excel Connected to Office Online

Sheet1 Sheet2 Sheet3

Ready 100%

Microsoft Excel

Home Insert Page Layout Formulas Data Review View Acrobat

From Access From Web From Text From Other Sources Existing Connections Refresh All Properties Edit Links Connections Sort & Filter Filter Clear Reapply Advanced Text to Columns Remove Duplicates Data Validation Consolidate What-If Analysis Group Ungroup Subtotal Outline Analysis

A1 fx

Book1

	A	B	C	D	E	F	G	H
1								
2								
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29								

Sheet1 Sheet2 Sheet3

Excel Help

histogram Search

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All Excel Connected to Office Online

Microsoft Excel

Home Insert Page Layout Formulas Data Review View Acrobat

Get External Data Refresh All Edit Links Connections Sort & Filter Filter Clear Reapply Advanced Data Tools Text to Columns Remove Duplicates Data Validation Consolidate What-If Analysis Outline Analysis

D17 fx

Book1

	A	B	C	D	E	F	G	H	I	J	K	L
2	Students	Test #1	Test #2		Bin Range							
3	A	75			50							
4	B	78			55							
5	C	68			60							
6	D	69			65							
7	E	72			70							
8	F	71			75							
9	G	81			80							
10	H	76			85							
11	I	74			90							
12	J	95			95							
13	K	82			100							
14	L	63										
15	M	72										
16	N	72										
17	O	68										
18	P	91										
19	Q	79										
20	R	82										
21	S	73										
22	T	78										
23	Count	20										
24	Minimum	63										
25	Maximum	95										
26	Average	75.95										
27	Std. Dev.	7.721978										
28												

Sheet1 Sheet2 Sheet3

Histogram

Input

Input Range:

Bin Range:

☐ Labels

Output options

☐ Output Range:

☒ New Worksheet Ply:

☐ New Workbook

☐ Pareto (sorted histogram)

☐ Cumulative Percentage

☐ Chart Output

OK Cancel Help

B3

Book1

	A	B	C	D	E	F	G	H	I	J	K	L	M
2	Students	Test #1	Test #2		Bin Range								
3	A	75			50								
4	B	78			55								
5	C	68			60								
6	D	69			65								
7	E	72			70								
8	F	71			75								
9	G	81			80								
10	H	76			85								
11	I	74			90								
12	J	95			95								
13	K	82			100								
14	L	63											
15	M	72											
16	N	72											
17	O	68											
18	P	91											
19	Q	79											
20	R	82											
21	S	73											
22	T	78											
23	Count	20											
24	Minimum	63											
25	Maximum	95											
26	Average	75.95											
27	Std. Dev.	7.721978											
28													
29													
30													
31													
32													

Histogram

Input

Input Range:

Bin Range:

☐ Labels

Output options

☒ Output Range:

☐ New Worksheet Ply:

☐ New Workbook

☐ Pareto (sorted histogram)

☐ Cumulative Percentage

☒ Chart Output

OK Cancel Help

Microsoft Excel

Chart Tools

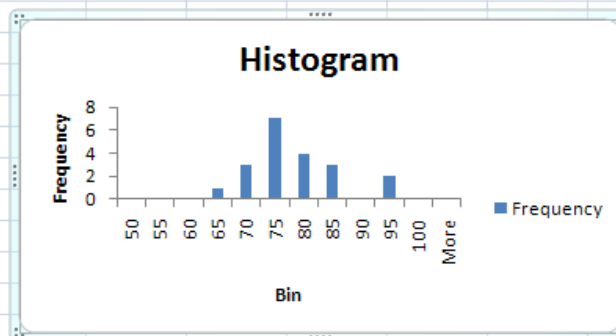
Home Insert Page Layout Formulas Data Review View Acrobat Design Layout Format

Get External Data Refresh All Properties Edit Links Connections Sort & Filter Filter Clear Reapply Advanced Text to Columns Remove Duplicates Data Tools Data Validation Consolidate What-If Analysis Group Ungroup Subtotal Outline Analysis

Chart 7

Book1

	A	B	C	D	E	F	G	H	I	J	K	L	M
2	Students	Test #1	Test #2		Bin Range	Bin	Frequency						
3	A	75			50	50	0						
4	B	78			55	55	0						
5	C	68			60	60	0						
6	D	69			65	65	1						
7	E	72			70	70	3						
8	F	71			75	75	7						
9	G	81			80	80	4						
10	H	76			85	85	3						
11	I	74			90	90	0						
12	J	95			95	95	2						
13	K	82			100	100	0						
14	L	63			More		0						
15	M	72											
16	N	72											
17	O	68											
18	P	91											
19	Q	79											
20	R	82											
21	S	73											
22	T	78											
23	Count	20											
24	Minimum	63											
25	Maximum	95											
26	Average	75.95											
27	Std. Dev.	7.721978											



Histogram

