Statistical treatment of data

Including statistical analysis using Microsoft® Excel®

Mean and standard deviation

Suppose that we make N measurements of the same quantity x. For the measurements to be comparable we usually arrange for the conditions under which x is measured to be as closely matched as possible. For example, if you wanted a meaningful idea of how much you weigh, you wouldn't jump on the bathroom scale right after the big Thanksgiving dinner and then try to compare that result with how much you weigh after running a marathon, would you? Of course not – instead, you might try to weigh yourself first thing every morning for a week just after you wake up.

Despite our best efforts, however, N measurements of the same quantity x can never be made under exactly matched conditions. There are many reasons for this fact. Some are psychological and physiological: the more times we repeat an operation, the better (or worse) we get at it and the manner in which a scientist executes a measurement (i.e., technique) influences the experimental outcome. Some are physical: the system under study changes with the passage of time in ways we cannot fully control. Given that individual measurements of the same quantity vary, what is the best way to report the data?

One approach is to determine the mean of the measurements of x and to report the variation in the data as the standard deviation. The mean of the N measurements of x is denoted by the symbol \overline{x} and is defined by

$$\bar{x} = \frac{x_1 + x_2 + x_3 + \dots + x_N}{N} = \frac{\sum_{i=1}^{i=N} x_i}{N}$$

where the x_i represent the individual measurements of the quantity x and the standard deviation σ is defined by

$$\sigma = \sqrt{\frac{(x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + (x_3 - \bar{x})^2 + \dots + (x_N - \bar{x})^2}{N}} = \sqrt{\frac{\sum_{i=1}^{i=N} (x_i - \bar{x})^2}{N}}$$

The mean expresses the central tendency in a set of data. The standard deviation expresses the theoretical expectation that 68.27% of the measurements of x will lie within one standard deviation on either side of the mean when x is measured an infinite number of times.

Example

Table A-1 presents the rainfall measured at Boston during September from 1999 to 2003 and the quantities needed to determine the mean September rainfall and its standard deviation. The mean is

Table A-1 September rainfall at Boston, 1999–2003 Quantities needed in the calculation of the mean and of the standard deviation

i		x_i	$x_i - \overline{x}$	$(x_i - \bar{x})^2$	
	Year	Rainfall [inch]	Deviation from the mean [inch]	Deviation squared [inch ²]	
1	1999	9.86	5.65	31.92	
2	2000	2.87	-1.34	1.80	
3	2001	2.29	-1.92	3.69	
4	2002	3.39	-0.82	0.67	
5	2003	2.65	-1.56	2.43	
	Sum	21.06		40.51	

$$\bar{x} = \frac{9.86 + 2.87 + 2.29 + 3.39 + 2.65}{5} = \frac{21.06}{5} = 4.2$$
 (to one decimal)

The standard deviation is

$$\sigma = \sqrt{\frac{(9.86 - 4.212)^2 + (2.87 - 4.212)^2 + (2.29 - 4.212)^2 + (3.39 - 4.212)^2 + (2.65 - 4.212)^2}{5}}$$

= 2.8 (to one decimal)

Thus, the best way to report the mean September rainfall is 4.2 ± 2.8 inch.

Recall that σ expresses the theoretical expectation that 68.27% of an infinite number of measurements will lie within one standard deviation on either side of the mean, that is, between 4.2 - 2.8 = 1.4 inch and 4.2 + 2.8 = 7.0 inch for the rainfall data set we are considering. Because the rainfall was measured only five and not an infinite number of times, four (2.87, 2.29, 3.39, 2.65) of the five measurements (80%) fall within one standard deviation on either side of the mean. Agreement with the theoretical expectation improves as the number of measurements increases.

The t-test

Calculating the standard deviation of a mean is one way of quantitatively assessing experimental variance. As useful as it is, the standard deviation suffers from the weakness of its being rigorously defined only when $N = \infty$ and we can never measure anything an infinite number of times. Another technique, the t-test, is useful when the mean is calculated from a small (N < 30) number of measurements. In the t-test, we calculate a confidence interval about the mean calculated from N < 30 measurements. The confidence interval specifies a range of values within which we would expect to find the mean if we were to measure a quantity an infinite number of times. The confidence interval about a mean is defined by

Table A-2 *t*-Scores at the 99% and 95% confidence levels as a function of the number of measurements *N*

N	<i>t</i> 99%	<i>t</i> 95%
2	63.657	12.706
3	9.925	4.303
4	5.841	3.182
5	4.604	2.776
6	4.032	2.571
7	3.707	2.447
8	3.499	2.365
9	3.355	2.306
10	3.250	2.262

confidence interval =
$$\pm \frac{t_c \sigma}{\sqrt{N}}$$

where t_c is the t-score at the c% confidence level, σ is the standard deviation of the mean, and N is the number of measurements from which the mean is determined. Table A-2 lists t-scores at the 99% and 95% confidence levels as a function of the number of measurements N.

Example

Suppose we measure the rainfall at Boston during September from 1999 to 2003 (i.e., N = 5) and obtain a mean of 4.2 inch and a standard deviation of 2.8 inch. What are the values of the confidence intervals at the 99% and 95% confidence levels?

To compute the confidence interval at the 99% level, select $t_{99\%}$ for N=5 from Table A-2 (i.e., 4.604). The confidence interval is given by

99% confidence interval =
$$\pm \frac{t_{99\%}\sigma}{\sqrt{N}} = \pm \frac{(4.604)(2.8)}{\sqrt{5}}$$

 $=\pm5.8$ (to one decimal)

Thus, if we were to measure September rainfall at Boston an infinite number of times, we would be 99% sure that the mean would lie somewhere between 4.2 - 5.8 = -1.6 inch and 4.2 + 5.8 = 10.0 inch – a pretty big spread indeed.

In like fashion, to construct the confidence interval at the 95% level, select $t_{95\%}$ for N=5 from Table A-2 (i.e., 2.776). The confidence interval is given by

95% confidence interval =
$$\pm \frac{t_{95\%}\sigma}{\sqrt{N}} = \pm \frac{(2.776)(2.8)}{\sqrt{5}}$$

 $=\pm3.5$ (to one decimal)

Hence, we can be 95% certain that, if we to measure September rainfall at Boston an infinite number of times, the mean would lie somewhere between 4.2 - 3.5 = 0.7 inch and 4.2 + 0.00

3.5 = 7.7 inch. Note that the confidence interval shrinks (from ± 5.8 inch at 99% confidence to ± 3.5 inch at 95% confidence) if we are willing to hazard a lesser degree of certainty.

Incidentally, more than a century of record keeping has shown that the average September rainfall at Boston is 3.47 inch – a value that lies within both the 99% and the 95% confidence intervals.

Linear least-squares

Suppose a data set relating two variables *x* and *y* is expected to obey the linear relationship

$$y = mx + b$$

where m is the slope of the line and b is the value of the y-intercept. Because of uncertainties in measurement, a plot of the x values versus the y values will not, in general, yield a graph in which all of the points lie on a single straight line. We could crudely estimate m and b by "eyeballing" a line, that is, by drawing a line above which there are as many points as below, but a more sophisticated approach is available.

The least-squares line is the best straight line that can be drawn through a set of data points. Deriving the equation of the least-squares line is a difficult enterprise involving differential calculus, solution of simultaneous equations and statistics: we will simply present the computational formulas here.

For *N* data pairs $\{x_1, y_1\}$, $\{x_2, y_2\}$, $\{x_3, y_3\}$, ..., $\{x_N, y_N\}$, the slope *m* of the least-squares line is given by

$$m = \frac{\sum_{i=1}^{i=N} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{i=N} (x_i - \bar{x})^2}$$

and b, the least-squares line's y-intercept, is given by

$$b = \overline{y} - m\overline{x}$$

where \bar{x} is the mean of the x_i and \bar{y} is the mean of the y_i .

The least-squares slope itself is subject to uncertainty. One way to express the variation in the data is to report the standard error of estimate σ_m in the least-squares slope:

$$\sigma_{m} = \sqrt{\frac{\sum_{i=1}^{i=N} (y_{i} - \bar{y})^{2}}{\sum_{i=1}^{i=N} (x_{i} - \bar{x})^{2}} - m^{2}}$$

where \bar{x} is the mean of the x_i , \bar{y} is the mean of the y_i , m is the least-squares slope and N is the number of data pairs used in constructing the least-squares line. The standard error of estimate σ_m indicates that, because of uncertainties in measurement, the least-squares slope m could be as high as $m + \sigma_m$ or as low as $m - \sigma_m$.

Example

Just in case you don't hit the lottery, it might be interesting to investigate whether there is a relationship between income

Table A-3 Years of school attended (x) and average household income (y) in thousands of dollars (k\$); Calculation of the linear least-squares slope m and intercept b

i	x _i [year]	<i>yi</i> [k\$]	$x_i - \overline{x}$ [year]	$y_i - \bar{y}$ [k\$]	$(x_i - \overline{x})(y_i - \overline{y})$ [year·k\$]	$(x_i - \bar{x})^2$ [year ²]
1	11	32	-3	-30	90	9
2	12	46	-2	-16	32	4
3	13	57	-1	-5	5	1
4	14	60	0	-2	0	0
5	16	83	2	21	42	4
6	18	94	4	32	128	16
Sum	84	372			297	34
Mean	14	62				

What is your situation in life?
Are you the typical college freshman who has already gone to school for 12 years? If so, the least-squares relationship says that you can expect an average annual household income of \$44,400 if you drop out of school now. On the other hand, finishing college typically boosts your annual income to \$79,200.

and the number of years you go to school. Table A-3 lists data collected by the United States Census Bureau on years of school attended by the head of a household and average household income; the quantities needed to compute the linear-least squares slope and intercept are also presented.

The least-squares slope m is given by

$$m = \frac{\sum_{i=1}^{i=N} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{i=N} (x_i - \bar{x})^2} = \frac{297}{34} = 8.7 \text{ (to one decimal)}$$

The slope suggests that you will earn \$8,700 per year for every year of school you complete. The least-squares *y*-intercept *b* is given by

$$b = \overline{y} - m\overline{x} = 62 - (8.7)(14) = -60$$

Table A-4 presents the quantities needed to compute the standard error of estimate σ_m in the least-squares slope; σ_m is given by

$$\sigma_{m} = \sqrt{\frac{\sum_{i=1}^{i=N} (y_{i} - \overline{y})^{2}}{\sum_{i=1}^{i=N} (x_{i} - \overline{x})^{2}} - m^{2}} = \sqrt{\frac{2650}{34} - (8.7)^{2}} = 0.8$$

Thus, the data suggest that annual household income in thousands of dollars (*y*) and the number of years that the head of the household attends school (*x*) follow the linear relationship

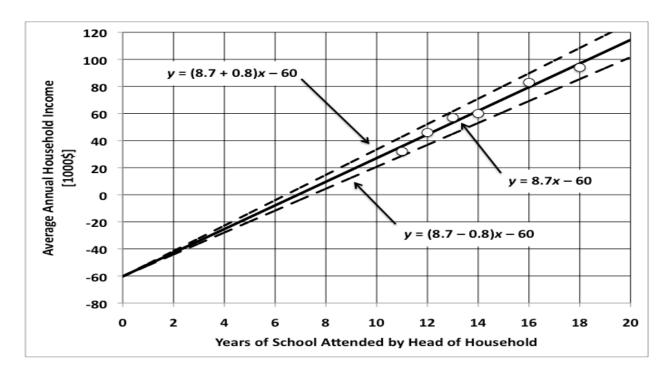
$$y = (8.7 \pm 0.8)x - 60$$

Table A-4 Years of school attended (x) and average household income (y) in thousands of dollars (k\$); Calculation of the standard error of estimate σ_m in the least-squares slope m

i	x _i [year]	<i>yi</i> [k\$]	$x_i - \overline{x}$ [year]	$y_i - \overline{y}$ [k\$]	$(x_i - \bar{x})^2$ [year·k\$]	$ \frac{(y_i - \overline{y})^2}{[\text{year}^2]} $
1	11	32	-3	-30	9	900
2	12	46	-2	-16	4	256
3	13	57	-1	-5	1	25
4	14	60	0	-2	0	4
5	16	83	2	21	4	441
6	18	94	4	32	1	1024
Sum	84	372			34	2650
Mean	14	62				

Figure A-1 shows a plot of the least-squares line and of the two lines indicating the uncertainty in the slope.

Figure A-1 A plot of the number of years of school completed by the head of the household (x) and average annual household income in thousands of dollars (y). The solid line represents the least-squares line; the dashed lines indicate the uncertainty in the slope caused by the variation in the data.



Statistical analysis of data using Microsoft® Excel®

Statistical analysis is an important part of this course because this is how scientists evaluate the quality of the data collected after performing an experiment. However, computing essential statistical quantities such as the standard deviation, linear least-squares slope, *y*-intercept and standard error of estimate of a data set can be an arduous task if the only tool at your disposal is a calculator. In order to make the calculations less burdensome, we offer a guide to using the popular Microsoft® Excel® spreadsheet application.

Open Excel® and in row 1 of column A enter the heading **xi**, then enter the heading **yi** in row 1 of column B. The data in the **xi** column represents the year from the previously discussed September rainfall example; the data in the **yi** column represents the September rainfall data in inches. Now enter the data in the appropriate cells. The spreadsheet should look something like this:

<>	А	В	С	D	Е	F	G
1	хi	yi					
2	1999	9.86					
3	2000	2.87					
4	2001	2.29					
5	2002	3.39					
6	2003	2.65					
7							
8							
9							
10							
11							
12							

You calculate quantities in Excel® by typing a *formula* in the cell where you want the result to be displayed. Formulas

- begin with an equal sign (=)
- may include *operators* that operate on *operands*. The most commonly employed operators are + for addition, for sub-

traction, * for multiplication, / for division, and ^ for exponentiation. The operands are cell locations denotated in the column–row system (e.g., A2). Thus, the formula that multiplies the number in cell A2 by the number in cell B2 is =A2*B2.

• may include *functions* that take *arguments*. The arguments of a function are most commonly, but not necessarily, cell locations. Arguments are written in parentheses following the name of that function. Some functions take the values in a range of cells as their arguments. A range of cells is specified by denoting the locations of the first and last cell in the range separated by a colon (:).

We now need a place to store the results of the statistical calculations we are about to perform. In Column D enter the headings shown below: the results will be placed in Column E next to the corresponding heading.

<>	А	В	С	D	Е	F	G
1	хi	yi					
2	1999	9.86		Nx			
3	2000	2.87		sum y			
4	2001	2.29		mean y			
5	2002	3.39		std dev y			
6	2003	2.65		99% conf int			
7				95% conf int			
8				slope			
9				y int			
10				dev sq x			
11				dev sq y			
12				std error			

We will use Excel®'s built-in functions (listed below) to perform the calculations. We caution you against using these functions uncritically and blindly trusting the answer: if you input the data incorrectly, or if the syntax of the formula in which these functions are used is incorrect, the result will be wrong. Remember: Garbage in, garbage out.

COUNT(range)

This function counts the number of cells that contain numbers in the specified range; thus, the **COUNT()** function can be used to calculate the number of measurements N in a data set. Suppose we wish to find the number of x values in the spreadsheet. The x value data starts at cell A2 and ends at cell A6: entering the formula **=COUNT(A2:A6)** in cell E2 returns N = 5.

SUM(range)

This function sums the numbers in the specified range. Suppose we wish to find the sum of the y values in the spreadsheet (i.e., $\sum y$). The y value data starts at cell B2 and ends at cell B6: entering the formula **=SUM(B2:B6)** in cell E3 returns $\sum y = 21.06$.

AVERAGE(range)

This function calculates the mean of the numbers in the specified range. Suppose we wish to find the mean of the y values in the spreadsheet (i.e., \bar{y}). The y value data starts at cell B2 and ends at cell B6: entering the formula **=AVERAGE(B2:B6)** in cell E4 returns $\bar{y} = 4.212$.

STDEVP(range)

This function calculates the standard deviation σ of the numbers in the specified range. Suppose we wish to find the standard deviation of the y values in the spreadsheet. The y value data starts at cell B2 and ends at cell B6: entering the formula **=STDEVP(B2:B6)** in cell E5 returns σ = 2.8464181.

TINV(probability, degrees of freedom)

Excel® lacks a built-in function for calculating a confidence interval when the number of measurements N < 30; instead, the required formula must be constructed by the user. Recall that the confidence interval about a mean is defined by

confidence interval =
$$\pm \frac{t_c \sigma}{\sqrt{N}}$$

where t_c is the t-score at the c% confidence level, σ is the standard deviation of the mean, and N is the number of measure-

ments from which the mean is determined. Excel® employs the TINV(probability,degrees of freedom) function to determine the appropriate *t*-score. The probability argument of the TINV() function corresponds to the confidence level and the degrees of freedom argument of the TINV() function corresponds to the number of measurements, but the correspondences makes sense only to a statistician.

If you are calculating a 99% confidence interval, the **probability** argument of the **TINV()** function is **0.01**. If you are calculating a 95% confidence interval, the **probability** argument of the **TINV()** function is **0.05**. If you are calculating a 90% confidence interval, the **probability** argument of the **TINV()** function is **0.10**, and so on.

The **degrees of freedom** argument of the **TINV()** function equals the number of measurements N-1. If the number of measurements N=3, the **degrees of freedom** argument of the **TINV()** function **2**. If the number of measurements N=4, the **degrees of freedom** argument of the **TINV()** function is **3**. If the number of measurements N=5, the **degrees of freedom** argument of the **TINV()** function is **4**, and so on.

Because N = 5 in the spreadsheet we are considering, the t-score at the 99% confidence level is given by **TINV(0.01,4)** whereas the t-score at the 95% confidence level is given by **TINV(0.05,4)**.

Suppose we wish to find the 99% confidence interval of the five y values in cells B2 to B6 in the spreadsheet. There are several ways to proceed. The easiest method is first to calculate the standard deviation σ and to store the result in a cell. Let's say you enter the formula **=STDEVP(B2:B6)** in cell E5. Entering the formula **=TINV(0.01,4)*E5/SQRT(5)** in cell E6 returns the 99% confidence interval = 5.860814209. The formula **=TINV(0.01,4)*STDEVP(B2:B6)/SQRT(5)** gives the same result. If you are an Excel® animal, try

=TINV(0.01,COUNT(B2:B6)-1)*STDEVP(B2:B6)/SQRT(COUNT(B2:B6))

Suppose we wish to find the 95% confidence interval of the five y values in cells B2 to B6 in the spreadsheet. We can first calculate the standard deviation σ : enter the formula **=STDEVP(B2:B6)** in cell E5. Entering the formula

=TINV(0.05,4)*E5/SQRT(5) in cell E7 returns the 95% confidence interval = 3.534294878, as does entering the formula **=TINV(0.05,4)*STDEVP(B2:B6)/SQRT(5)**, as does entering the formula

=TINV(0.05, COUNT(B2:B6)-1)*STDEVP(B2:B6)/SQRT(COUNT(B2:B6))

SLOPE(y value range,x value range)

This function calculates the linear least-squares slope m in one step! In our spreadsheet the x values start at cell A2 and end at cell A6 and the y values start at cell B2 and end at cell B6: entering the formula **=SLOPE(B2:B6,A2:A6)** in cell E8 returns m = -1.39. Note that the y value range is entered as the first argument of the **SLOPE()** function.

INTERCEPT(y value range,x value range)

This function calculates the linear least-squares y-intercept b. In our spreadsheet the x values start at cell A2 and end at cell A6 and the y values start at cell B2 and end at cell B6: entering the formula **=INTERCEPT(B2:B6,A2:A6)** in cell E9 returns b = 2785.602. Note that the y value range is entered as the first argument of the **INTERCEPT()** function.

DEVSQ(range)

Excel® lacks a built-in function for calculating the standard error of estimate σ_m of a linear least-squares line; the required formula must be constructed by the user. Recall that σ_m is defined by

$$\sigma_{m} = \sqrt{\frac{\sum_{i=1}^{i=N} (y_{i} - \bar{y})^{2}}{\sum_{i=1}^{i=N} (x_{i} - \bar{x})^{2}} - m^{2}}$$

where \bar{x} is the mean of the x_i , \bar{y} is the mean of the y_i , m is the least-squares slope and N is the number of data pairs used in constructing the least-squares line.

The function **DEVSQ()** calculates the quantities $\Sigma (x_i - \overline{x})^2$ and $\Sigma (y_i - \overline{y})^2$ required in the calculation of σ_m . In our spreadsheet the x values start at cell A2 and end at cell A6 and the y values start at cell B2 and end at cell B6: entering the formula **=DEVSQ(A2:A6)** in cell E10 returns the quantity $\Sigma (x_i - \overline{x})^2 = 10$. Likewise, entering the formula **=DEVSQ(B2:B6)** in cell E11 returns the quantity $\Sigma (y_i - \overline{y})^2 = 40.51048$.

Let's suppose that we already calculated the linear least-squares slope m of the N=5 data pairs and placed the result in cell E8. We just placed the value of $\Sigma(x_i-\bar{x})^2$ in cell E10 and the value of $\Sigma(y_i-\bar{y})^2$ in cell E11. The value of σ_m is determined by entering the formula **=SQRT(((E11/E10)-E8^2)/3)** in E12; the value returned is $\sigma_m=0.840426082$. Note that we have made liberal use of parentheses in constructing the formula for σ_m so that Excel® doesn't get confused about what it's multiplying, squaring, dividing, and what's supposed to be the argument of the **SQRT()** function. You must be very careful about using parentheses when entering Excel® formulas: faulty grouping may return a result, but that result will be wrong.