Institut for Matematik og Datalogi
Syddansk Universitet – Odense Universitet

September 11, 2001
JFB

Introduction to Information Technology
E00 – Lecture 2

Lecture, September 7

We began with an introduction to the course and a definition of an algorithm. The concept of a tree structure was introduced, motivated by the organization of files in folders. Sections 1.1, 1.2, and 1.3 and section 11.3.1 in the textbook.

Lecture, September 21

We will start with section 1.4 in the textbook. Then, we will be talking about algorithms from chapters 2 and 3 in the textbook (sections 2.1 through 2.3.1 and the algorithm from 3.5.3), and we will introduce spreadsheets from section 11.2 (we will skip most of subsection 11.2.4, since it assumes knowing much about what was covered earlier in the textbook - you could read it later when you know more about computer science).

Lecture, October 1, in U45

We will continue talking about algorithms from chapters 2 (from 2.3.3 to the end of the chapter) and 3 in the textbook. We will also talk about Maple, a program for symbolic computation. Read section 11.4 in the text, but keep in mind that the syntax you will you use with Maple is different from the syntax in Mathematica, which is used for the examples in the textbook.

Primary Lab 2 - for week 39

Bring your booklet on Excel if you have one. Help for this lab can be found from the home page for this course.

The motivation for this lab comes from an elective course in the second semester, BM102. It concerns enzyme kinetics, which you can read about in chapter 6 of your biology text, *Biology*, by Campbell. Although this lab concerns enzyme kinetics, the skills used are more generally relevant, since this type of plotting is done frequently in the biological sciences and is important for writing reports about experimental data.

Exercise 1

The purpose of this lab is to learn about a spreadsheet program, called Excel. The version of Excel you will be using is part of Microsoft's *Office 2000*. First, change your version of Office 2000 to Danish. Click on **Start** → **Programmer** → **Microsoft Office Tools** → **Microsoft Office Language Settings**. Find Danish in the dialog box under "Display menu and Dialog boxes in:". Click on **OK**.

To start Excel, click on **Start** → **Programmer** → **Microsoft Excel**. Since this is the first of those programs you will be using, when you start up the program, you will be asked for your name and initials. Just give them as asked.

If you are more experienced with Excel, do exercise 8 before continuing here. If you do exercises 7 and 8, you can just type in every second pair of numbers below, starting with the second.

You should type in two columns of numbers and some headings. The first column will contain concentrations of the substrate and the second will contain the absorption changes per minute observed experimentally. Your two columns and the headings should contain the following:

Substrate	**Reaction rate**	
[isocitrate] mM	**ΔA/min**	**μM/min**
0,025	0,009	
0,050	0,016	
0,100	0,023	
0,150	0,026	
0,200	0,030	
1,000	0,040	
2,000	0,041	
3,000	0,041	
4,000	0,040	

Note that a comma is used instead of a decimal point, since you have the Danish version of Excel. When we use Maple, you will decimal points, since there is no Danish version.

Note that Δ is D in the "Symbol" type font, and μ is m in the "Symbol" type font.

The third heading is present because of a calculation you will now.

Exercise 2

From the observed values for the absorption rate, calculate the reaction rate in μM/min. This can be done by dividing the absorption rate by the extinction coefficient which in this case is 6.22mM^{-1}/min to get mM/min and then multiplying by 1000. (Note that the numbers are very small if you use the units mM/min.) Do these calculations in column C and give three digits of precision past the decimal point. The result should be:

1,447
2,572
3,698
4,180
4,823
6,431
6,592
6,592
6,431

Exercise 3

Plot your data from columns A and C in a graph. The horizontal axis should be labelled **Isocitrate concentration (mM)** and the vertical **Reaction rate μM/min**. (The symbol μ is m in the "Symbol" type font.) Use squares for experimental points.

Note that you should follow several important standard practices in making this plot:

- Label both axes.
- Indicate which units of measure are being used (mM and μM/min).
- Use different symbols for different data sets. (Not relevant here since there is only one data set so far.)
- Use circles or squares for experimental points and $\times$ or $+$ for calculated points.
- All points should lie within axes, so there are numbers on the axis at least as far out as the data goes.
- Sketch smooth lines through the points or draw straight lines between points, but be consistent. The curve should not extend beyond the points, except when extrapolating.
- Include the point $(0, 0)$ if it is appropriate; axes should usually start at zero.
- Choose the orientation of your plot to spread out the points, and consider using logarithmic scales to spread points. (Not relevant here.)

Try changing one of the data point values to see it change in the plot. Then change it back to the original value.

Exercise 4

Compute the inverses of your data in two new columns. Thus, if a value s appeared in column A, $1/s$ should appear in column D. Similarly, if a value v appeared in the column C, $1/v$ should appear in column E. Your columns should end up with the following, where the numbers should be calculated, not typed in.

1/s	**1/v**
40,000	0,691
20,000	0,389
10,000	0,270
6,667	0,239
5,000	0,207
1,000	0,156
0,500	0,152
0,333	0,152
0,250	0,156

Exercise 5

In order to get good estimates for a formula which could predict the experimental data, you can use a graph of the two columns you just calculated. The formula should have the form: $v = \frac{V_{\max} \cdot s}{k_m + s}$. Notice that this is equivalent to $1/v = (\frac{k_m}{V_{\max}})(1/s) + \frac{1}{V_{\max}}$, so the points should fall almost on a line which intercepts the x-axis at $-1/k_m$ and the y-axis at $1/V_{\max}$. The value $V_{\max}$ is especially interesting because the limit of $\frac{V_{\max} \cdot s}{k_m + s}$ as s approaches infinity is $V_{\max}$.
Plot these two new columns from exercise 4 in a graph. The horizontal axis should be labelled **1/s** and the vertical **1/v**.

Exercise 6

Try to estimate where a "good" line through the points in your last graph would intersect the axes. Use these values for $1/V_{\max}$ and $1/k_m$ to create a formula which would predict the values in column C in your spreadsheet. Calculate these values in column H, and label the column **calculated**. Try adjusting your estimates for $1/V_{\max}$ and $1/k_m$ to get a little closer to your experimental values. Now plot these calculated points and the experimental points so that you can compare them. The new calculated points can be added to the plot you made in Exercise 3.

Exercise 7 - no help on the Web

One possible method of checking how close your experimental values are to your predicted ones is just to check how many are larger and how many are smaller. (The next lab will concern better statistical tests.) Use the function `HVIS` to determine for each experimental value and the corresponding predicted one, which is larger. You can have the result 1 if the experimental is larger and 0 if the predicted is. Then, summing will say how many are larger. If you have too many ones or zeros, you can go back to exercise 6 and try some other estimates for $1/V_{\max}$ and $1/k_m$.

Exercise 8 - more advanced, no help

Create a macro to adjust headings and columns after you have typed the headings in. Make the headings boldface, make the font a little larger, and adjust the column size automatically to fit the text you have typed. Use **Hjælp** and search for **makro** to find information about how to do this. Then make all your headings this way. Go back to exercise 1.

Exercise 9

Save your worksheet (in a file with a meaningful name, so it can be found again). E-mail your worksheet, with at least the first 6 exercises completed correctly, to your lab instructor. Remember to logoff your computer, but do not push any buttons on it.