# COLLABORATIVE LABORATORY FOR QUANTITATIVE DATA ANALYSIS

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## ABSTRACT

In this project, students share experimental results to perform data analysis and to develop an appreciation of precision, accuracy and reliability of experimental data and of the scientific method. The number of students taking Junior Chemistry means that the data sets are large and naturally contain random, systematic, and even deliberate errors. By forcing students to work with a wide range of measurements including their own, students develop an appreciation of the importance of the role of human error in the physical sciences. In doing so and in using spreadsheet software, key generic attributes including quantitative, problem solving and inquiry skills are developed and deficiencies in the computer skills are addressed. The project has led to real improvements in the development of generic attributes in our courses, at minimal expense.

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## INTRODUCTION

Graduate attributes are those skills and qualities that students should possess alongside discipline knowledge upon graduation (Bowden, Hart, King, Trigwell & Watts, 2000). There are generic graduate attributes that should be achieved by all graduates, irrespective of their degree program. Universities use these qualities to differentiate their graduates and to increase their marketability to prospective employers because they are deemed "work ready" and capable of ongoing learning and development (Barrie, 2007). By stressing the employability of its graduates, a university can in turn seek to make a distinction when marketing their courses.

Science graduates, however, should acquire additional specific generic and science procedural skills (Jones, 2009). They should be trained in and ready to apply the scientific method in their professional lives. It is just these quantitative, problem solving and inquiry skills that make science students so employable in a variety of graduate careers outside science (Jones, Dermoudy, Hannan, James, Osborn & Yates, 2007). Science graduates should possess the employability skills required in a competitive and global employment market (DEST, 2002). Whilst subject specific knowledge is important in research and a narrow range of other careers, the ability to tackle new problems using the scientific method is the key attribute that science graduates can also use to differentiate themselves in other careers.

The types of skills and attributes that are distinctive of the scientific method are (or should be) an integral and explicit enabling component of the science degree (Barrie, 2007). However, these transferrable skills should be central learning outcomes not only for students who graduate in scientific disciplines but also for the many more who only take Junior Science units. For such students, the exposure to the scientific method and to the ways in which scientists work is arguably much more important than the acquisition of subject specific knowledge.

In the design of a Junior Science unit, the overriding facet is commonly its preparation for the Intermediate Science units for which it is a pre-requisite. This often translates to a focus on subject specific, content 'dot points' and a first year of the BSc degree which is extremely content heavy (Leggett, Kinnear, Boyce & Bennett, 2004). There is usually considerably less focus on the development of quantitative, problem solving and inquiry skills leading to an uneven skill set in Second Year students (Green, Hammer & Star, 2009). The development of these skills occurs in the 3<sup>rd</sup> and 4<sup>th</sup> years of the degree where there is a focus on research projects, and many of the attributes may only be taught at a foundation level in the first year curriculum (Barrie, 2006; Peat, Taylor & Franklin, 2005).

The rationale for the implicit introduction and development of the scientific method in Junior Science thus covers both students who will ultimately graduate as scientists and those taking science units as part of a professional degree, for interest or simply to collect credit points. Many first year students do not recognise the generic skills that are developed in first year science units and do not appreciate where their deficiencies in these areas may lie. This can lead to low student engagement in activities specifically designed to develop the scientific method, including laboratory work (Leggett, Kinnear, Boyce & Bennett, 2004). As a result, course and unit evaluation scores pertaining to graduate attributes are, perhaps not surprisingly, traditionally low.

This paper describes one initiative in our ongoing attempts to embed graduate attributes and to develop the scientific method in our Junior Chemistry units. Its aim is to develop skills in data analysis, team work and information technology and to develop an appreciation of how real science works. It seeks to take advantage of the large number of students taking first year Chemistry to provide a large database. It also utilises the range of abilities and attitudes of these students to highlight that even physical sciences like chemistry are human activities (Mahaffy, 2006) and hence open to all the failings and biases of the humans that are engaged in it.

### **METHODS AND RESULTS**

A large number of students, around 2000 students in semester 1 and around 1600 students in semester 2, take Junior Chemistry units at The University of Sydney. We provide 8 units in semester 1 and 7 units in semester 2, including service units for Pharmacy, Veterinary Science and Medical Science degrees and 4 levels of units taken by students in other faculties, including Science. These 4 levels ("Fundamentals", "Mainstream", "Advanced" and "Special Studies") allow us to design units for specific levels of prior knowledge.

In many of our laboratory classes, students record measurements. In this project, all such data is pooled. The students will then download the measurements from around 2000 separate observations and manipulate them. In doing this, they develop skills in dealing with large datasets including graphing and presenting data, statistical analysis and dealing with outliers. They collaborate with a large number of fellow scientists and, hopefully, come to appreciate the meaning of accuracy, precision and significance in numerical results by making value judgements about the reliability and relevance of information in a scientific context.

In this project, data collection and analysis has been performed on 4 experiments. In each case, the experimental instructions were unchanged compared to those used before the intervention. After recording their measurements at the bench, each student enters their data via an online form. The data was collected in this way over the course of the week and automatically released on Friday afternoon in the cross-platform csv (comma separated values) format for students to download and open in any spreadsheet software. The data analysis is performed entirely using the spreadsheet software. The instructions are deliberately tailored towards Excel because this is the spreadsheet software available in the university computer rooms and library and because this is the most common data analysis software used in workplaces. However, all of the tasks can also be tackled using other spreadsheet programs, including Apple iWork and the free OpenOffice and Google documents. Below, we outline the procedures and results for 2 of the 4 experiments.

In the 'Properties of Gases' experiment, students obtain the molar mass of an unknown gas in two ways: from density and from flow times measurements. Figure 1 shows the distribution of masses obtained in semester 1 of 2010. As can be seen from the figure, the measurements obtained by the students naturally fit a Gaussian distribution centred on the molar mass of carbon dioxide. The main aim of asking students to plot this data was to illustrate how a normal distribution arises even in a relatively simple experiment performed under apparently identical conditions. Students were asked to consider and comment on the precision and accuracy of the two experimental methods using both the graphical results and through calculation of the averages, standard deviations and standard errors. Students were asked to report the unknown mass including a justification of the number of significant figures based on the analysis.



## Figure 1: Distribution of experimental molar mass masses from (a) flow times experiment (•) and (b) density experiment (×) obtained by Junior Chemistry students in semester 1 of 2010.

During the assessment period for this task, it was clear from discussion board activity and from an informal focus group that a significant proportion of students do not know how to use the basic functions of spreadsheet software, such as drawing simple charts. It appears that despite such software being available in high schools and despite being both relatively high achievers and reasonably motivated, these "generation-Y" students manage to avoid such exercises at school. Clearly, "the assumption that some Academic staff make, that students already have computer literacy skills, is often erroneous." (Reid, 1997). This assumption is certainly one that we made and is common in many science units. As a result, students are now given access to targeted support in Excel using the exSite available on the learning management system.

It is also clear that, whilst many students lack necessary computer skills, few will attend separate courses. The teaching of computer skills is more effective when built into academic subjects and assessment, rather than as an add-on (Link & Marz, 2006). It is also important to design activities that help to solve practical problems and show the benefits of using computers in order to engage students from the whole spectrum of computer literacy.

As noted above, a consequence of using a data set in the analysis which is real and large is that it naturally fits a normal distribution. Of course, another consequence is that it contains points which are suspect. No doubt, this may be due to data entry errors, a failure of equipment or incompetence. Another source of outliers is "fraud". The data entry is deliberately designed to be anonymous, ideally to ensure that students enter their actual results. However, it also, in a large class, invites a number of students to intentionally submit wrong (and often ridiculous) results. These results are *not* removed from the data set prior to its release to students. Instead, students are confronted with such factors as a reality of the scientific endeavour. The methods used to assess the reliability of individual measurements are introduced and students use Chauvenet's criterion (Taylor, 1997) as a statistical indicator of reliability.

In the 'Enantiomers - Chirality in Organic Chemistry' experiment, students measure the optical rotation of the isomers of limonene at different concentrations. The equipment used for this is really designed to illustrate the general principle that optically active molecules rotate polarised light and that a pair of enantiomers do so in opposite directions. In the experiment, each student therefore records the rotation of light by each enantiomer at a single concentration. Repeating the experiment multiple times at different concentrations is required to obtain a meaningful numerical result but is not a task that a typical student enjoys and is irrelevant to the main learning outcome of the actual experiment. Such a task is, however, ideally suited as a large group activity and, over a week, the data set contains multiple measurements at each concentration.

Using the linear regression facility of Solver within Excel, the students obtain the specific rotation of limonene. Figure 2 shows the result of this analysis obtained in semester 2 of 2009. The gradient and its standard error are used by students to calculate the specific rotation of limonene. In the 4 occasions that this analysis has been performed using large classes, the value obtained is close to the literature value despite the scatter in the data and the simplicity of the experimental set up. On 2 occasions, the analysis was performed using a small class of less than 50 students and this leads to poor results. The analysis uses a relatively advanced feature of Excel to show how information can be extracted from experimental data, and the value of repeating experiments.



Figure 2: The dependence of the optical rotation on concentration of (+)-limonene  $(\times)$  and (-)-limonene  $(\bullet)$  obtained by Junior Chemistry students in semester 2 of 2009.

The task is completed by students analysing the residuals, the difference between the measured optical rotation and that calculated using the value for the specific rotation, obtained from the regression. Figure 3 shows the residuals for the (-)-enantiomer from the same analysis as shown in Figure 2. The distribution of the residuals is an indication of the nature of the error in the experiment. Typically, the residuals for this experiment suggest that there is a bias towards overestimating rotation at low concentrations and underestimating it at higher concentrations. The students are asked to assess this and hence comment on ways in which the experimental set up can be improved.



Figure 3: Residuals obtained from the linear regression for (-)-limonene obtained by Junior Chemistry students in semester 2 of 2009.

Figure 4 shows the student evaluation scores for the question "This unit of study helped me develop valuable graduate attributes" on the unit of study evaluation for a selection of our units. The figures for 2008, before the introduction of the work described in this paper, are consistent with those from previous years, and with qualitative comments by students. Although the figures for 2009 and 2010 suggest that we still have much to do, they show a consistent and pleasing improvement across all units. It should be noted that the students were made directly aware of the importance of graduate attributes in the course and the particular skills which this activity seeks to develop.



Figure 4: Student evaluation scores relating to graduate attributes (out of 5) for science (CHEM1001 – Fundamentals, CHEM1101 – Mainstream and CHEM1901 – Advanced) and service units (CHEM1108 – Life Sciences and CHEM1611 – Pharmacy). All students were invited to complete evaluations with around 300 choosing to do so in each of the years shown.

#### CONCLUSIONS

The primary aim of the project was to improve the ability of students to perform data analysis and their appreciation of the precision, accuracy and reliability of experimental data. This formed part of a general strategy to develop generic attributes more thoroughly in our courses and to address deficiencies in the computer skills of our students.

Using a relatively simple web interface, students' experimental results are collected leading to large data sets for the subsequent analysis which naturally include random, systematic, and even deliberate errors. These factors are often not appreciated in undergraduate classes in the physical sciences where there is traditionally a strong desire to reproduce a theoretical result. This motivation is completely against the way science is conducted at research level and opposes the critical skills that our graduates should possess. This project aims to confront this attitude by developing an inquiry and student-centred approach to the analysis of data. The project is also built around the role of peer interaction in science. By forcing students to work with a wide range of measurements including their own, students will appreciate the importance of the role of human error in the physical sciences.

The project has successfully met its objectives of improving the quantitative, problem solving and inquiry skills and computer literacy in Junior Chemistry students. Student feedback has been positive, with a noticeable increase in the percentage of students finding the task useful for developing valuable graduate attributes.

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