NUMERICAL ALGORITHMS - ENHANCING PRESENTATION WHILE MAINTAINING RIGOUR IN INTRODUCTORY COURSES.
A minimalist approach to course modernisation

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ABSTRACT

Recent academic developments which include a changing student profile, the focus of contemporary research, and social trends have combined to pose significant challenges in first year undergraduate mathematics courses. Issues which arise include the content level, the need to maintain rigour, addressing the needs of specialist and non-specialist students, the need to equip students with useful, applicable, techniques, and our desire to present a picture of the important problems and directions in modern mathematics and its beauty and excitement.

Calculus reform has made a significant impact but more needs to be done. There are large areas of research in which the computer has the role of an experimental tool. The use of software packages is widespread. This has produced the need for something akin to an instinct which can identify the correct or incorrect functioning of a package or black box. To acquire this instinct some knowledge and experience of the behaviour of numerical algorithms is needed. As a consequence the way in which calculus is taught needs to be changed. It also needs to change because the computer has caused major changes in the theoretical directions of mathematics.

These influences can be used to enhance courses whose content contains the essential foundations of the subject. The foundations will not change, but investigations of numerical algorithms, for example, can pose the same fundamental questions that are to be found in texts dating back a century at least. Well founded approximation methods provide exact rigorous statements. Numerical experimentation can provide insight. There is no need to present a grab bag of computations whose output is of doubtful validity.

This presentation will briefly review the knowledge levels of entering students; it will describe some important applications and it will attempt to show how some of the challenges can be met.

Keywords: Algorithms, Numerical Analysis, Calculus, Linear Algebra, Biomathematics

1. Introduction

The pace of change in universities and other tertiary institutions closely follows that of the world at large. Scientific discoveries, changing social structures, and reforms of education all combine to exert a strong influence on the practice of mathematics whether it be in the workplace, in school and college or at the cutting edge of research.

In the context of teaching, Mathematics needs to respond to these changes. What the response should be is a topic which needs careful consideration and how a perceived response should take place is a second important issue. It is the author's view that the mathematics community in Australia and, perhaps, worldwide, has been slow to recognise that change has taken place. Many who feel the need for mathematics to support their work share this view. At the author's university the biological scientists are eager for the mathematicians to lend support to their research (arguably the most important in the 21st century) and they realise that this support cannot be sustained without a strong undergraduate degree.

The focus of this meeting is undergraduate teaching and, since many students take a first year course and may not proceed with further mathematics, suggestions for changes will be in this context. Apart from a couple of sentences in conclusion, the proposals here are modest, necessarily so against a background of inaction imposed by those who resist change.

A review and assessment of the background of the entrants to first year courses will be made initially. This will be followed by an overview of major developments in discipline areas which draw on mathematics and mathematicians as a resource. Instances of responses to these stimuli will be described and inferences regarding curriculum content will be drawn from these observations. Finally, in the last section it will be argued by example that the important values in a traditional curriculum can be maintained while presenting a more forward looking account of the subject.

2. First year undergraduate entrants

Whereas, in times hitherto, high school curricula consisted of a small number of subjects, the need for a breadth of choice to address students with diverse talents and abilities has led to a proliferation of options. The effect has been that mathematics occupies a significantly smaller fraction of school activity. In Queensland, Australia, in the past, many university matriculants would study two mathematics subjects, amounting to 200 hours each year, however no more than one of these subjects is needed for university entrance so that the time spent on mathematics has been reduced by 50% in many cases. Statistics from the Queensland Board of Secondary School Studies web site at http://www.qbssss.edu.au/statisticsandpublications/statistics/Subject_stats.html show that the percentage of students taking both Mathematics B and C as a percentage of those taking only Mathematics B fell from 29% in 1992 to 20% in 2001. Data for 2000 and 1999 suggests that these numbers have now stabilised.

It has to be recognised too that the depth of knowledge of the subject has reduced in other ways. Informal tests at the University of Queensland carried out on first year entrants on their knowledge of content indicated a substantial fall over the period 1973-1990 (Belward and Pemberton 1996). Now the content is problem driven, thus more time is spent on problem solving rather than on an accumulation of knowledge strengthening and technique. There are compensations however, the syllabi now require students to have some proficiency with graphics calculators or computers and they may have assessment instruments which are take home projects of two to three weeks duration. More details are available at the Queensland Board of Senior Secondary School Studies site http://www.qbssss.edu.au/Curriculum/subjectguides/MathsB.html.

3. Mathematics and Research

There was once a time when a mathematics researcher only needed to look at the journals whose titles bore mathematics connotations. At least it appeared so. Today there are many subject areas where a large amount of content is concerned with mathematics. Many IEEE journals (see http://shop.ieee.org/store/Overviews/periodicals.asp#list) contain large amounts of mathematics and there are many such journals where mathematics is a major element of the work reported. The problems under review may be engineering problems but removal of the mathematics would most often remove the content of the problem. Operations Research is another rich source of mathematics. The Simplex method for linear programming has had immense success and its development continues (Zakeri, Philpott, A. and Ryan 2000). As computing power has increased problems such as the travelling salesman problem can be solved for larger numbers of variables and the search for efficient algorithms has been pivotal in the development of stochastic algorithms and evolutionary algorithms. Much work in these areas has been done by computer scientists. Many problems in financial mathematics have a large stochastic component. The introduction of a stochastic element is necessary to model the behaviour of many investment instruments. This, concurrent with present computing power, has been a catalyst for widespread interest in the solution of stochastic differential equations (Kuechler and Platen 2000).
Utilising the biological analogies drawn by the developers of by genetic and other evolutionary optimisation algorithms we find ourselves lead into life science itself. The sequencing of DNA is a problem which has been confronted by several different approaches leading to a large variety of optimisation algorithms. There is no doubt that bio-physics, bio-mathematics and bio-informatics are all manifestations of the current surge in research in the life sciences whose major problems have been said to offer the largest intellectual challenges of the 21st century. Recent numbers of the journal *Bioinformatics* raise this matter regularly. In a recent editorial (Pearson, 2001) the view is expressed that "Genome biology presents a different scale, whose promise will not be fulfilled without an infrastructure of well-trained researchers in Bioinformatics, Computational Biology and Biomathematics … ".

4. Some responses to research stimuli

Research institutions and universities worldwide have taken steps to meet the challenge of updating and focussing their research on the rapidly developing areas noted in the previous section. Specialist groups, centres and semi-autonomous institutes and commercial organisations have been set up to deal with these problems. This permits an initial response, however in order that this be sustained an increase is needed in the number of graduates. If the research programmes are successful, large numbers of graduates with expertise in the appropriate area will be needed.

At the University of Queensland federal funding has been made available for six emerging researchers to set up a computational biology program. The outcome will be a degree course which will be the life science counterpart to an engineering degree. The University is a participant in the Queensland Parallel Supercomputing Foundation which has an educational programme wherein materials will be made available through the internet as support materials in advanced undergraduate and master‘s programmes in high performance computing and visualisation. On a smaller scale the university has an honours programme in Financial Mathematics as a joint operation between the departments of commerce and mathematics.

5. The course for mathematics

On the evidence presented in the previous sections it is imperative that the content of first year mathematics change if some sort of mismatch between current content and expected outcome is to be avoided. Educational programmes must reform in the way that research programmes keep abreast of modern developments. While research in both pure and applied mathematics has gone ahead at pace, teaching methods and course content have progressed only a little. Admittedly the evidence is anecdotal, but all too often colleagues (respected and successful) from other disciplines who are users of mathematics tell me that "I didn't learn a single useful thing in my maths courses".

The task is not easy; many competing pressures are apparent. Besides those noted already, departments have reduced resources due to budgetary pressures and those same forces have resulted in classes being merged into one large single stream. Often course structures prevent potential users from completing more than first year mathematics.

Another source of pressure is the duty to remain true to ones subject; in other words to maintain integrity. This means that there are certain fundamental concepts which are important and cannot be rejected, the sorts of ideas which are essential in a degree majoring in Mathematics.

Finally there is the need to put on courses addressing the interests both of those who want to specialise in the subject and those who will use mathematics to support their chosen discipline. Mathematics is useful, but it is also exciting and beautiful. Thus it is crucial that an effort be made to show those who want to specialise in mathematics a glimpse of the modern ideas. On the other hand, believing as we do that all intellectual investigation can benefit with the application of mathematics we have to convince students that in their chosen subjects mathematics will be important and may provide important benefits to them.

6. Examples of enhancement of first year courses

In this section a minimalist approach to some reform is presented. Without rewriting a typical calculus or linear algebra syllabus it is possible to address the problem of "… not learning a single useful thing …" while meeting the needs of both the application oriented and potential specialist students. This is possible because scientific computation uses methods whose validity relies on the analytical and algebraic foundations of the subject. Thus the material can take on a more modern appearance without loss of integrity.

Approximation theory includes application of the functional analysis to numerical approximation schemes. It is worth emphasising that approximation theory is exact, in the sense that error bounds are given on the results of calculations and therefore careful choices of numerical algorithms can be validated by these error bounds. Therefore many good numerical techniques can enjoy standards of rigour on a par with those of calculus and other areas of mathematics.

Each of the topics below appear in many first year courses. All of them merit a thorough treatment. Despite their algorithmic character a "cook book" presentation should be avoided.

Solution of nonlinear equations

In the absence of an analytical expression for the roots of a nonlinear equation a sequence of values is desired converging to an x satisfying the equation $f(x) = 0$.

Newton's method appears almost always in first year calculus books. Sometimes it is portrayed as a single step method, but in a practical situation a sequence $\{\alpha_n\}$ is generated by the rule

$$a_n = a_{n-1} - \frac{f(a_{n-1})}{f'(a_{n-1})}$$

This works very efficiently when it converges, but to be able to give bounds on the solution we require values of x which bracket a sign change in f and the knowledge that f is continuous on the interval defined by the bracket. A robust root finding program must find values, which bracket a solution, particularly when the algorithm is a component inside some other routine. For these reasons the humble bisection method, wherein intervals bracketing the root are halved repeatedly until some tolerance level is reached, should not be ignored. It might then be possible to introduce Brents algorithm which implements the secant method safeguarded by the bisection method.

Here we immediately introduce the notions of convergence and continuity without the need for contrived examples. The idea of fixed point iteration is introduced whose convergence analysis can be used as a vehicle for introducing the mean value theorem, see (Belward 1999) for an example and further details.

Numerical integration

An enunciation of Simpson's rule or the trapezoidal rule without some discussion of the error committed by their application is poor mathematics. Further to simply derive the formulae by fitting parabolas or evaluating the areas of trapezia will not equip the class with the methodology which will enable them to deal with more difficult situations later. An integration rule should be presented as the integration of an approximant to the integrand, thus we approximate $f(x)$ by $a(x)$ with an error $e(x)$. Then we integrate the relation

$$f(x) = a(x) + e(x)$$

and obtain

$$\int_a^b f(x)dx = \int_b^b a(x)dx + \int_a^b e(x)dx = \text{ quadrature approximation } + \text{ error}$$

Presenting the method in this way enables more advanced methods (e.g. product integration rules) to be understood and provides a methodology to deal with singularities.

It is also important that some numerical experience be obtained. For appropriately smooth integrands the error committed is proportional to $1/n^2$ and $1/n^4$, respectively, for the trapezoidal rule and Simpson's rule, n being the number of steps. A feeling for convergence rates may then be inculcated and experimental curiosity aroused by application to functions with and without the smoothness assumptions of the error formulae.

number of subintervals	*exp(x)*	*sin(100x)*	$x^{1/2}$
4	3.7013e-005	-2.6068e-001	-1.0140e-002
8	2.3262e-006	-2.6068e-001	-3.5874e-003
16	1.4559e-007	-2.6068e-001	-1.2685e-003
32	9.1027e-009	8.5074e-002	-4.4848e-004
64	5.6897e-010	6.3366e-005	-1.5856e-004
128	3.5562e-011	3.0707e-006	-5.6061e-005
256	2.2224e-012	1.8138e-007	-1.9820e-005
512	1.3789e-013	1.1181e-008	-7.0076e-006
Exact value	1.71828 …	1.3768e-003	.666666…
Remarks	Because the function is so smooth the convergence rate is attained immediately	Until enough points are chosen results are bad, then rapid convergence is observed	Moderate accuracy from the start, given the number of points but the convergence rate never improves

Table 1. Errors in Simpson's rule for the integral of three functions on (0,1) against the number of intervals.

The data in table 1 summarises the results which may be obtained by experimenting with 3 functions for which we know the value of the integral on (0, 1) and therefore the accuracy for each example. Insight into these results can be gained by plotting the integrands and superimposing the quadrature points. Sketching the piecewise parabolic pieces which are used in Simpson's rule then reveals that until enough points are taken to follow the integrand the results will be unreliable. The square root function example, however, shows that understanding its results cannot be deduced from the graphical information. One needs the error formula to see why the convergence is slower.

It is not often that bounds on the accuracy of numerical integration schemes are available. It is therefore useful to note a nice example wherein upper and lower bounds on a numerical integration scheme can be found (Hughes-Hallett, Gleason, et al. 1998).

Linear algebra

There is little doubt that the solution of linear equations is one of the most useful techniques, which can be given to users of mathematics. Furthermore this both necessitates and motivates the study of linear vector space theory ; it is fully exploited in the approach of Strang in his book on linear algebra (Strang 1998). By attempting to interpolate data with unsuitable choices of basis functions one can give simple examples of systems with one, none and an infinity of solutions. (Fit a quadratic to 3 data points at -1, 0, 1. Then use 1, x^2 and x^4 as a basis with data values that are different and then the same at -1 and 1, see (Belward 1999) for further details)

Here again we have used a practical problem to introduce important abstract ideas. An important point is that one should not stray too far from the problem source. Although solving linear systems by pencil and paper using augmented matrices looks attractive, in using the algorithm students tend to forget what problem they are solving. Preference should therefore be given to the idea of always carrying equivalent sets of equations. In this way absurdities introduced by arithmetic error are more easily detected.

Using equation sets rather than matrices carries over to the simplex algorithm where many students have no idea what is happening when a tableau is processed. In comparison the dictionary method of Chvatal (Chvatal 1983) carries the constraints and an explicit expression for the objective function expressed in terms of the non-basic variables, whereupon the choices of entering and leaving variables, not to mention the optimality criterion, are made clear. Once again by keeping to the practical problem one has both algorithmic efficiency and rigour.

7. Conclusion

This article has attempted to show that the pace of change in universities and research institutions is considerable and that, as a consequence, undergraduate mathematics, particularly in first year, needs considerable adjustment. It may not be possible to make wholesale changes to large first year courses where enrolments are measured in hundreds and sometimes thousands. Nevertheless a good teacher can enliven the most turgid material and a good choice of examples can also provide considerable insight.

The author has adopted this minimalist approach. Students have found the material stimulating, they have realised that there is interesting mathematics beyond calculus and linear algebra. Interest in Scientific Computation is steadily increasing. In the past students often did not meet these ideas until their second year. With the extra emphasis put on this material in first year they are now informed of attractive opportunities in visualisation, plant architecture informatics, and genomics. Through the medium of this brief introduction they are able to make more informed choices when planning their later year studies.

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