

UNIVERSITY COLLEGE DUBLIN
Mathematical Physics Department
Master of Computational Science

NUMERICAL ALGORITHMS

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First Semester 2004-2005

Wed. 2pm - 4pm

This course is an introduction to the fundamentals of numerical computation. The formal purpose is to introduce students of the sciences to some of the numerical algorithms that form basis of all numerical computation on digital computers. To understand numerical algorithms students must be familiar with the following essentials :

- Computation with a small set of primitive operators $\{+, -, *, /\}$.
- Computation with finite (limited) precision.
- Construction and analysis of algorithms.
- Perturbation analysis of problems and error estimation of algorithms.
- Testing and evaluation of numerical software.

The informal purpose of the course is to demonstrate that high-quality mathematical software writing is a very demanding and difficult task which is best left to experts. A corollary to this is that there is a lot of junk software in use today because of the inability of users to distinguish between good and bad mathematical software.

Hence, the ultimate purpose of this course is to make you critical mathematical software users or consultants.

This is a copy of the Class Webpage at

www.derekroconnor.net/NA/na2col.html

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APPENDIX I. AN ALGORITHMIC LANGUAGE

APPENDIX II. ANALYSIS OF ALGORITHMS

NOTES and TEXTBOOKS

There is no required text for this course. The notes and links above are required reading. You are responsible for downloading and printing these and to have the appropriate notes with you for each class. Nonetheless, you should make yourself familiar with some, if not all, of the books below.

Matlab Notes & Textbooks

1. Griffiths, David F. : *An Introduction to Matlab Version 2.2*, Aug 2001. Download from course webpage. www.derekroconnor.net/NA/na2col.html
2. Higham, Desmond J. & Higham, Nicholas J. : *MATLAB Guide*, SIAM. 2000.
3. Neuman, Edward : Matlab Tutorials. Download from course webpage. www.derekroconnor.net/NA/na2col.html
4. Moler, Cleve : *Numerical Computing with MATLAB*. This book is available in PDF format at www.mathworks.com/moler/. This is an excellent book by the inventor of MATLAB. It may be used as a text, tutorial, or reference.
5. MATLAB reference manuals are downloadable from the Mathworks website www.mathworks.com.

Modern Texts

1. Coleman, T.F., and Van Loan, C. : *Handbook for Matrix Computations*, SIAM, 1988.
2. Demmel, James W. : *Applied Numerical Linear Algebra*, SIAM, 1997
3. Gill, P., Murray, W., and Wright, M : *Numerical Linear Algebra and Optimization, Vol 1*, Addison-Wesley, 1991.
4. Golub, Gene H, and Van Loan, Charles F. : *Matrix Computations 3rd Ed*, The Johns Hopkins University Press, 1996.
5. Hager, William W. : *Applied Numerical Linear Algebra*, Prentice-Hall, 1988. (Out of print by P-H, but available from the author)
6. Higham, N.J. : *Accuracy and Stability of Numerical Algorithms 2nd Ed*, SIAM. 2002.
7. Kahaner, D., Moler, C., and Nash, S. : *Numerical Methods and Software*, Prentice-Hall, 1989.
8. Moler, Cleve : *Numerical Computing with MATLAB*, SIAM, 2004. This book is available in PDF form at www.mathworks.com/moler/ (Moler is the inventor of MATLAB). SIAM (the Society for Industrial and Applied Mathematics).
9. Stewart, G.W. : *Afternotes on Numerical Analysis*, SIAM, 1996.
10. Stewart, G.W. : *Matrix Computations, Volume 1 : Basic Decompositions*, SIAM, 1998.
11. Trefethen, Lloyd, N. and Bau III, David, *Numerical Linear Algebra*, SIAM, 1997.
12. Van Loan, Charles , F : *Introduction to Scientific Computing : A Matrix-Vector Approach using Matlab*, Prentice-Hall, 2000.
13. Watkins, D.S. : *Fundamentals of Matrix Computations*, Wiley, 1991.

Classic Texts

1. Forsythe, G.E. and Moler C.B. : *Computer Solution of Linear Algebraic Systems*, Prentice-Hall, 1967.
2. Forsythe, G.E., Malcolm, M., and Moler, C.B. : *Computer Methods for Mathematical Computations*, Prentice-Hall, 1977.
3. Whittaker, Sir E.T. and Robinson, G. : *The Calculus of Observations : An Introduction to Numerical Analysis*, Dover, 1967, a republication of the 4th ed., 1944. First edition, Blackie & Sons, 1924. From the Preface of the First Edition, 1924:

[Numerical Analysis] is now included in the syllabus for the Open Competitive Examination for appointments in the Home and Indian Civil Services, the Colonial Service, etc. The present volume represents courses of lectures given at different times during the years 1913–1923 by Professor Whittaker to undergraduate and graduate students in the Mathematical Laboratory of the University of Edinburgh, . . . etc.

4. Wilkinson, James H. : *Rounding Errors in Algebraic Processes*, Notes on Applied Science 32, Her Majesty's Stationary Office, 1963. Also Prentice-Hall, 1963.
5. Wilkinson, James H. : *The Algebraic Eigenvalue Problem*, Oxford University Press, 1965.

Not Recommended Texts

1. Press, W.H., Flannery, B.P., Teukolsky, S.A., and Vetterling, W.T. : *Numerical Recipes*, Cambridge University Press, 1986, and 2nd Ed 1992 (See NR-Critics link on class webpage)

EXERCISES and ASSIGNMENTS

- After many of classes you will be given a small set of problems which you will solve and hand in at the end of the next class. These will require you to use MATLAB, and to a limited extent, MAPLE .
- You will be given three (3) MATLAB programming assignments which you must work on individually and complete to pass this course.
- These exercises and assignments are designed to test and reinforce your understanding of the lecture material. As such it is vital that you keep up to date by submitting them on the due dates. Solutions to the assignments and exercises will be posted on the class webpage shortly after the due dates.

No submissions will be accepted after the solutions have been posted.

GRADING

The final grade will have this composition :

1. Exercises : 15%
2. Assignments : 15%
3. Exam : 70%