A Personal Perspective on Numerical Analysis and Optimization

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Abstract

I give a brief, non-technical, historical perspective on numerical analysis and optimization. I also touch on emerging trends and future challenges. This content is based on the short presentation that I made at the opening ceremony of The International Conference on Numerical Analysis and Optimization, which was held at Sultan Qaboos University, Muscat, Oman, on January 6–9, 2020. Of course, the material covered here is necessarily incomplete and biased towards my own interests and comfort zones. My aim is to give a feel for how the area has developed over the past few decades and how it may continue.

1 Definitions

Mathematicians love to make definitions. But defining an area of mathematics is a thankless task. The best one-sentence definitions that I can come up with for numerical analysis and optimization are as follows.

Numerical Analysis: the design, analysis and implementation of computational algorithms to deliver approximate solutions to problems arising in applied mathematics.

Optimization: the design, analysis and implementation of computational algorithms to approximate the best solution to a problem arising in applied mathematics when there may be many feasible solutions.

For alternative versions, I refer to the references [3, 24, 29].
The unstoppable growth of interest in the use of computational algorithms can be attributed to two main factors. First, technology has advanced rapidly and consistently since the digital computing era began in the 1950s. The CDC6600, widely acknowledged to be the world’s first “supercomputer”, was introduced in 1964, achieving a speed of 3 megaflops (that is, $3 \times 10^6$ floating operations per second) \[17\]. Today’s fastest supercomputers can achieve petaflop speeds ($10^{15}$ floating operations per second). By contrast, in his 1970 Turing Award Lecture \[28, 1971\], James Wilkinson discussed the use of mechanical desk calculators:

“It happened that some time after my arrival [at the National Physical Laboratory in 1946], a system of 18 equations arrived in Mathematics Division and after talking around it for some time we finally decided to abandon theorizing and to solve it . . . The operation was manned by Fox, Goodwin, Turing, and me, and we decided on Gaussian elimination with complete pivoting.”

Leslie Fox \[12\] noted that the computation referred to in this quotation took about two weeks to complete. By my estimation, this corresponds to around 0.003 floating operations per second!

A second, and equally important, factor behind the rise of scientific computation is the availability of ever-increasing sources of data, caused by improvements in experimental techniques and, perhaps most notably, by the inexorable sensorization and digitization of our everyday lives. Hence, although numerical analysis and optimization build on classical ideas that can be attributed to the likes of Newton, Euler, Lagrange and Gauss, they continue to be shaped by current developments. Of course, many disciplines make extensive use of computational techniques. For example, the word “Computational” often appears before the words Biology, Chemistry, Physics, and Social Science. Furthermore, Computational Science and Engineering \[23\] is a well established discipline that is often referred to as the third leg of the science and engineering stool, equal in stature to observation and theory. In addition, many graduate schools now offer courses with titles such as “Data Analytics” and “Data Science.” Although there is clearly much overlap, my view is that numerical analysis and optimization have a distinct role of focusing on the design and analysis of algorithms for problems in applied mathematics, in terms of complexity, accuracy and stability, and hence they are informed by, but not driven by, application fields.

3 Reflections

My own exposure to numerical analysis and optimization dates back to the mid 1980s when I enrolled on an MSc course on “Numerical Analysis and
History of Numerical Analysis Programming” at the University of Manchester. The course, in which optimization was treated as a branch of numerical analysis, made heavy use of the series of textbooks published by Wiley that was written by members of the highly influential numerical analysis group at the University of Dundee [27]. Here are the topics, and most recent versions of these books: approximation theory [26], numerical methods for ODEs [18], numerical methods for PDEs [22, 25] and optimization [11]. An additional topic was numerical linear algebra [14]. Each of these topics remains active and highly relevant. Numerical linear algebra and optimization are often important building blocks within larger computational tasks, and hence their popularity has never waned. Partial differential equations lie at the heart of most models in the natural and engineering sciences, and they come in many varieties, giving rise to an ever-expanding problem set. Timestepping methods for ODEs gained impetus through the concept of geometric integration [15] and now play a prominent role in the development of tools for statistical sampling [6]. ODE simulation also forms a key component in certain classes of neural network, as described in [7], which received a Best Paper Award at NeurIPS 2018, a leading conference in machine learning. Approximation theory lies at the heart of the current deep learning revolution [16, 19], and, in particular, understanding very high dimensional data spaces and/or parameter spaces remains a fundamental challenge.

4 Impact

In a special issue of the journal Computing in Science and Engineering, Jack Dongarra and Francis Sullivan published their top-ten list of algorithms that had the “greatest influence on the development and practice of science and engineering in the 20th century” [9]. These were

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

Here, the word “algorithm” is being used in a very general sense, but it is clear that most of these achievements have ideas from numerical analysis and optimization at their heart.
Researchers in numerical analysis and optimization are in the advantageous position that their work is not only recorded in journals and textbooks, but may also be made operational through public domain software. Many authors now deposit code alongside their academic publications, and state-of-the-art code is available in a wide range of languages and platforms, including FORTRAN, C, R, MATLAB, Maple, (Scientific) Python and the more recent Julia [4].

5 Momentum

Judging by the level of activity around graduate classes, seminar series, conferences and journals, there is a strong pull for further research in numerical analysis and optimization. Particularly active, and overlapping, directions include

- dealing with, or exploiting, randomness, both in the simulation of mathematical models that are inherently stochastic [20] and in the use of randomization in solving deterministic problems [8, 21],
- accurately and efficiently simulating mathematical models that operate over a vast range of temporal or spatial scales [10, 13],
- tackling problems of extremely high dimension, notably large-scale optimization and inverse problems in machine learning and imaging [2, 5],
- exploiting the latest computer architectures and designing algorithms that efficiently trade off between issues such as memory bandwidth, data access, communication and, perhaps most topically, the use of low precision special function units [1].

Such items, and may others, emphasize that important challenges remain for researchers in numerical analysis and optimization in the design, evaluation and extension of the modern computational scientist’s toolbox.

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References

1. A. Abdel fattah, H. Anzt, E. G. Boman, E. Carson, T. Cojean, J. Dongarra, M. Gates, T. Grützmacher, N. J. Higham, S. Li, N. Lindquist, Y. Liu, J. Loe, P. Luszczek, P. Nayak, S. Pranesh, S. Rajamanickam, T. Ribizel, B. Smith, K. Swirydowicz, S. Thomas, S. Tomov, Y. M. Tsai, I. Yamazaki, and U. M. Yang, A survey of numerical methods utilizing mixed precision arithmetic, ArXiv:2007.06674, July 2020.
2. S. Arridge, P. Maass, O. Öktem, and C.-B. Schönlieb, Solving inverse problems using data-driven models, Acta Numerica, 28 (2019), pp. 1–174.
3. J. Barrow-Green and R. Siegmund-Schultze, *The history of applied mathematics*, in The Princeton Companion to Applied Mathematics, N. J. Higham, M. R. Dennis, P. Glendinning, P. A. Martin, F. Santos, and J. Tanner, eds., Princeton University Press, Princeton, NJ, USA, 2015, pp. 55–79.
4. J. Bezeroson, A. Edelman, S. Karpinski, and V. B. Shah, *Julia: A fresh approach to numerical computing*, SIAM Review, 59 (2017), pp. 65–98.
5. L. Bottou, F. E. Curtis, and J. Nocedal, *Optimization methods for large-scale machine learning*, SIAM Review, 60 (2018), pp. 223–311.
6. S. Brooks, A. Gelman, G. L. Jones, and X.-L. Meng, eds., *Handbook of Markov Chain Monte Carlo*, CRC Press, Boca Raton, 2011.
7. R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. K. Duvenaud, *Neural ordinary differential equations*, in Advances in Neural Information Processing Systems 31, S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, eds., Curran Associates, Inc., 2018, pp. 6571–6583.
8. M. P. Connolly, N. J. Higham, and T. Mary, *Stochastic rounding and its probabilistic backward error analysis*, MIMS EPrint 2020.12, Manchester Institute for Mathematical Sciences, 2020.
9. J. Dongarra and F. Sullivan, *Guest editors’ introduction to the top 10 algorithms*, Computing in Science and Engineering, 2 (2000), pp. 22–23.
10. W. E, *Principles of Multiscale Modeling*, Cambridge University Press, Cambridge, 2011.
11. R. Fletcher, *Practical Methods of Optimization*, John Wiley and Sons, Chichester, 2000.
12. L. Fox, *James Hardy Wilkinson, 1919–1986*, Biographical Memoirs of Fellows of the Royal Society, 33 (1987), pp. 671–708.
13. M. G. D. Geers, V. G. Kouznetsova, K. Matou, and J. Yvonnet, *Homogenization methods and multiscale modeling: Nonlinear problems*, in Encyclopedia of Computational Mechanics, Second Edition, Wiley, 2017, pp. 1–34.
14. G. H. Golub and C. F. Van Loan, *Matrix Computations*, The Johns Hopkins University Press, 3rd ed., 1996.
15. E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer, Berlin, 2nd ed., 2006.
16. C. F. Higham and D. J. Higham, *Deep learning: An introduction for applied mathematicians*, SIAM Review, 61 (2019), pp. 860–891.
17. S. Hongwei, *Seymour Cray: The father of world supercomputer*, History Research, 7 (2019), pp. 1–6.
18. J. D. Lambert, *Numerical Methods for Ordinary Differential Systems: The Initial Value Problem*, John Wiley and Sons, Chichester, 1991.
19. Y. LeCun, Y. Bengio, and G. Hinton, *Deep learning*, Nature, 521 (2015), pp. 436–444.
20. G. J. Lord, C. E. Powell, and T. Shardlow, *An Introduction to Computational Stochastic PDEs*, Cambridge University Press, Cambridge, 2014.
21. P.-G. Martinsson and J. Tropp, *Randomized numerical linear algebra: Foundations and algorithms*, Acta Numerica, to appear, (2020).
22. A. R. Mitchell and D. F. Griffiths, *The Finite Difference Method in Partial Differential Equations*, John Wiley and Sons, Chichester, 1980.
23. U. Rüde, K. Willcox, L. C. McInnes, H. D. Sterck, G. Biros, H. Bungartz, J. Corones, E. Cramer, J. Crowley, O. Ghatta, M. Gunzburger, M. Hanke, R. Harrison, M. Heroux, P. J. Jan Hesthaven, C. Johnson, K. E. Jordan, D. E. Keyes, R. Krause, V. Kumar, S. Mayer, J. Meza, K. M. Mørken, J. T. Oden, L. Petzold, P. Raghavan, S. M. Shontz, A. Trefethen, P. Turner, V. Voevodin, B. Wohlmuth, and C. S. Woodward, *Research and education in computational science and engineering*, SIAM Review, 60 (2018), pp. 707–754.
24. L. N. Trefethen, *The definition of numerical analysis*, SIAM News, 25 (1992).
25. R. Wait and A. Mitchell, *Finite Element Analysis and Applications*, John Wiley and Sons, Chichester, 1985.
26. G. A. Watson, *Approximation Theory and Numerical Methods*, John Wiley and Sons, Chichester, 1980.
27. ———, *The history and development of numerical analysis in Scotland: a personal perspective*, in *The Birth of Numerical Analysis*, World Scientific, London, 2009, pp. 161–177.
28. J. H. Wilkinson, *Some comments from a numerical analyst*, J. Assoc. Comput. Mach., 18 (1971), pp. 137–147.
29. S. J. Wright, *Continuous optimization (nonlinear and linear programming)*, in *The Princeton Companion to Applied Mathematics*, N. J. Higham, M. R. Dennis, P. Glendinning, P. A. Martin, F. Santosa, and J. Tanner, eds., Princeton University Press, Princeton, NJ, USA, 2015, pp. 281–293.