矩阵计算

Matrix Computations

数值线性代数

Numerical Linear Algebra

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数值算法

In the history of science, there were two periods of time that made the most impact for applied mathematics. The first was the time of Newton, during which it was established that **mathematics should be the language of science**. The second was the time of von Neumann, during which it was proposed that **numerical algorithms should be the main bridge between mathematics and science**.

— Weinan E, "A Mathematical Perspective on Machine Learning", ICM 2022.

- ICM 2022 一小时报告, ICML 2022 (国际机器学习大会) 开场特邀报告
- ICIAM Maxwell Prize (2023), ICIAM Collatz Prize (2003), ACM Gordon-Bell Prize (2020)

计算数学

计算科学是 21 世纪确保国家核心竞争能力的战略技术之一.

—— 计算科学: 确保美国竞争力，2005 年总统信息技术咨询委员会报告

科学计算是 20 世纪重要科学技术进步之一, 已与理论研究和实验研究相并列成为科学研究的第三种方法. 现今科学计算已是体现国家科学技术核心竞争力的重要标志, 是国家科学技术创新发展的关键要素.

—— 国家自然科学基金 · 重大项目指南, 2014

1947 年 Von Neumann 和 Goldstine 在《美国数学会通报》发表了题为“高阶矩阵的数值求逆”的著名论文, 开启了现代计算数学的研究.

计算数学的主要研究内容

一般来说, 计算数学主要研究各种数学问题的有效数值计算方法及其相关的数学理论, 包括算法的设计与分析 (收敛性, 稳定性, 复杂性等).

计算数学的主要研究内容

- 数值代数
- 数值逼近
- 最优化方法
- 微分方程计算方法

科学计算:科技创新的第三种方法*

文/陈志明
中国科学院数学与系统科学研究院 北京 100190

“数值代数主要研究代数方程组, 代数特征值问题和最小二乘问题的数值求解方法, 数值代数的算法在科学计算中具有基础作用” — 陈志明, 中科院院刊, 2012.

国家自然科学基金委员会关于计算数学的分类 (2020)

- 计算数学与科学工程计算 (A0117)
  - 偏微分方程数值解 (A011701)
  - 流体力学中的数值计算 (A011702)
  - 一般反问题的计算方法 (A011703)
  - 常微分方程数值计算 (A011704)
  - 数值代数 (A011705)
  - 数值逼近与计算几何 (A011706)
  - 谱方法及高精度数值方法 (A011707)
  - 有限元和边界元方法 (A011708)
  - 多重网格技术与区域分解 (A011709)
  - 自适应方法 (A011720)
  - 并行计算 (A011711)
- 运筹学 (数值最优化, 非线性方程, ...)

国家自然科学基金委员会关于计算数学的分类 (2021)

- A05 计算数学
  - A0501 算法基础理论与构造方法
  - A0502 数值代数
  - A0503 数值逼近与计算几何
  - A0504 微分方程数值计算
  - A0505 反问题建模与计算
  - A0506 复杂问题的可计算建模与数值模拟
  - A0507 新型计算方法
- A04 统计与运筹: 连续优化, 离散优化, 随机优化与统计优化, ...
- A06 数学与其他学科的交叉: 符号计算, 人工智能, 数据科学
- - A0813 计算固体力学
- - A0910 计算流体力学
- F02 计算机科学: 信息安全, 数据科学与大数据计算
- F06 人工智能

MSC (Mathematics Subject Classification) 2020: Numerical analysis

65Axx Tables in numerical analysis
65Bxx Acceleration of convergence in numerical analysis
65Cxx Probabilistic methods, stochastic differential equations
65Dxx Numerical approximation and computational geometry (primarily algorithms)
65Exx Numerical methods in complex analysis (potential theory, etc.)
65Fxx Numerical linear algebra
65Gxx Error analysis and interval analysis
65Hxx Nonlinear algebraic or transcendental equations
65Jxx Numerical analysis in abstract spaces
65Kxx Numerical methods for mathematical programming, optimization and variational techniques
65Lxx Numerical methods for ordinary differential equations
65Mxx Numerical methods for partial differential equations, initial value and time-dependent initial-boundary value problems
65Nxx Numerical methods for partial differential equations, boundary value problems
65Pxx Numerical problems in dynamical systems
65Qxx Numerical methods for difference and functional equations, recurrence relations
65Rxx Numerical methods for integral equations, integral transforms
65Sxx Graphical methods in numerical analysis
65Txx Numerical methods in Fourier analysis
65Yxx Computer aspects of numerical algorithms
65Zxx Applications to the sciences

数值线性代数

If any other mathematical topic is as fundamental to the mathematical sciences as **calculus** and **differential equations**, it is **numerical linear algebra**.

— Trefethen & Bau, *Numerical Linear Algebra*, 1997/2022.

Lloyd N. Trefethen

- Professor of University of Oxford / Harvard (2023.9–)
- First customer to buy MATLAB
- Royal Society (英国皇家学会), National Academy of Engineering (美国国家工程院), Chinese Academy of Sciences, Academia Europaea (欧洲人文与自然科学院)
- President of SIAM, Fellow of SIAM and AMS
- IMA Gold Medal, LMS Naylor Prize, SIAM Pólya Prize
- SIAM John von Neumann Prize
- Invited speaker at ICIAM, ICM, and ECM congresses
- Author of SIAM's all-time bestseller
- Winner of teaching prizes at MIT, Cornell and Oxford
- Winner of the first Fox Prize in Numerical Analysis

Linear algebra — in particular, the solution of linear systems of equations — lies at **the heart** of most calculations in scientific computing.

— Dongarra & Eijkhout, 2000.

J.J. Dongarra and V. Eijkhout, Numerical linear algebra algorithms and software, *JCAM*, 123 (2000), 489–514.

Jack J. Dongarra

- 世界知名的超级计算机与并行计算专家
- 美国田纳西大学电子工程与计算机科学杰出教授
- Director of Innovative Computing Laboratory
- Distinguished Research Staff, Oak Ridge National Laboratory
- Turing Fellow at Manchester University
- National Academy of Engineering, British Royal Society, Russian Academy of Sciences
- Fellow of AAAS, ACM, IEEE and SIAM
- first IEEE Medal of Excellence in Scalable Computing,
  first recipient of the SIAM Special Interest Group on Supercomputing's award, ...
- **EISPACK, LINPACK, BLAS, LAPACK, ScaLAPACK, Netlib, PVM, MPI, Top500, ...**
- 图灵奖(2021)

数值线性代数基本问题

数值线性代数主要研究以下问题:

- 线性方程组求解 $Ax = b$, $A \in \mathbb{R}^{n\times n}$ 非奇异
- (线性) 最小二乘问题 $\min\limits_{x\in\mathbb{R}^n} \|Ax - b\|_2^2$, $A \in \mathbb{R}^{m\times n}$, $m \geq n$
- 矩阵特征值问题 $Ax = \lambda x$, $A \in \mathbb{R}^{n\times n}$, $\lambda \in \mathbb{C}$, $x \in \mathbb{C}^n$, $x \neq 0$
- 矩阵奇异值问题 $A^{\mathsf{T}}Ax = \sigma^2 x$, $A \in \mathbb{R}^{m\times n}$, $\sigma \geq 0$, $x \in \mathbb{R}^n$, $x \neq 0$
- 其它: 广义特征值问题, 非线性特征值问题, 矩阵方程, 张量计算, ...

MSC 2020: Numerical Linear Algebra

65F05 Direct numerical methods for linear systems and matrix inversion
65F08 Preconditioners for iterative methods
65F10 Iterative numerical methods for linear systems
65F15 Numerical computation of eigenvalues and eigenvectors of matrices
65F18 Numerical solutions to inverse eigenvalue problems
65F20 Numerical solutions to overdetermined systems, pseudoinverses
65F22 Ill-posedness and regularization problems in numerical linear algebra
65F25 Orthogonalization in numerical linear algebra
65F35 Numerical computation of matrix norms, conditioning, scaling
65F40 Numerical computation of determinants
65F45 Numerical methods for matrix equations
65F50 Computational methods for sparse matrices
65F55 Numerical methods for low-rank matrix approximation; matrix compression
65F60 Numerical computation of matrix exponential and similar matrix functions
65F99 None of the above, but in this section

数值线性代数常用方法（技术、技巧或工具）

- 矩阵分解: LU, Cholesky, QR, SVD, ...
- 矩阵分裂: 定常迭代法, 预处理技术, ...
- 矩阵降维: 子空间迭代法, 大规模特征值计算, 随机算法, ...

- 问题的特殊结构对算法的设计具有非常重要的影响.
- 自己动手编程实现算法对理解和掌握算法非常有帮助.
- 在实际应用中, 要充分利用现有的优秀程序库.

二十世纪十大优秀算法 (SIAM News, 2000)

1. Monte Carlo method (1946)
2. Simplex Method for Linear Programming (1947)
3. **Krylov Subspace Iteration Methods** (1950)
4. **The Decompositional Approach to Matrix Computations** (1951)
5. The Fortran Optimizing Compiler (1957)
6. **QR Algorithm for Computing Eigenvalues** (1959-61)
7. Quicksort Algorithm for Sorting (1962)
8. Fast Fourier Transform (1965)
9. Integer Relation Detection Algorithm (1977)
10. Fast Multipole Method (1987)

The Best of the 20th Century: Editors Name Top 10 Algorithms, B. A. Cipra, SIAM News, 2000.

课程主要内容

- 预备知识: 线性代数基础 (第一讲)
- 线性方程组的直接解法 (第二讲)
- 线性最小二乘问题的数值算法 (第三讲)
- 非对称矩阵特征值计算 (第四讲)
- 对称矩阵矩阵特征值计算与奇异值计算 (第五讲)
- 线性方程组的定常迭代方法 (第六讲)
- 线性方程组的 Krylov 子空间方法 (第七讲)

成绩评定

平时成绩（考勤 + 小测 + 编程作业等）50%，期末成绩（笔试）50%

主要参考资料

- G.H. Golub and C. F. van Loan, **Matrix Computations (4th)**, 2013.
- J.W. Demmel, **Applied Numerical Linear Algebra**, 1997.
- L.N. Trefethen and D. Bau, III, **Numerical Linear Algebra**, 1997/2022.

- 本课程需要编程, 请自学编程语言, 如北太天元, MATLAB, Python
- 课程主页: http://math.ecnu.edu.cn/~jypan/Teaching/MatrixComp/


谢 谢
THANK YOU