

An Introduction To Numerical Computation

An Introduction To Numerical Computation An Introduction to Numerical Computation An introduction to numerical computation is essential for understanding how modern scientists, engineers, and data analysts solve complex mathematical problems using computers. Numerical computation involves designing algorithms to obtain approximate solutions to problems that may be difficult or impossible to solve analytically. This field bridges pure mathematics and computer science, enabling solutions across diverse areas such as physics, finance, engineering, and data science. As computational power continues to grow, so does the importance of numerical methods in practical applications, making it a cornerstone of scientific computing.

--- What is Numerical Computation? Numerical computation refers to the use of algorithms to perform mathematical operations on data, often involving approximation techniques when exact solutions are unattainable or impractical. Unlike symbolic computation, which seeks precise symbolic solutions, numerical methods aim for sufficiently accurate approximations within acceptable error bounds.

Key Objectives of Numerical Computation

- Accuracy: Achieving results that are close enough to the true solution for practical purposes.
- Efficiency: Maximizing computational speed and minimizing resource usage.
- Stability: Ensuring that small errors do not magnify uncontrollably during calculations.
- Robustness: Providing reliable results across a wide range of problems and input data.

--- Importance of Numerical Computation Numerical methods are vital because many real-world problems cannot be solved analytically. For example:

- Complex Differential Equations: Many physical systems are described by differential equations that lack closed-form solutions.
- Large-scale Data Analysis: Handling massive datasets requires efficient numerical algorithms.
- Optimization Problems: Finding minima or maxima in high-dimensional spaces often relies on numerical techniques.
- Simulation and Modelling: Numerical simulation of weather patterns, fluid dynamics, and structural analysis depends heavily on computational methods.

--- Fundamental Concepts in Numerical Computation Understanding numerical computation involves grasping several core concepts:

1. Approximation and Error - Numerical methods typically produce approximate results.
2. Numerical Stability - A stable algorithm ensures that errors do not grow exponentially during computation.
3. Convergence - An algorithm converges if its output approaches the exact solution as the number of iterations increases.

- Errors can be classified as:

- Round-off errors: Due to finite precision in computer arithmetic.
- Truncation errors: From approximating infinite processes or series.

- Convergence rate impacts computational efficiency.

--- Common Numerical Methods and Techniques Numerical computation employs various methods tailored to specific types of problems:

1. Numerical Linear Algebra - Solving systems of linear equations (e.g., Gaussian elimination)
- 2 - Eigenvalue and singular value decomposition - Matrix factorization techniques
2. Numerical Differentiation and Integration - Finite difference methods for derivatives - Numerical quadrature (e.g., Simpson's rule, trapezoidal rule)
3. Root-Finding Algorithms - Bisection method - Newton-Raphson method - Secant method
4. Optimization Algorithms - Gradient descent - Newton's method - Genetic algorithms
5. Differential Equation Solvers - Euler's method - Runge-Kutta methods - Finite element analysis

--- Applications of Numerical Computation Numerical computation is pervasive across numerous fields:

- Engineering - Structural analysis and design - Control systems simulation
- Signal processing
- Physics and Chemistry - Quantum mechanics simulations - Molecular modeling - Electromagnetic field calculations
- Economics and Finance - Risk assessment models - Option pricing algorithms
- Portfolio optimization
- Data Science and Machine Learning - Numerical optimization in training models - Handling large datasets efficiently - Dimensionality reduction techniques

--- Challenges in Numerical Computation Despite its power, numerical computation faces several challenges:

- Ill-Conditioned Problems: Small changes in input

can cause large variations in output. - Computational Cost: High-precision calculations can be resource-intensive. - Error Propagation: Errors can accumulate through iterative processes. - Algorithm Selection: Choosing the appropriate method for a problem requires expertise. --- Best Practices for Numerical Computation To ensure reliable and efficient results, practitioners should follow best practices: - Understand the problem domain thoroughly. - Select algorithms suited for the specific problem and data. - Analyze the stability and convergence properties of algorithms. - Implement error analysis and validation checks. - Use high-precision arithmetic when necessary. - Leverage existing libraries and software packages (e.g., LAPACK, MATLAB, NumPy). --- Future Trends in Numerical Computation The field continues to evolve with technological advances: - Parallel Computing: Distributing computations across multiple processors for speed. - Machine Learning Integration: Using AI to improve algorithms. - Quantum Computing: Potential for solving certain problems exponentially faster. - Adaptive Algorithms: Automatically adjusting parameters for optimal performance. --- Conclusion An introduction to numerical computation reveals its vital role in solving real-world problems where analytical solutions are unavailable or impractical. By leveraging algorithms that approximate solutions efficiently and accurately, numerical computation enables advancements across science, engineering, finance, and beyond. As computational resources expand and algorithms become more sophisticated, the importance of understanding numerical methods will only grow, empowering professionals to tackle increasingly complex challenges with confidence and precision. --- References - Chapra, S. C., & Canale, R. P. (2010). Numerical Methods for Engineers. McGraw-Hill Education. - Higham, N. J. (2002). Accuracy and Stability of Numerical Algorithms. SIAM. - Press, W. H., Teukolsky, S. A., Vetterling, W. T., & Flannery, B. P. (2007). Numerical Recipes: The Art of Scientific Computing. Cambridge University Press. --- This article 3 provides a comprehensive overview of the fundamental aspects of numerical computation, aiming to serve as a foundational resource for students, researchers, and professionals interested in the field. QuestionAnswer What is numerical computation and why is it important? Numerical computation involves using algorithms and mathematical methods to solve problems approximately with computers. It is crucial for handling complex mathematical models, simulations, and data analysis in science, engineering, and technology where exact solutions are often impossible. What are common methods used in numerical computation? Common methods include finite difference methods, finite element analysis, numerical integration, root-finding algorithms, and iterative methods such as Jacobi and Gauss-Seidel. These techniques approximate solutions to differential equations, algebraic equations, and optimization problems. How do numerical errors affect computation results? Numerical errors, such as truncation and round-off errors, can accumulate and impact the accuracy of results. Understanding and controlling these errors through techniques like error analysis and stability assessment is essential for reliable numerical computations. What role does stability play in numerical algorithms? Stability refers to an algorithm's ability to produce accurate results despite small errors during calculations. Stable algorithms prevent errors from amplifying, ensuring that solutions are reliable even with imperfect data or computational limitations. What is the significance of convergence in numerical methods? Convergence indicates that an iterative numerical method approaches the true solution as the number of iterations increases. Ensuring convergence is critical to guarantee that the algorithm yields meaningful and accurate approximations. How does computational complexity influence numerical computation? Computational complexity measures the amount of resources, such as time and memory, required by an algorithm. Efficient numerical methods optimize resource use, enabling the solution of large-scale problems within reasonable time frames. What are some popular software tools for numerical computation? Popular tools include MATLAB, NumPy and SciPy in Python, Mathematica, and Julia. These platforms provide extensive libraries and functions for implementing numerical algorithms efficiently and effectively. What are practical applications of numerical computation? Numerical computation is used in engineering simulations (like fluid dynamics), financial modeling, machine learning, image processing, weather forecasting, and solving scientific problems where analytical solutions are infeasible. 4 What skills are essential for someone working in numerical computation? Key skills include strong mathematical knowledge, programming proficiency, understanding of numerical analysis principles, problem-solving abilities, and familiarity with computational tools and algorithms to develop accurate and efficient solutions. Introduction to

Numerical Computation Numerical computation is a fundamental aspect of modern scientific research, engineering, and data analysis. It involves the development and application of algorithms to solve mathematical problems numerically rather than symbolically. In essence, numerical computation enables us to approximate solutions to complex equations that are often impossible or impractical to solve analytically. As the backbone of scientific computing, it bridges the gap between theoretical mathematics and real-world applications, offering powerful tools to model, simulate, and analyze phenomena across various disciplines.

--- **Understanding Numerical Computation**

Numerical computation is centered around designing algorithms that can efficiently and accurately approximate mathematical operations. Unlike symbolic computation, which manipulates symbols algebraically, numerical methods work with numerical values, often involving floating-point arithmetic. This approach allows for the handling of problems that are otherwise intractable analytically, such as differential equations, large systems of linear equations, and optimization problems. The primary goal is to obtain solutions that are sufficiently precise within acceptable error margins, considering the constraints of finite precision arithmetic. Numerical computation is indispensable in fields like physics, engineering, finance, and machine learning, where exact solutions are seldom feasible.

--- **Core Concepts in Numerical Computation**

Error Analysis Understanding and managing errors is crucial in numerical computation. Errors can arise from various sources:

- **Round-off errors:** Due to finite precision in representing numbers.
- **Truncation errors:** From approximating infinite processes (like Taylor series) with finite terms.
- **Propagation of errors:** When multiple operations compound errors. Strategies for managing errors include choosing stable algorithms, using appropriate precision levels, and analyzing the bounds of errors to ensure reliability.

Stability and Convergence

- **Stability:** refers to an algorithm's ability to control error amplification during computation.
- **Convergence:** indicates whether an iterative method approaches the true solution as the number of iterations increases. Understanding these properties helps in selecting the right An Introduction To Numerical Computation 5 algorithms for specific problems, ensuring accurate and efficient results.

--- **Common Numerical Methods and Techniques**

Solving Linear Systems

Linear systems are prevalent in modeling physical phenomena, and their solutions form the basis for many numerical techniques.

- **Gaussian elimination:** A straightforward method for small systems.
- **LU decomposition:** For more stable and efficient solving, especially for multiple right-hand sides.
- **Iterative methods:** Such as Jacobi, Gauss-Seidel, and Conjugate Gradient methods, suitable for large sparse systems.

Numerical Differentiation and Integration

- **Differentiation:** Approximates derivatives using finite differences.
- **Integration:** Techniques like Simpson's rule, trapezoidal rule, and Gaussian quadrature approximate definite integrals.

Root-Finding Algorithms

Methods to find zeros of functions include:

- **Bisection method:** Simple, reliable but slow.
- **Newton-Raphson method:** Faster convergence but requires derivative information.
- **Secant method:** Does not require derivatives, balancing speed and simplicity.

Interpolation and Approximation

Constructing functions that fit data points:

- **Polynomial interpolation** (e.g., Lagrange, Newton).
- **Spline interpolation:** Piecewise polynomials providing smooth fits.

--- **Numerical Solutions to Differential Equations**

Differential equations model dynamic systems and are central to physics and engineering. Numerical methods for solving these equations include:

- **Euler's method:** Simple but suffers from stability issues.
- **Runge-Kutta methods:** More accurate and stable, especially the classical fourth-order method.
- **Finite difference and finite element methods:** Discretize continuous problems into algebraic systems suitable for computation. These techniques enable simulations of complex systems such as weather patterns, mechanical structures, and biological processes.

--- **Features and Advantages of Numerical Computation**

Handling Complex Problems

Capable of solving problems that lack closed-form solutions.

Flexibility

Applicable across various fields and problem types.

Computational Power

Leveraging modern hardware for large-scale computations.

Approximate but An Introduction To Numerical Computation 6

Sufficiently Accurate: Provides solutions that are practically useful even if not exact.

Limitations and Challenges

While powerful, numerical computation has its challenges:

- **Accumulation of Errors:** Finite precision can lead to significant inaccuracies.
- **Stability Issues:** Some algorithms may produce unreliable results if not carefully chosen.
- **Computational Cost:** Large problems can demand significant processing time and resources.
- **Sensitivity:** Some problems are highly sensitive to initial conditions or parameters, requiring careful analysis.

--- **Implementing Numerical Computation:** Tools and Software

Numerical

computation relies heavily on software tools that facilitate algorithm implementation and data analysis: - MATLAB: Widely used in engineering and scientific computing for its extensive library of numerical routines. - Python (with NumPy, SciPy): Open-source, versatile, and increasingly popular for scientific computation. - Fortran and C/C++: High-performance languages for computationally intensive tasks. - R: Popular in statistics and data analysis. Choosing the right tool depends on the problem complexity, performance requirements, and user familiarity. --- Applications of Numerical Computation Numerical methods underpin innovations and solutions across many domains: - Engineering: Structural analysis, fluid dynamics, control systems. - Physics: Simulation of particle interactions, astrophysics modeling. - Finance: Risk assessment, option pricing, portfolio optimization. - Biology and Medicine: Modeling biological systems, image reconstruction. - Data Science and Machine Learning: Optimization algorithms, large-scale data analysis. --- Future Directions and Trends The field of numerical computation continues to evolve with advancements in hardware, algorithms, and interdisciplinary applications: - High-Performance Computing (HPC): Utilizing parallel and distributed systems to handle large-scale problems. - Machine Learning Integration: Combining numerical methods with AI for enhanced predictive modeling. - Adaptive Algorithms: Developing methods that dynamically adjust parameters for efficiency and accuracy. - Quantum Computing: Emerging potential to revolutionize numerical problem-solving. --- Conclusion Numerical computation remains an essential discipline that empowers scientists, engineers, and data analysts to solve complex problems that are otherwise intractable analytically. Its core principles—error analysis, stability, convergence—guide the An Introduction To Numerical Computation 7 development of robust algorithms capable of approximating solutions with high accuracy. While it faces challenges such as error propagation and computational demands, continuous advancements in algorithms, hardware, and software ensure its relevance and expanding capabilities. As technology progresses, numerical computation will further integrate with fields like artificial intelligence and quantum computing, opening new horizons for innovation and discovery. Whether modeling physical phenomena, optimizing systems, or analyzing large datasets, numerical methods serve as a vital toolset in the modern scientific landscape. numerical analysis, algorithms, computational mathematics, approximation methods, error analysis, iterative methods, linear algebra, differential equations, programming, scientific computing

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this book serves as a set of lecture notes for a senior undergraduate level course on the introduction to numerical computation which was developed through 4 semesters of teaching the course over 10 years the book requires minimum background knowledge from the students including only a three semester of calculus and a bit on matrices the book covers many of the introductory topics for a first course in numerical computation which fits in the short time frame of a semester course topics range from polynomial approximations and interpolation to numerical methods for odes and pdes emphasis was made more on algorithm development basic mathematical ideas behind the algorithms and the implementation in matlab the book is supplemented by two sets of videos available through the author s youtube channel homework problem sets are provided for each chapter and complete answer sets are available for instructors upon request the second edition contains a set of selected advanced topics written in a self contained manner suitable for self learning or as additional material for an honored version of the course videos are also available for these added topics

our intention in this book is to cover the core material in numerical analysis normally taught to students on degree courses in computer science the main emphasis is placed on the use of analysis and programming techniques to produce well designed reliable mathematical software the treatment should be of interest also to students of mathematics science and engineering who wish to learn how to write good programs for mathematical computations the reader is assumed to have some acquaintance with pascal programming aspects of pascal particularly relevant to numerical computation are revised and developed in the first chapter although pascal has some drawbacks for serious numerical work for example only one precision for real numbers the language has major compensating advantages it is a widely used teaching language that will be familiar to many students and it encourages the writing of clear well structured programs by careful use of structure and documentation we have produced codes that we believe to be readable particular care has been taken to ensure that students should be able to understand the codes in conjunction with the descriptive material given in the book

published to honor the late jim wilkinson the respected pioneer in numerical analysis this book includes contributions from his colleagues and collaborators leading experts in their own right the breadth of wilkinson s research is reflected in the topics covered which include linear algebra error analysis and computer arithmetic algorithms and mathematical software an invaluable reference the book is completely up to date with the latest developments on the lanczos algorithm qr factorizations error propagation models parameter estimation problems sparse systems and shape preserving splines reflecting the current growth and vitality of this field the volume is an essential reference for all numerical analysts

this book deals with various aspects of scientific numerical computing no at tempt was made to be complete or encyclopedic the successful solution of a numerical problem has many facets and consequently involves different fields of computer science computer numerics as opposed to computer algebra is thus based on applied mathematics numerical analysis and numerical computation as well as on certain areas of computer science such as computer architecture and operating systems applied mathemalies i i numerical analysis analysis algebra i i numerical computation symbolic computation i operating systems computer hardware each chapter begins with sample situations taken from specific fields of application abstract and general formulations of mathematical problems are then presented following this abstract level a general discussion

about principles and methods for the numerical solution of mathematical problems is presented relevant algorithms are developed and their efficiency and the accuracy of their results is assessed it is then explained as to how they can be obtained in the form of numerical software the reader is presented with various ways of applying the general methods and principles to particular classes of problems and approaches to extracting practically useful solutions with appropriately chosen numerical software are developed potential difficulties and obstacles are examined and ways of avoiding them are discussed the volume and diversity of all the available numerical software is tremendous

designed for non expert student enthusiast or researcher this two volume text provides an accessible introduction to numerical computation and its applications in science and engineering it assumes no prior knowledge beyond undergraduate calculus and elementary computer programming fundamental and practical issues are discussed in a unified manner with a generous but not excessive dose of numerical analysis topics are introduced on a need to know basis to concisely illustrate the practical implementation of a variety of algorithms and demystify seemingly esoteric numerical methods algorithms that can be explained without too much elaboration and can be implemented within a few dozen lines of computer code are discussed in detail and computer programs in fortran c and matlab are provided algorithms whose underlying theories require long elaborate explanations are discussed at the level of first principles and references for further information are given the book uses numerous schematic illustrations to demonstrate concepts and facilitate their understanding by providing readers with a helpful interplay between ideas and visual images real world examples drawn from various branches of science and engineering are presented updated information on computer technology and numerical methods is included many new and some original topics are introduced additional solved and unsolved problems are included

computer science and applied mathematics introduction to numerical computations second edition introduces numerical algorithms as they are used in practice this edition covers the usual topics contained in introductory numerical analysis textbooks that include all of the well known and most frequently used algorithms for interpolation and approximation numerical differentiation and integration solution of linear systems and nonlinear equations and solving ordinary differential equations a complete discussion of computer arithmetic problems that arise in the computer evaluation of functions and cubic spline interpolation are also provided this text likewise discusses the newton formulas for interpolation and adaptive methods for integration the level of this book is suitable for advanced undergraduate students and readers with elementary mathematical background

julia is an open source and fast growing programming language for scientific computing that offers clarity and ease of use for beginners but also speed and power for advanced applications fundamentals of numerical computation julia edition provides a complete solution for teaching julia in the context of numerical methods it introduces the mathematics and use of algorithms for the fundamental problems of numerical computation linear algebra finding roots approximating data and functions and solving differential equations a clear progression from simple to more advanced methods allows for use in either a one semester course or a two semester sequence the book includes more than 40 functions and 160 examples fully coded in julia and available for download online supplemental content including tested source materials for student projects and in class labs related to every chapter and over 600 exercises evenly split between mathematical and computational work and solutions to most exercises for instructors

designed for a one semester course introduction to numerical analysis and scientific computing presents fundamental concepts of numerical mathematics and explains how

to implement and program numerical methods the classroom tested text helps students understand floating point number representations particularly those pertaining to ieee simple an

this text is for an introductory course in what is commonly called numerical analysis numerical methods or even numerical calculus while it parallels the development in course b4 on numerical calculus in the proposed curriculum in computer science issued by the association for computing machinery this book is designed for any science or engineering student who has completed his first course in calculus and who has at least a passing knowledge of elementary computer programming in fortran this is a practical book for the student who in addition to seeing the theory of numerical methods also likes to see the results the predominant emphasis is on specific methods and computer solutions it often points out where the theory departs from practice and it illustrates each method of computer solution by an actual computer program and its results

designed for the many applied mathematicians and engineers who wish to explore computerized numerical methods this text communicates an enthusiasm for the power of c an object oriented language as a tool for this kind of work this revision of the successful first edition includes for the first time information on programming in windows based environments in addition this revision includes new topics and methods throughout the text that clarify and enhance the treatment of the subject from reviews of the first edition if you are interested in numerical methods or are looking for a course text this book is worth your attention journal of the association of c and c users

designed for the non expert student enthusiast or researcher this text provides an accessible introduction to numerical computation and its applications in science and engineering it assumes no prior knowledge beyond undergraduate calculus and elementary computer programming fundamental and practical issues are discussed in a unified manner with a generous but not excessive dose of numerical analysis topics are introduced on a need to know basis to concisely illustrate the practical implementation of a variety of algorithms and demystify seemingly esoteric numerical methods algorithms that can be explained without too much elaboration and can be implemented within a few dozen lines of computer code are discussed in detail and computer programs in fortran c and matlab are provided algorithms whose underlying theories require long elaborate explanations are discussed at the level of first principles and references for further information are given the book uses numerous schematic illustrations to demonstrate concepts and facilitate their understanding by providing readers with a helpful interplay between ideas and visual images real world examples drawn from various branches of science and engineering are presented updated information on computer technology and numerical methods is included many new and some original topics are introduced additional solved and unsolved problems are included

this textbook is a comprehensive introduction to computational mathematics and scientific computing suitable for undergraduate and postgraduate courses it presents both practical and theoretical aspects of the subject as well as advantages and pitfalls of classical numerical methods alongside with computer code and experiments in python each chapter closes with modern applications in physics engineering and computer science features no previous experience in python is required includes simplified computer code for fast paced learning and transferable skills development includes practical problems ideal for project assignments and distance learning presents both intuitive and rigorous faces of modern scientific computing provides an introduction to neural networks and machine learning

this book is the second part of a modern two volume introduction to numerical computation which strongly emphasizes software aspects it can serve as a textbook for

courses on numerical analysis particularly for engineers the book can also be used as a reference book and it includes an extensive bibliography the author is a well known specialist in numerical analysis who was involved in the creation of the software package quadpack

numerical algorithmic science and engineering nas e or more compactly numerical algorithmics is the theoretical and empirical study and the practical implementation and application of algorithms for solving finite dimensional problems of a numeric nature the variables of such problems are either discrete valued or continuous over the reals or and as is often the case a combination of the two and they may or may not have an underlying network graph structure this re emerging discipline of numerical algorithmics within computer science is the counterpart of the now well established discipline of numerical analysis within mathematics where the latter s emphasis is on infinite dimensional continuous numerical problems and their finite dimensional continuous approximates a discussion of the underlying rationale for numerical algorithmics its foundational models of computation its organizational details and its role in conjunction with numerical analysis in support of the modern modus operandi of scientific computing or computational science engineering is the primary focus of this short monograph it comprises six chapters each with its own bibliography chapters 2 3 and 6 present the book s primary content chapters 1 4 and 5 are briefer and they provide contextual material for the three primary chapters and smooth the transition between them mathematical formalism has been kept to a minimum and whenever possible visual and verbal forms of presentation are employed and the discussion enlivened through the use of motivating quotations and illustrative examples the reader is expected to have a working knowledge of the basics of computer science an exposure to basic linear algebra and calculus and perhaps some real analysis and an understanding of elementary mathematical concepts such as convexity of sets and functions networks and graphs and so on although this book is not suitable for use as the principal textbook for a course on numerical algorithmics nas e it will be of value as a supplementary reference for a variety of courses it can also serve as the primary text for a research seminar and it can be recommended for self study of the foundations and organization of nas e to graduate and advanced undergraduate students with sufficient mathematical maturity and a background in computing when departments of computer science were first created within universities worldwide during the middle of the twentieth century numerical analysis was an important part of the curriculum its role within the discipline of computer science has greatly diminished over time if not vanished altogether and specialists in that area are now to be found mainly within other fields in particular mathematics and the physical sciences a central concern of this monograph is the regrettable downward trajectory of numerical analysis within computer science and how it can be arrested and suitably reconstituted resorting to a biblical metaphor numerical algorithmics nas e as envisioned herein is neither old wine in new bottles nor new wine in old bottles but rather this re emerging discipline is a decantation of an age old vintage that can hopefully find its proper place within the larger arena of computer science and at what appears now to be an opportune time

this textbook provides an accessible and concise introduction to numerical analysis for upper undergraduate and beginning graduate students from various backgrounds it was developed from the lecture notes of four successful courses on numerical analysis taught within the mphil of scientific computing at the university of cambridge the book is easily accessible even to those with limited knowledge of mathematics students will get a concise but thorough introduction to numerical analysis in addition the algorithmic principles are emphasized to encourage a deeper understanding of why an algorithm is suitable and sometimes unsuitable for a particular problem a concise introduction to numerical analysis strikes a balance between being mathematically comprehensive but not overwhelming with mathematical detail in some places where further detail was felt to be out of scope of the book the reader is referred to further reading the book uses matlab implementations to demonstrate the workings of the method and thus matlab s own implementations are avoided unless they are used as building blocks of an algorithm in some cases the listings are printed in the book but all

are available online on the book's page at crcpress.com most implementations are in the form of functions returning the outcome of the algorithm also examples for the use of the functions are given exercises are included in line with the text where appropriate and each chapter ends with a selection of revision exercises solutions to odd numbered exercises are also provided on the book's page at crcpress.com this textbook is also an ideal resource for graduate students coming from other subjects who will use numerical techniques extensively in their graduate studies

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Introduction

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