A COURSE IN

LINEAR ALGEBRA FOR CHEMICAL ENGINEERS

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A first-year graduate course (or sequence of courses) in applied mathematics has become an integral part of the curriculum in a large number of chemical engineering departments. Among the diverse subjects taught in these courses, linear algebra usually enjoys a prominent position. The reason for this popularity perhaps lies in the fact that linear algebra is as central a subject and as applicable as calculus. The pioneering work of Neal Amundson, and of his students and disciples as well as other prominent scholars, has established beyond any doubt that many significant and complex chemical engineering problems may be solved by advanced linear algebra techniques [1].

Linear algebra can also serve as an ideal stepping stone for introducing the first-year graduate student to the formal mathematical language of functional analysis. The basic concepts of matrix algebra, already familiar to the student, can be formulated using the abstract framework of linear vector spaces. The same abstraction can also be used to unify apparently diverse problems in finite dimensional spaces under this common framework. Thus, the groundwork is laid out for the introduction of functional analysis in infinite dimensional spaces, which is necessary for the study of differential and integral operator problems [2].

Our linear algebra course strives to combine both elements of mathematics—abstraction and application. Many of the fundamental theorems of linear algebra are rigorously derived in class.

TABLE 1
Course Materials

COURSE TEXTBOOK

ADDITIONAL COURSE REFERENCES

The theory, however, is motivated and reinforced by examples derived from a wide range of chemical engineering problems. Particular emphasis is placed upon the important aspects of computational linear algebra. In our opinion, it is imperative to expose the students to some fundamental computational methods and to study their efficiency as well as their convergence problems. Student responses to the course evaluation questionnaire indicate that they particularly enjoy the computational part of the course since it points out some of the real problems to which linear algebra theory can be applied.

COURSE ORGANIZATION

Eleven weeks (out of a total of fifteen) of the fall semester course, "Applied Mathematics for Chemical Engineers I," are devoted to the study of linear algebra and its applications. The remaining time is devoted to a brief review of complex analysis and complex integration, which is the final preparation step for the second course in applied mathematics taught at Rice. This

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second course covers the theory of differential and integral operators, again using the functional analysis approach.

The course meets twice a week for two hours and runs largely as a lecture, although active student participation is encouraged by frequent questions from the instructor. The lectures are accompanied by tutoring sessions which are designed to help the students with their computer projects as well as for the discussion of homework assignments in an informal way.

The students are urged to keep a complete set of notes, which are regularly supplemented by handouts providing lengthy theorem proofs or summarizing the results established up to that point.

The assigned textbook is *Linear Algebra and its Applications* (2nd Edition), by Gilbert Strang. Although it is an extremely well-written book, it is not followed closely (especially in the first part of the course). The students are strongly encouraged to consult additional references (see Table 1).

Homework problems are assigned almost every week. In addition, the students are required to complete one or two computational projects. They also have to take a mid-semester and a final exam, which consist of both open- and closed-book parts.

### COURSE CONTENTS

The linear algebra part of the course (see Table 2) consists of four parts:

- Vector spaces and linear transformations
- The solution of systems of linear equations

### TABLE 2

Topical Outline of the Linear Algebra Course

1. VECTOR SPACES AND LINEAR TRANSFORMATIONS
   - Overview of the problem of solving systems of linear equations. Which applications give rise to such systems? Which are the theoretical problems that must be answered?
   - Vector spaces and subspaces.
   - Linear dependence, basis and dimension.
   - Linear transformations between finite-dimensional spaces and their matrix representation.
   - Rank and nullity of linear transformations.
   - Elementary matrices and the computation of the rank of a matrix.
   - The theory of simultaneous linear equations. Homogeneous and nonhomogeneous systems.
   - The Fredholm alternative.

2. SOLUTION OF SYSTEMS OF LINEAR EQUATIONS $A \mathbf{x} = \mathbf{b}$
   - Gaussian elimination. LU—decomposition, pivoting, operation count.
   - Error analysis. Ill-conditioned matrices.
   - Overview of iterative methods for solving linear equations.
   - Comparison of the various numerical algorithms.

3. THE EIGENVALUE PROBLEM $A \mathbf{x} = \lambda \mathbf{x}$
   - Determinants.
   - Inner products, norms, orthogonality.
   - Eigenvalues and eigenvectors of matrices.
   - Diagonalization and similarity transformations.
   - Systems of difference equations.
   - Functions of matrices.
   - Unitary transformations. Normal matrices.
   - Spectral decomposition of operators.

4. QUADRATIC FORMS AND VARIATIONAL PRINCIPLES
   - Positive definite quadratic forms.
   - Minimization problems. Least squares.
   - Rayleigh quotient. Maximum and minimax principles.
   - Numerical computation of eigenvalues and eigenvectors.
   - Overview of the finite elements method.
The students are thus presented with our objectives for the first part of the course. A brief review of the algebra of matrices follows, reminding the student of the familiar concepts of multiplying a matrix by a scalar to obtain another matrix and of summing two matrices to obtain a third one.

- The Eigenvalue problem
- Quadratic forms and variational principles

The Linear Equation Problem $A \mathbf{x} = \mathbf{b}$

The course starts with an introduction to the problem of solving systems of linear equations of the form $A \mathbf{x} = \mathbf{b}$. Several applications that give rise to such large systems are discussed and the three fundamental questions are introduced:

- Do these problems have a solution?
- If they do, is the solution unique?
- How can the solution be computed?

The students are thus presented with our objectives for the first part of the course. A brief review of the algebra of matrices follows, reminding the student of the familiar concepts of multiplying a matrix by a scalar to obtain another matrix and of summing two matrices to obtain a third one. It is also pointed out that these operations satisfy certain properties such as associativity, commutativity, distributivity, etc. This discussion serves as the motivation to introduce the notion of abstract linear vector spaces. Several examples of vector spaces are then presented, covering sets of functions, polynomials, solutions of differential or integral equations, etc. The students come to realize that seemingly different mathematical systems may be considered as vector spaces and that this abstract framework can unify these diverse phenomena into a single study.

The basic concepts of linear combinations, basis sets, and dimension are then discussed. Thus, the abstract quantities called vectors can be represented now in terms of their coefficients of expansion with respect to a particular basis set.

The first milestone is reached with the introduction of linear transformations between finite-dimensional spaces and their matrix representation. Most of the important theorems here are rigorously derived in class and the concepts of rank and nullity of transformations are formally introduced. Armed with the conclusion that all the results established for linear transformations can be used for matrices (and conversely), we can then establish the conditions for existence and uniqueness of solutions of the first fundamental problem of linear algebra $A \mathbf{x} = \mathbf{b}$. This is accomplished in one lecture using the previously derived theorems.

Throughout this part of the course, emphasis is placed on the generality of this approach, and the students have the opportunity to see how the results apply to linear differential and integral operators, as well as to chemical engineering problems. Such examples include first-order reaction systems and the determination of the number of independent chemical reactions in a closed system using experimental measurements.

The practical problem of efficiently computing the solution of systems of linear equations can now be considered. The Gauss elimination procedure and the LU decomposition are introduced, which lead naturally to the idea of the operation count as a measure of the computational effort required. An important application which gives rise to large systems of linear equations is then studied by introducing the finite-difference method for solving ordinary and partial differential equations subject to specified boundary conditions. The students learn how to take advantage of the matrix structure (band or positive-definite matrices) in order to speed up the computational process and how to use the LU-decomposition for the efficient solution of iterative problems that arise in the solution of nonlinear differential equations. The problem of ill-conditioned matrices is outlined in sketchy form, along with a rudimentary introduction to error analysis. Iterative methods for the solution of linear systems of equations are also briefly covered.

At this point a computer project is assigned. The students are asked to solve a two-dimensional partial differential equation using finite differences. They must use different grid sizes and compare the numerical results to the true solutions in each case.

The students must demonstrate that they can correctly formulate the system of linear equations. Following that, they use the library programs available at our computer center to obtain the results. The library programs LINPACK and ITPACK (for the direct and iterative solution of linear systems) have proven to be invaluable aids.
Thus, the emphasis is shifted from the drudgery of computer programming to the analysis of the results. The numerical simulations permit the students to evaluate the relative efficiency of numerical schemes (i.e. execution speeds, memory requirements) and to determine which ones must be used for the various structures and sizes of the resulting matrices. Thus, the theoretical results derived in class are reinforced and justified.

The second part of the computer assignment exposes the students to the pitfalls which may befall the unwary and uninstructed user of computer software packages. The students are asked to solve a system of equations for which the matrix of the coefficients of the unknowns is badly ill-conditioned (the notorious Hilbert matrix has served as the perfect example in this respect). The students are asked to compute the known solution of a system of equations using single and double precision computer arithmetic. They are then asked to explain why the solution deteriorates as the order of the system increases by monitoring the magnitude of the pivoting elements, the condition number of the matrix, and using the theory presented in class.

The Eigenvalue Problem \( A \mathbf{x} = \lambda \mathbf{x} \)

The second part of the course starts with a brief review of the theory of determinants. Their properties are presented along with the basic formulas for their computation. The operation count for solving systems of linear equations using Cramer’s rate is derived and most of the students are surprised to find out that even the most powerful computer would need about \(10^{15}\) years to solve a 100 x 100 system using this method. They are reminded, however, that determinants give a very useful invertibility test for square matrices, whose main application will be used later on in the course for the development of the theory of eigenvalues. The concepts of inner products of vectors and of the norm of a vector are then presented as abstract mappings of vectors into the field of real (or complex) numbers and are related to the familiar notions of angle between vectors and of magnitude respectively.

A discussion of the solution of a simple 2 x 2 system of linear ordinary differential equations motivates the introduction of the eigenvalues of a matrix \( A \). The main emphasis here is on the development of the theoretical results needed for the solution of systems of difference and ordinary differential equations. The cases of operators with distinct and non-distinct eigenvalues are treated in detail, although the case of defective matrices and the Jordan canonical form are only briefly covered.

Throughout this part of the course it is continuously emphasized that the eigenvalues are the most important feature of any dynamical system. The students have the opportunity to solve a large variety of chemical engineering problems. They study:

- The difference equations describing a cascade of CSTR’s.
- The differential equations describing isothermal and non-isothermal CSTR’s and their stability.
- The problem of N first-order chemical reactions taking place in a catalyst pellet.
- The difference equations resulting when a continuous system is subject to piecewise constant inputs, which provides them with an introduction to sampled-data system theory.
- The problem of N first-order reactions taking place in a batch reactor. This is a long assignment, which leads the students in a step-by-step fashion to derive the theoretical results necessary to determine all the rate constants, through a set of carefully designed experiments [3]. This problem encompasses almost everything the students have learned so far in the course. As such, it has come to be known as the “Everything you always wanted to know about first-order reactions in batch (... and more!)” assignment.

The final part of the course introduces the students to the concept of formulating the two main problems of linear algebra, namely \( A \mathbf{x} = \mathbf{b} \) and \( A \mathbf{x} = \lambda \mathbf{x} \), as minimization problems. The emphasis now shifts to pointing out the advantages of this approach for numerical computations. The problem of minimization of a multivariable function serves as the starting point for an introduction of the concepts of quadratic forms and positive definite matrices. The least squares method is then developed formally, and its practical implications are considered. The course closes with the formulation of the eigenvalue problem as a minimization one. The Rayleigh and the min-max principles are presented, followed by a brief

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this method. However, emphasis is placed on when such an approximation can be invoked by developing ideas on multiple time scale analysis. The method is illustrated by considering shrinking unreacted core model in gas-solid reactions and evaporation of a drop in a stagnant fluid.

Additional topics covered in the course are listed in Table 3. These include non-Newtonian fluid flow, turbulent flow, some cases of exact solution of Navier-Stokes equations, evaluations of Nusselt and Sherwood numbers in laminar and turbulent flow, and some cases of mass transfer where no analogs in heat transfer are available. Finally, some examples of macroscopic balances are also solved.

SUMMARY

The course is essentially a survey in transport processes. An attempt is made to give students a thorough understanding of the topics covered, so that they can formulate the necessary differential equations. They are given sufficient insight into some of the powerful tools available to analyze and solve these equations. It is emphasized that the answers obtained must be checked to see if the assumptions made in deriving them are fulfilled. It is also stressed that in most cases, knowing the distribution of velocity, temperature, and concentration is not as important as knowing the fluxes at the interface. These in turn are related to friction factor, Nusselt, and Sherwood numbers respectively. The course as described here has been well received by the students. Good students tend to feel they are ready to tackle more difficult topics. Terminal master’s students feel they have a solid foundation in transport phenomena on which they can continue to build their practical experience.

REFERENCES

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discussion of simple numerical methods for the computation of eigenvalues. In order to further establish the importance of the variational methods, the finite element method is briefly outlined at the end of the course, using tools that the students already possess.

CONCLUDING REMARKS

Our course attempts to introduce the students to the essentials of linear algebra and, at the same time, to convey the fact that these elegant results can be applied to a wide range of engineering problems. Significant emphasis is placed upon the development of basic and efficient computational methods. There is hardly any need to stress again the importance of exposing the chemical engineering graduate student to the basics of numerical analysis. Our experience indicates that the essentials of computational linear algebra can be successfully integrated into an applied mathematics course. A large number of students go on to take a rigorous numerical analysis course given by the Mathematical Sciences Department at Rice, which covers methods for the solution of ordinary and partial differential equations. They have discovered that their background in computational linear algebra was adequate.

We plan to introduce still another computer project in future offerings of this course, in order to familiarize the students with some of the most useful methods for the numerical computation of eigenvalues and eigenvectors of large matrices. The emphasis will again be on the understanding of the physical problem and the resulting mathematical one, and on the study of the relative advantages of the various algorithms.

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REFERENCES