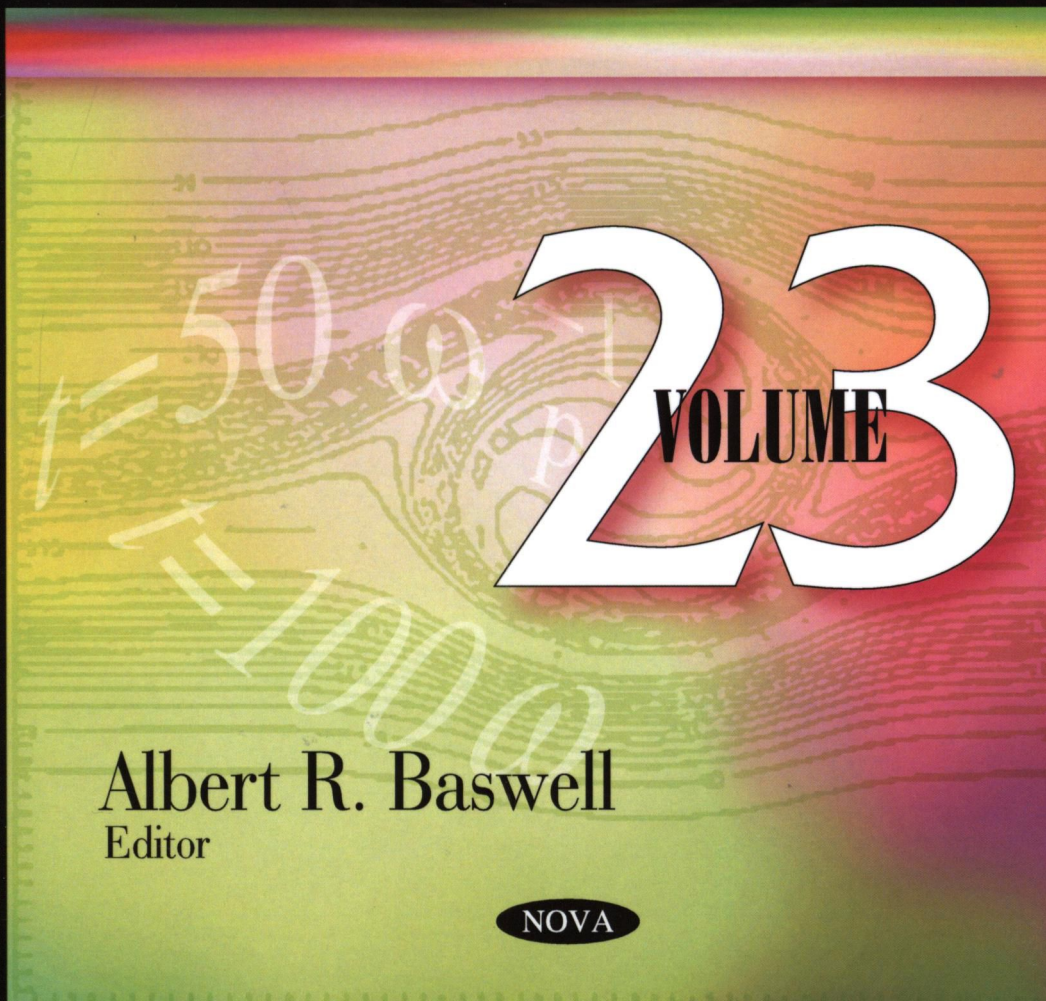
Advances in Mathematics Research



VOLUME 23

Albert R. Baswell
Editor

NOVA

ADVANCES IN MATHEMATICS RESEARCH

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NOTICE TO THE READER

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PREFACE

In the opening chapter by Victor Martinez-Luaces, two kinds of matrices related to chemical problems are examined and an outline of their main properties about their eigenvalues is exhibited in order to demonstrate that all the ODE solutions are either stable or asymptotically stable. In chapter two by Ivan Kyrchei, the Cramer rules for the weighted Moore-Penrose solutions of left and right systems of quaternion linear equations are obtained. Next, in chapter three, Tadeusz Antczak showcases numerous sets of saddle point criteria for a new class of nonconvex nonsmooth discrete minimax fractional programing problems. Marcia de F. B. Binelo, Airam T. Z. R. Sausen, Paulo S. Sausen, and Manuel O. Binelo provide a summary of electric mathematical models used for the prediction of batteries charge and discharge behavior in chapter four. In chapter five, general methodology for the precise modeling and performance assessment of launch vehicles dedicated to microsatellites is proposed by M. Pontani, M. Palloney, and P. Teofilattoz. In chapter six, Nodari Vakhania exemplifies ties and relationships among some optimization problems such as scheduling and transportation issues. In chapter seven, a geometry without using points in established by N. L. Bushwick, bringing the book to a close.

In Chapter 1, two kinds of matrices related to chemical problems are analyzed. Firstly, the focus will be put on first order chemical kinetics mechanisms (FOCKM), which are modeled through ODE linear systems, where their associated matrices (FOCKM-matrices) have a particular structure. A summary of the main properties of their eigenvalues will be discussed in this Chapter. Taking into account these results it is possible to prove that all the ODE solutions are stable or asymptotically stable.

The second class of problems to consider are mixing problems (MP), also analyzed in previous works. These problems led to linear ODE systems, for which the associated matrices (MP-matrices) have different structures depending on whether or not there is recirculation of fluids. It can be observed that all the matrix eigenvalues have a non-positive real part and if the mixing problem involves three or less components, then all the eigenvalues have a negative real part and so, the corresponding ODE solutions are asymptotically stable.

Both types of matrices (FOCKM and MP matrices) have similarities and differences and the latter are important enough to obtain different qualitative behaviors of the ODE solutions as analyzed in Chapter 1.

The theory of noncommutative column-row determinants (previously introduced by the author) is extended to determinantal representations of the weighted Moore-Penrose inverse over the quaternion skew field in Chapter 2. To begin with, the authors introduce the weighted singular value decomposition (WSVD) of a quaternion matrix.

Similarly as the singular value decomposition can be used for expressing the Moore-Penrose inverse, Chapter 2 gives the representation of the weighted Moore-Penrose inverse by WSVD. Using this representation, limit and determinantal representations of the weighted Moore-Penrose inverse of a quaternion matrix are derived within the framework of the theory of column-row determinants. By using the obtained analogs of the adjoint matrix, the authors get the Cramer rules for the weighted Moore-Penrose solutions of left and right systems of quaternion linear equations, and for solutions of two-sided restricted quaternion matrix equation in all cases with respect to weighted matrices.

Numerical examples to illustrate the main results are given.

In Chapter 3, the authors present several sets of saddle point criteria for a new class of nonconvex nonsmooth discrete minimax fractional programming problems in which the involving functions are (Ψ, Φ, ρ)-univex and/or (Ψ, Φ, ρ)-pseudounivex. The results extend and generalize the corresponding results established earlier in the literature for such nonsmooth optimization problems.

Battery behavior modeling, under different use conditions, can be relatively complex due to the nonlinear nature of the charge and discharge processes. Understanding these dynamics by leveraging mathematical models, favors the development of more efficient batteries and also provides tools for software developers to better manage device resources. A review of electrical mathematical models used in the prediction of battery charge and discharge

behavior is presented in Chapter 4. The class of electrical models has been used in various battery modeling applications, including mobile devices and electrical vehicles. The scientific investigation of such models is motivated by their capacity to provide important electrical information such as current, voltage, state of charge, and also some nonlinear aspects of the problem while keeping a relatively low complexity. Six subclasses of electrical models (Simple models, Thévenin-based models, Impedance-based models, Runtime-based models, Combined models and Generic models) along with a discussion of the main characteristics of each. This will demonstrate the evolution of electrical models through successive modification and combination, resulting in varying levels of accuracy and complexity.

Multistage launch vehicles of reduced size, such as "Super Strypi" or "Sword", are currently investigated for the purpose of providing launch opportunities for microsatellites. Chapter 5 proposes a general methodology for the accurate modeling and performance evaluation of launch vehicles dedicated to microsatellites. For illustrative purposes, the approach at hand is applied to the Scout rocket, a micro-launcher used in the past. Aerodynamics and propulsion are modeled with high fidelity through interpolation of available data. Unlike the original Scout, the terminal optimal ascent path is determined for the upper stage, using a firework algorithm in conjunction with the Euler-Lagrange equations and the Pontryagin minimum principle. Firework algorithms represent a recently-introduced heuristic technique, not requiring any starting guess and inspired by the firework explosions in the night sky. The numerically results prove that this methodology is easy-to-implement, robust, precise and computationally effective, although it uses an accurate aerodynamic and propulsive model.

Scheduling and transportation problems are important real-life problems having a wide range of applications in production process, computer systems and routing optimization when the goods are to be distributed to the customers using scarce available resources. In Chapter 6, the authors illustrate ties and relationships among some of these optimization problems. They consider scheduling problem with release and due dates, batch scheduling and vehicle routing problems. As the authors will show here, although these problems seem to have a little in common, a closer look at their parametric and structural properties can give us more insight into the "hidden" ties among these problems that may lead to efficient solution methods.

The construction presented in Chapter 7, like systems of Aristotelian continua presented elsewhere, is designed to establish a geometry without using points. However, it goes further in that the foundation consists of

elements that are completely abstract, rather than line segments whose universe is a line. Furthermore, the result could be modified to represent elements and spaces of multiple dimensions.

CONTENTS

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Chapter 1

MATRICES IN CHEMICAL PROBLEMS: CHARACTERIZATION, PROPERTIES AND CONSEQUENCES ABOUT THE STABILITY OF ODE SYSTEMS

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Abstract

In this chapter, two kinds of matrices related to chemical problems are analyzed. Firstly, the focus will be put on first order chemical kinetics mechanisms (FOCKM), which are modeled through ODE linear systems, where their associated matrices (FOCKM-matrices) have a particular structure. A summary of the main properties of their eigenvalues will be discussed here. Taking into account these results it is possible to prove that all the ODE solutions are stable or asymptotically stable.

The second class of problems to consider are mixing problems (MP), also analyzed in previous works. These problems led to linear ODE systems, for which the associated matrices (MP-matrices) have different structures depending on whether or not there is recirculation of fluids. It can be observed that all the matrix eigenvalues have a non-positive real part and if the mixing problem involves three or less components, then all the eigenvalues have a negative real part and so, the corresponding ODE solutions are asymptotically stable.

Both types of matrices (FOCKM and MP matrices) have similarities and differences and the latter are important enough to obtain different qualitative behaviors of the ODE solutions as analyzed in the chapter.

1. Introduction

Several classical books show the strong relation between chemistry and mathematics, particularly in differential equations, Laplace transform, statistics and numerical methods [1, 2]. This relation was explored in previous papers and book chapters, including five books released by NOVA Publishers [3, 4, 5, 6, 7].

The mathematical tools used in these works included Laplace transform [6, 7, 8, 9, 10], Fourier transform [10, 11], ODE linear systems [5, 12, 13], parabolic PDE [6, 7, 10], numerical methods [14, 15, 16], non parametric statistics [17, 18] and experimental design [19, 20, 21], etc.

The connection of chemical problems with linear algebra was examined in previous works in two different directions. Firstly, chemical kinetics mechanisms were analyzed, with a special interest in first order reactions (called FOCKM-problems). Those FOCKM-problems and the corresponding FOCKM-matrices were the main subject in many papers and book chapters [3, 5, 13, 22, 23]. Also, another area explored in previous papers [12, 24] refers to mixing problems (MP), that can be modeled using linear ODE systems and for which the associated matrices (MP-matrices) have different structures, depending on whether or not there is recirculation of fluids.

Here, both kind of matrices – FOCKM and MP – are analyzed, including a characterization of each class (see section 2 and 4), followed by a study of some of their properties (see section 3 and 5).

In the last section their similarities and differences will be commented on, focusing on ODE solutions corresponding to both FOCKM and MP. In particular, the qualitative behavior of these solutions will be the main interest of the conclusion section.

2. Characterization of FOCKM-Matrices

A typical problem that involves first order ODE appears when a first order unimolecular chemical reaction is studied. This mathematical model is usually included in classical textbooks such as Courant [25], who adapted the original paper written by Wilhelmy in 1850 [26].

In a simplified version, a first order reaction can be easily schematized as follows: $A \xrightarrow{k} B$ where A represents reactant, k is the kinetic constant and B is the reaction product.

The corresponding ODE mathematical model for this chemical kinetics problem is:

$$\frac{d[A]}{dt} = -k[A], \tag{1}$$

where $[A]$ represents the concentration of substance, t is time and the negative sign indicates that the reactant is being transformed, so its concentration diminishes with time.

When several substances react and all these reactions are first order ones, we will call this system a FOCKM. The main purpose of this section is to obtain a general mathematical model (i.e., an ODE system) that describes accurately the FOCKM-problem. For this purpose, let us consider n chemical species E_1, E_2,..., E_n and suppose that all the possible first order chemical reactions $E_i \xrightarrow{k_{ij}} E_j$ take place. If any of these reactions does not occur, then, the corresponding kinetic constant will be considered null.

In this situation, direct reactions involving species E_1 are:

$$E_1 \xrightarrow{k_{12}} E_2,\ E_1 \xrightarrow{k_{13}} E_3,\ \ldots,\ E_1 \xrightarrow{k_{1n}} E_n \tag{2}$$

and the opposed reactions are:

$$E_2 \xrightarrow{k_{21}} E_1,\ E_3 \xrightarrow{k_{31}} E_1,\ \ldots,\ E_n \xrightarrow{k_{n1}} E_1. \tag{3}$$

Consequently, the corresponding ODE for the variation of E_1 concentration with time is:

$$\frac{d[E_1]}{dt} = -k_{12}[E_1] - k_{13}[E_1] - \ldots - k_{1n}[E_1] + k_{21}[E_2] + k_{31}[E_3] + \ldots + k_{n1}[E_n] \tag{4}$$

or in a condensed form:

$$\frac{d[E_1]}{dt} = -s_1[E_1] + k_{21}[E_2] + k_{31}[E_3] + \ldots + k_{n1}[E_n] \tag{5}$$

where

$$s_1 = k_{12} + k_{13} + \ldots + k_{1n} = \sum_{j \neq 1} k_{1j} \tag{6}$$

Following a similar reasoning for species E_i we have:

$$\frac{d[E_i]}{dt} = -s_i[E_i] + k_{1i}[E_1] + \ldots + k_{i-1,i}[E_{i-1}] + k_{i+1,i}[E_{i+1}] \ldots + k_{ni}[E_n] \tag{7}$$

where

$$s_i = k_{i1} + \ldots + k_{i,i-1} + k_{i,i+1} \ldots + k_{in} = \sum_{j \neq i} k_{ij} \tag{8}$$

Then, the ODE system that corresponds to a general FOCKM is:

$$\begin{pmatrix} [E_1] \\ [E_2] \\ \vdots \\ [E_n] \end{pmatrix}' = \begin{pmatrix} -s_1 & k_{21} \cdots & k_{n1} \\ k_{12} & -s_2 \cdots & k_{n2} \\ \vdots & \vdots & \vdots \\ k_{1n} & k_{2n} \cdots & -s_n \end{pmatrix} \begin{pmatrix} [E_1] \\ [E_2] \\ \vdots \\ [E_n] \end{pmatrix} \tag{9}$$

and its associated matrix is:

$$A = \begin{pmatrix} -s_1 & k_{21} \cdots & k_{n1} \\ k_{12} & -s_2 \cdots & k_{n2} \\ \vdots & \vdots & \vdots \\ k_{1n} & k_{2n} \cdots & -s_n \end{pmatrix} \tag{10}$$