

# Contents

- 1. Determinants and Their Properties** 1
- 1.1 Introduction and definition, 1. 1.2 Elementary operations, 3. 1.3 Minors and cofactors, 5. 1.4 Laplace's development of a determinant, 6. 1.5 Solution of linear simultaneous algebraic equations, 8. 1.6 Multiplication of determinants, 10. 1.7 Differentiation of a determinant, 11.*
- 2. Linear Algebraic Equations and Elementary Properties of Matrices** 14
- 2.1 Definition, 14. 2.2 Elementary operations and properties, 15. 2.3 The adjoint and the inverse matrices, 17. 2.4 The reversal rule for transposes and inverses, 20. 2.5 Rank of a matrix, 21. 2.6 Elementary matrix operations on rows and columns, 24. 2.7 Sylvester's law of nullity, 26. 2.8 Linear simultaneous algebraic equations: The general theory, 27. 2.9 Further implications of rank, 33. 2.10 The solution of homogeneous linear equations, 35. 2.11 Comparison of solution of linear equations by determinants and elimination, 38. 2.12 Computation of the inverse of a matrix by the method of elimination, 40. 2.13 Derivation of linear equations by the method of least squares, 41. 2.14 Related matrices, 43. 2.15 Partitioned matrices, 43. 2.16 Differentiation and integration of matrices, 44.*

**3. Vectors and Matrices**

47

3.1 Introduction, 47. 3.2 Sets of vectors, 48. 3.3 Application to chemical equilibrium, 50. 3.4 Application to dimensional analysis, 54. 3.5 Expansion of vectors in a basis, 56. 3.6 Application of vector expansion to the solution of linear equations and matrix inversion, 60. 3.7 Application to chemical reaction systems, 61.

**4. Linear Programming**

70

4.1 Introduction, 70. 4.2 The problem and its dual, 75. 4.3 Transformation of the problem, 76. 4.4 Convex sets, 77. 4.5 Fundamental theorems in linear programming, 79. 4.6 The simplex method of Dantzig, 82. 4.7 Feasible solution for the dual problem, 89. 4.8 Optimality criterion, 93. 4.9 Duality, 94. 4.10 The general problem of linear programming, 101. 4.11 Matrix solution of the linear programming problem, 102. 4.12 Degeneracy and its solution, 105. 4.13 Optimal solutions, 109.

**5. Eigenvalues and Eigenvectors**

111

5.1 Introduction, 111. 5.2 Eigenvectors, 113. 5.3 The biorthogonality property of distinct eigenvectors, 114. 5.4 The symmetric case, 116. 5.5 The expansion of an arbitrary vector, 117. 5.6 Examples, 119. 5.7 Application to a system of first-order differential equations, 121. 5.8 Air-water interaction process, 124. 5.9 The Hamilton-Cayley theorem, 127. 5.10 A useful lemma, 128. 5.11 Proof of the Hamilton-Cayley theorem, 128. 5.12 Some deductions from the Hamilton-Cayley theorem, 130. 5.13 Sylvester's theorem, 132. 5.14 An alternative form for Eq. (5.13.3) 135. 5.15 Gram-Schmidt orthogonalization process, 138. 5.16 The calculation of eigenvalues and eigenvectors, 139. 5.17 Eigenvalues of the Jacobi matrix, 143. 5.18 Sturmian functions, 145.

**6. Some Problems in Staged Operations**

149

6.1 Introduction, 149. 6.2 Multicomponent rectification, 149. 6.3 The solution as a difference equation, 153. 6.4 The solution by separation of variables, 157. 6.5 The transient analysis of a staged absorber, 160. 6.6 Reactions in stirred tank reactors and batch reactors, 167. 6.7 Multicomponent distillation, 170.

**7. Further Properties of Matrices**

177

7.1 Introduction, 177. 7.2 Reduction of a matrix to diagonal form, 177. 7.3 Quadratic forms, 180. 7.4 The reduction of a quadratic form to canonical form, 183. 7.5 An associated problem, 185. 7.6 Definite

*quadratic forms*, 186. 7.7 *Maxima and minima of functions of several variables*, 187. 7.8 *The minimal properties of the eigenvalues*, 188. 7.9 *Functions defined on matrices. Infinite series*, 191. 7.10 *Systems of first-order differential equations*, 196. 7.11 *The matrizant*, 199. 7.12 *Reduction of a system of equations to normal form*, 204. 7.13 *The Routh-Hurwitz criterion for eigenvalues*, 207. 7.14 *The exploration of response surfaces*, 208. 7.15 *Maxima or minima with restrictions*, 214. 7.16 *Simultaneous maxima*, 216. 7.17 *Transformations*, 218. 7.18 *Transformations in oblique coordinate systems*, 221.

## 8. Complex Monomolecular Kinetics and Staged Dynamics 224

8.1 *Introduction*, 224.

A. *Analysis of Complex Reaction Systems*, 225

8.2 *Preliminary remarks*, 225. 8.3 *Reduction to normal form*, 227. 8.4 *The character of the eigenvalues*, 229. 8.5 *Straight line reaction paths*, 232. 8.6 *A new set of vectors*, 236. 8.7 *The treatment of experimental data*, 237. 8.8 *An example of Wei and Prater for a four-component system*, 241. 8.9 *Time contours in the reaction simplex and their properties*, 247. 8.10 *Remarks on applicability of first-order systems*, 248. 8.11 *A simple irreversible consecutive reaction system*, 249.

B. *Distillation Column Dynamics*, 251

8.12 *Formulation of the equations*, 251. 8.13 *On the character of the eigenvalues of  $G_i$* , 254. 8.14 *The mathematical solution*, 256. 8.15 *The numerical procedure*, 258. 8.16 *The computation of eigenvectors and eigenvalues*, 259.

## References 262

## Index 265