

# Meschach

## Matrix Computations in C

|   |           |
|---|-----------|
| <b>1 Tutorial</b>   | <b>1</b>  |
| 1.1 The data structures and some basic operations . . . . .                           | 1         |
| 1.2 How to manage memory . . . . .  | 5         |
| 1.2.1 No deallocation . . . . .   | 6         |
| 1.2.2 Allocate and deallocate . . . . .   | 6         |
| 1.2.3 Resize on demand . . . . .  | 6         |
| 1.2.4 Registration of workspace . . . . .   | 7         |
| 1.3 Simple vector operations: An RK4 routine . . . . .                                | 8         |
| 1.4 Using routines for lists of arguments . . . . .                                   | 14        |
| 1.5 A least squares problem . . . . .   | 15        |
| 1.6 A sparse matrix example . . . . .   | 18        |
| 1.7 How do I . . . ? . . . . .  | 20        |
| 1.7.1 . . . solve a system of linear equations . . . . .                              | 20        |
| 1.7.2 . . . solve a least-squares problem . . . . .                                   | 20        |
| 1.7.3 . . . find all the eigenvalues (and eigenvectors) of a general matrix . . . . . | 20        |
| 1.7.4 . . . solve a large, sparse, positive definite system of equations              | 21        |
| <b>2 Data structures</b>  | <b>23</b> |
| 2.1 General principles . . . . .  | 23        |
| 2.2 Vectors . . . . .   | 24        |
| 2.2.1 Integer vectors . . . . .   | 25        |
| 2.2.2 Complex vectors . . . . .   | 25        |
| 2.3 Matrices . . . . .  | 26        |
| 2.3.1 Complex matrices . . . . .  | 27        |
| 2.3.2 Band matrices . . . . .   | 27        |
| 2.4 Permutations . . . . .  | 28        |
| 2.5 Basic sparse operations and structures . . . . .                                  | 29        |
| 2.6 The sparse data structures . . . . .  | 30        |
| 2.7 Sparse matrix factorisation . . . . .   | 33        |
| 2.8 Iterative techniques . . . . .  | 34        |
| 2.9 Other data structures . . . . .   | 36        |
| <b>3 Numerical Linear Algebra</b>   | <b>37</b> |
| 3.1 What numerical linear algebra is about . . . . .                                  | 37        |
| 3.2 Complex conjugates and adjoints . . . . .   | 38        |
| 3.3 Vector and matrix norms . . . . .   | 38        |
| 3.4 “Ill conditioning” or intrinsically bad problems . . . . .                        | 39        |

|          |  |            |
|----------|--|------------|
| 3.5      | Least squares and pseudo-inverses . . . . .              | 41         |
| 3.5.1    | Singular Value Decompositions . . . . .                  | 42         |
| 3.5.2    | Pseudo-inverses . . . . .                                | 42         |
| 3.5.3    | QR factorisations and least squares . . . . .            | 43         |
| 3.6      | Eigenvalues and eigenvectors . . . . .                   | 44         |
| 3.7      | Sparse matrix operations . . . . .                       | 46         |
| <b>4</b> | <b>Basic Dense Matrix Operations</b>                     | <b>49</b>  |
| <b>5</b> | <b>Dense Matrix Factorisation Operations</b>             | <b>115</b> |
| <b>6</b> | <b>Sparse Matrix &amp; Iterative Operations</b>          | <b>148</b> |
| <b>7</b> | <b>Installation and copyright</b>                        | <b>181</b> |
| 7.1      | Installation . . . . .                                   | 181        |
| 7.1.1    | Installation on non-Unix systems . . . . .               | 183        |
| 7.1.2    | makefile . . . . .                                       | 184        |
| 7.1.3    | machine.h . . . . .                                      | 184        |
| 7.1.4    | machine.c . . . . .                                      | 185        |
| 7.2      | Backward compatibility . . . . .                         | 187        |
| 7.3      | Copyright . . . . .                                      | 187        |
| <b>8</b> | <b>Designing numerical libraries in C</b>                | <b>189</b> |
| 8.1      | Numerical programming in C . . . . .                     | 189        |
| 8.1.1    | On efficient compilers . . . . .                         | 190        |
| 8.1.2    | Strategies for using C . . . . .                         | 190        |
| 8.1.3    | Non-C programmers start here! . . . . .                  | 191        |
| 8.2      | The data structures . . . . .                            | 195        |
| 8.2.1    | Pointers to struct's . . . . .                           | 195        |
| 8.2.2    | Really basic operations . . . . .                        | 196        |
| 8.2.3    | Output . . . . .   | 198        |
| 8.2.4    | Copying . . . . .  | 199        |
| 8.2.5    | Input . . . . .  | 200        |
| 8.2.6    | Resizing . . . . .                                       | 202        |
| 8.3      | How to implement routines . . . . .                      | 203        |
| 8.3.1    | Design for debugging . . . . .                           | 203        |
| 8.3.2    | Workspace . . . . .                                      | 204        |
| 8.3.3    | Incorporating user-defined types into Meschach . . . . . | 206        |
| 8.3.4    | Output and object resizing . . . . .                     | 210        |
| 8.4      | User-defined functions . . . . .                         | 211        |
| 8.5      | Building the library . . . . .                           | 213        |
| 8.5.1    | Numerical aspects . . . . .                              | 214        |
| 8.6      | Debugging . . . . .                                      | 215        |
| 8.6.1    | Memory allocation bugs . . . . .                         | 216        |
| 8.6.2    | If all else fails . . . . .                              | 217        |

|                                  |   |            |
|----------------------------------|---|------------|
| 8.7                              | Suggestions for enthusiasts . . . . .   | 218        |
| 8.8                              | Pride and Prejudice . . . . .   | 218        |
| 8.8.1                            | What about Fortran 90? . . . . .  | 218        |
| 8.8.2                            | Why should people writing numerical code care about good<br>software? . . . . . | 218        |
| <b>For further reading . . .</b> |   | <b>220</b> |
| <b>Index</b>                     |   | <b>221</b> |
| <b>Function index</b>            |   | <b>229</b> |