## Chapter 8

## Conclusions and further work

In this thesis we have studied certain problems involving positive semi-definite matrix constraint. We have found that our implementations of the new unconstrained methods for solving the Euclidean distance matrix problem have performed well in comparison with the projection method. However, the hybrid methods in Chapter 4 performed even better, with very fast convergence, especially the projection-unconstrained method (Section 4.3) which is much better than the projection method and Method 3.4.2 from which it is composed. In determining the correct rank the projection method worked well and found the rank in a few iterations. Also we have successfully found methods for switching from one method to another.

A number of suggestions for further research about the methods that solves the Euclidean distance matrix problem are the following.

- It is clear that if the diagonal matrix $\Delta^{(k)}$ in (3.3.11) satisfies $P_{d} P_{M}\left(F+\Delta^{(k)}\right)=P_{M}\left(F+\Delta^{(k)}\right)$ then $P_{M}\left(F+\Delta^{(k)}\right)$ is the required solution where $F$ is a given matrix. Possibly from the structure of the given matrix $F$ that one can find the required diagonal matrix in one go. It is not clear how to do this but it might be worth trying.
- The unconstrained methods have a large number of variables $(\sim(r-1) n$ depending on the method) which means that the method takes a large number of line searches to solve the problem. Therefore it is worth trying to restate the problem with only the diagonal matrix $\Delta^{(k)}$ as variables and then finding methods for solving it.
- Method 3.4.3 needs more investigation because the number of variables is less than the
other unconstrained methods, whilst the number of line searches is larger. However number of possible reasons have been given in Section 3.6.

For the least distance problem in Chapter 5 two methods are developed, that is the projection method and the $l_{1}$ SQP method. The $l_{1}$ SQP method has performed well in comparison with the projection method which takes a huge number of iterations to solve the problem. Also the projection- $l_{1}$ SQP method (Section 4.3) has worked well in solving the problem. The few iterations taken by the projection method to determine the rank saves a large number of iterations taken by the $l_{1}$ SQP method. The integer $s$ in Algorithm 5.4.1 chosen to be small $(\sim 2)$ in Table 5.5.2. This reduces the number of iterations taken by projection method although the rank is not accurately estimated and the lower bound given by Fletcher [1985] has worked better in the case 1-18.

Two suggestions for further research about the methods that solves the least distance problem are given in the following.

- By looking at problem (5.4.3), there is a different problems with every different initial vector a. The projection Algorithm 5.2.2 solves this problem with the initial vector zero replaced by a. Extending the $l_{1}$ SQP method to solve problems of this type is worth investigation.
- A modified projection algorithm similar to Algorithm 4.2 .1 is needed for the least distance problem this enable us to use the result matrix from the $l_{1}$ SQP method as an initial matrix for the projection method. Then a more effective hybrid method could be obtained.

Two methods have given for solving the educational testing problem. One is the $l_{1} \mathrm{SQP}$ method by Fletcher [1985] the other is the projection method by Glunt [1991]. The hybrid methods developed in Chapter 7 have good rate of convergence specially the $l_{1}$ SQP-projection method (Section 7.3) as compared with the methods of Chapter 6. The projection method is not very effective in determining the rank when $n \geq 12$. This is because a small value of $s$ is shosen in Algorithms 7.2.1 and 7.3.1. In the other hand if $s$ is increased then a large number of iterations are consumed by the projection method. Hence a suitable way of chosing the integer $s$ is needs some investigation. Various examples are solved in Sections 6.5 and 7.4 with different $\tau$. The best way to choose $\tau$ is given there.

## References

Al-Baali, M. and Fletcher, R. [1985]. Variational methods for nonlinear least squares, J. Oper. Res. Soc., 36, pp. 405-421.

Bentler, P. M. [1972]. A lower-bound method for the dimension-free measurement of internal consistency, Social Sci. Res., 1, pp. 343-357.

Blumenthal, L. M. [1953]. Theory and Applications of Distance Geometry, Oxford Univ. Press, London.

Boyle, J. P. and Dykstra, R. L. [1986]. A method for finding projections onto the intersection of convex sets in Hilbert space, in Advances in Order Restricted Statistical Inference, (Eds. R. Dykstra, T. Robertson, and F. T. Wright), Lecture Notes in Statistics 37, Springer-Verlag, Berlin, pp. 28-47.

Browne, M. W. [1987]. The Young-Householder algorithm and the least squre multidimensional scaling of squared distance, J. of Classification, 4, pp. 175-190.

Broyden, C. G. [1970]. The convergence of a class of double rank minimization algorithms, parts I and II, J. Inst. Maths. Applns., 6, pp. 76-90 and 222-231.

Cheney, W. and Goldstein, A. [1959]. Proximity maps for convex sets, Proc. Amer. Math. Soc., 10, pp. 448-450.

Colledge, R. G. and Rushton, G. [1972]. Multidimensional scaling: review and geographical applications. Geographic technical papers series, no. 10. Association of American geographers. Washington.

Crippen, G. M. [1977]. A novel approach to calculation of conformation: distance gemotry. $J$. Computational Physics 24, pp. 96-107. *

Crippen, G. M. [1978]. Rapid calculation of coordinates from distance measures. J. Computational Physics 26, pp. 449-452.

De Leeuw, J. and Heiser, W. [1980]. Multidimensional scaling with restrictions on the configuration, in Multivariate Analysis V, (Ed. P. R. Krishnaiah), North Holland Pub. Co., pp. 502-522.

Deutsch, F. [1983]. Von Neumann's alternating method: the rate of convergence, in Approximation Theory IV, (Eds. C. Chui, L. Schumaker and J. Ward), Academic Press, New York-London, pp. 427-434.

Dykstra, R. L. [1983]. An algorithm for restricted least squares regression, J. Amer. Stat. Assoc. 78, pp. 839-842.

Fletcher, R. [1970]. A new approach to variable metric algorithms, Computer J., 13, pp. 317-322.

Fletcher, R. [1981a]. Numerical experiments with an exact $l_{1}$ penalty function method, in Nonlinear Programming 4, (Eds. O. L. Mangasarian, R. R. Meyer and S. M. Robinson), Academic Press, New York.

Fletcher, R. [1981b]. A nonlinear programming problem in statistics (educational testing), SIAM J. Sci. Stat. Comput., 2, pp. 257-267.

Fletcher, R. [1982]. Semi-definite matrix constraints in optimization, Dept. Mathematical Sciences, Numerical Analysis Report NA/61, Univ. Dundee, Scotland.

Fletcher, R. [1985]. Semi-definite matrix constraints in optimization, SIAM J. Control and Optimization, 23, pp. 493-513.

Fletcher, R. [1987]. Practical methods of optimization, John Wiley and Sons, Chichester.

Gaffke, N. and Mathar, R. [1989]. A cyclic projection algorithm via duality, Metrika, 36, pp. 29-54.

Gilbert, E. N. [1974]. Distortion in maps, SIAM Review, 16, pp. 47-62.

Glunt, W. [1991]. An alternating projections method for linear convex programming problems, Ph.D. Thesis, University of Kentucky.

Glunt,W. Hayden, T. L. Hong, S. and Wells, J. [1990]. An alternating projections method for computing the nearest Euclidian distance matrix, SIAM J. Matrix and App. , 4, pp. 589-600.

Goldfarb, D. [1970]. A family of variable metric methods derived by variaional means, Maths. Comp., 24, pp. 23-26.

Golub, G. H. and Van Loan, C. F. [1989]. Matrix Computations, Johns Hopkins Universty Press, Baltimore, MD.

Guttman, L. [1945]. A basis for analyzing test-retest reliability, Psychometrika, 10, pp. 255282.

Hald, J. and Madsen, K. [1981]. Combined LP and quasi-Newton methods for minmax optimization, Math. Programming, 20, pp. 49-62.

Han, S. P. [1977]. A globally convergent method for nonlinear programming, J. Optim. Theory Appl., 22, pp. 297-309.

Han, S. P. [1988]. A successive projection method, Math. Programming, 40, pp. 1-14.

Havel, T. Kuntz, I. and Crippen, G. [1983]. The theory and practice of distance geometry, Bull. Math. Biol., 45, pp. 665-720.

Hayden, T. L. and Wells, J. [1988]. Approximation by matrics positive semi-definite on a subspace, Linear Alg. and Appl., 109, pp. 115-130.

Higham, N. [1988]. Computing a nearest symmetric positive semi-definite matrix, Linear Alg. and Appl., 103, pp. 103-118.

Kendall, D. G. [1971]. Construction of maps from "odd" bits of information, Nature, 231, pp. 158-159.

Lalouel, J. M. [1977]. Linkage mapping from pairwise recombination data, Heredity, 38, pp. 61-77.

Menger, K. [1931]. New foundations of Euclidean geometry, Amer. J. Math., 53, pp. 721-745.

Meulman, J. [1986]. A distance approach to nonlinear multivariate analysis, DSWO Press, Leiden.

Powell, M. J. D. [1970]. A hybrid method for nonlinear equations, in Numerical Methods for Nonlinear Algebraic Equations, (Ed. P. Rabinowitz), Gordon and Breach, London.

Rockafellar, R. T. [1970]. Convex Analysis, Princeton Univ. Press, Princeton, NJ.

Rockafellar, R. T. [1981]. The Theory of Subgradients and Its Applications to Problems of Optimization. Convex and Nonconvex Functions, Research and Education in Mathematics 1, Heldermann Verlag, Berlin.

Schoenberg, I. J. [1935]. Remarks to M. Frechet's article "Sur la definition axiomatique d'une classe d'espace distances vectoriellement applicable sur l'espace de Hilbert", Ann. of Math., 36, pp. 724-732.

Shanno, D. F. [1970]. Conditioning of quasi-Newton methods for function minimization, Maths. Comp., 24, pp. 647-656.

Takane, Y. [1977]. On the relations among four methods of multidimensional scaling, Behaviormetrika 4, pp. 29-43.

Von Neumann, J. [1950]. Functional Operators II, The geometry of orthogonal spaces, Annals of Math. Studies No. 22, Princeton Univ. Press.

Woodhouse, B. [1976]. Lower bounds for the reliability of a test, M.Sc. Thesis, Dept of Statistics, University of Wales, Aberystwyth.

Woodhouse, B. and Jackson, P. H. [1977]. Lower bounds for the reliability of the total score on a test composed of non-homogeneous items: II. A search procedure to locate the greatest lower bound, Psychometrika 42, pp. 579-591.

Young, F. W. [1984]. Scaling, Ann. Rev. Psychol. 35, pp. 55-81.

Young, G. and Householder A. S. [1938]. Discussion of a set of points in terms of their mutual distances, Psychometrika 3, pp. 19-22.

