

Bibliography

- [1] R. Agrawal, J. Gehrke, D. Gunopulos, and P. Raghavan. Automatic subspace clustering of high dimensional data for data mining applications. In *Proc. ACM SIGMOD Int. Conf. on Management of Data*, pages 94–105, 1998.
- [2] M.P. Allen and D.J. Tildesley. *Computer Simulations of Liquids*. Clarendon Press, Oxford, 1990.
- [3] N. Allinson, H. Yin, L. Allinson, and J. Slack (editors). *Advances in Self-Organizing Maps*. Springer, 2001.
- [4] A. Amadei, A.B.M. Linssen, and H.J.C. Berendsen. Essential dynamics of proteins. *Proteins*, 17, 1993.
- [5] A. Ben-Dor, R. Shamir, and Z. Yakhini. Clustering gene expression patterns. *Journal of Computational Biology*, 6(3/4):281–297, 1999.
- [6] J. Bezdek and N. Pal. Some new indexes of cluster validity. *IEEE Trans. Syst. Man. Cybern.*, 28:301–315, 1998.
- [7] Ch.M. Bishop. *Neural networks for pattern recognition*. Oxford University Press, 1995.
- [8] H. Bothe and R. Rojas (editors). *Proceedings of the 2nd International ICSC Symposium on Neural Computation*. ICSC Academic Press, 2000.
- [9] S. Brooks and A. Gelman. General methods for monitoring convergence of iterative simulations. *J. Comp. Graph. Stat.*, (7):434–455, 1998.
- [10] D. R. Corey. Design and engineering of proteins as therapeutic agents. In [63], pages 187–204.
- [11] M. Cottrell, E. de Bodt, and M. Verleysen. Kohonen maps versus vector quantization for data analysis. In *Proc. of European Symposium on Artificial Neural Networks (ESANN)*. D-Facto, Brussel, 1997.
- [12] M. Cottrell, J. Fort, and G. Pages. Theoretical aspects of the som algorithm. *Neurocomputing*, (21):119–138, 1998.

- [13] P. Deuflhard and A. Hohmann. *Introduction to Scientific Computing*. Springer, 2nd edition, 2002.
- [14] P. Deuflhard, M. Dellnitz, O. Junge, and Ch. Schütte. Computation of essential molecular dynamics by subdivision techniques. In [15].
- [15] P. Deuflhard, J. Hermans, B. Leimkuhler, A.E. Mark, S. Reich, and R.D. Skeel (editors). *Computational Molecular Dynamics: Challenges, Methods, Ideas. Lecture Notes in Computational Science and Engineering*, volume 4. Springer, 1998.
- [16] P. Deuflhard, W. Huisenga, A. Fischer, and Ch. Schütte. Identification of almost invariant aggregates in nearly uncoupled markov chains. *Linear Algebra and its Applications* 315, pages 39–59, 2000.
- [17] M. Dittenbach, D. Merkl, and A. Rauber. The growing hierarchical self-organizing map. In *Proc. International Joint Conf. on Neural Networks (IJCNN), Como, Italy*, volume 6, pages 15–19. IEEE Computer Society, 2000.
- [18] B.S. Duran and P.L. Odell. *Cluster Analysis*. Springer, 1974.
- [19] M. Ester, H.-P. Kriegel, J. Sander, and X. Xu. Incremental clustering for mining in a data warehousing environment. In *Proc. 24th Int. Conf. on Very Large Databases (VLDB 98), New York City*, pages 323–333, 1998.
- [20] B.S. Everitt. *Cluster Analysis*. Arnold, 3rd edition, 1993.
- [21] U.M. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthurusamy (editors). *Advances in Knowledge Discovery and Data Mining*. AAAI Press / The MIT Press, California, 1996.
- [22] A. Fischer, F. Cordes, and Ch. Schütte. Hybrid Monte Carlo with adaptive temperature choice: efficient conformational analysis of RNA. *Comput. Phys. Comm.*, 121-122:37–39, 1998.
- [23] A. Fischer, Ch. Schütte, P. Deuflhard, and F. Cordes. Hierarchical uncoupling-coupling of metastable conformations. In [57]. Available as ZIB-Report 01-03 via <http://www.zib.de/bib/pub/pw>.
- [24] N.I. Fisher. *Statistical Analysis of Circular Data*. University Press, Cambridge, 1993.
- [25] C. Fraley and A. E. Raftery. How many clusters? Which clustering method? Answers via model-based cluster analysis. *Computer Journal*, (41):578–588, 1998.
- [26] B. Fritzke. Growing grid - a self-organizing network with constant neighborhood range and adaptation strength. *Neural Processing Letters*, 2(5):9–13, 1995.
- [27] K. Fukunaga. *Introduction to Statistical Pattern Recognition*. Academic Press, 1990.

- [28] T. Galliat. Clustering data of different information levels. Preprint SC-99-42, Konrad-Zuse-Zentrum, Berlin. Available via <http://www.zib.de/DataMining>, 1999.
- [29] T. Galliat and P. Deufhard. Adaptive hierarchical cluster analysis by self-organizing box maps. ZIB-Report 00-13, Konrad-Zuse-Zentrum, Berlin. Available via <http://www.zib.de/bib/pub/pw/>, 2000.
- [30] T. Galliat, P. Deufhard, R. Roitzsch, and F. Cordes. Automatic identification of metastable conformations via self-organized neural networks. In [57]. Available as ZIB-Report 00-51 via <http://www.zib.de/bib/pub/pw/>.
- [31] T. Galliat, W. Huiszinga, and P. Deufhard. Self-organizing maps combined with eigenmode analysis for automated cluster identification. In [8], pages 227–232.
- [32] V. Ganti, R. Ramakrishnan, J. Gehrke, A. Powell, and J. French. Clustering large datasets in arbitrary metric spaces. In *Proc. 15th International Conf. on Data Engineering, Sydney, Australia*, pages 502–511. IEEE Computer Society, 1999.
- [33] M. Garey and D. Johnson. *Computers and Intractability: a guide to the theory of NP-completeness*. Freeman, New York, 1979.
- [34] A. Gelman and D.B. Rubin. Inference from iterative simulation using multiple sequences. *Statistical Science*, (7):457–511, 1992.
- [35] A. Gersho and R.M. Gray. *Vector Quantization and Signal Compression*. Kluwer Academic Publishers, 1992.
- [36] D. Gibson, J. Kleinberg, and P. Raghavan. Clustering categorical data: An approach based on dynamical systems. In *Proc. 24th Int. Conf. on Very Large Databases (VLDB 98), New York City*, pages 311–323, 1998.
- [37] T.A. Halgren. Merck molecular force field.i-v. *J. Comp. Chem.*, 17(5&6):490–641, 1996.
- [38] T. Heskes. Energy functions for self-organizing maps. In [50], pages 303–316.
- [39] W. Huiszinga, C. Best, R. Roitzsch, C. Schütte, and F. Cordes. From simulation data to conformational ensembles: Structure and dynamic based methods. *J. Comp. Chem.*, 20(16):1760–1774, 1999.
- [40] M. Van Hulle. *Faithful Representations and Topographic Maps*. John Wiley Sons, Inc., 2000.
- [41] M. Hyvönen, Y. Hiltunen, W. El-Deredy, T. Ojala, J. Vaara, P. Kovanen, and M. Ala-Korpela. Application of self-organizing maps in conformational analysis of lipids. *J. Am. Chem. Soc.*, 123(5):810–816, 2001.
- [42] A. Jain and R. Dubes. *Algorithms for Clustering Data*. Prentice Hall, 1988.

- [43] M. Karpen, D. Tobias, and C. Brooks. Statistical clustering techniques for the analysis of long molecular dynamics trajectories. *Biochemistry*, 32(2):412–420, 1993.
- [44] S. Kaski. *Data Exploration Using Self-Organizing Maps*. PhD thesis, Helsinki University of Technology, 1997.
- [45] L. Kato. *Perturbation Theory for Linear Operators*. Springer, 1995.
- [46] L. Kaufman and P. Rousseeuw. *Finding Groups in Data: An Introduction to Cluster Analysis*. John Wiley and Sons, 1990.
- [47] T. Kohonen. Comparison of som point densities based on different criteria. *Neural Computation*, (11):2081–2095, 1999.
- [48] T. Kohonen. *Self-Organizing Maps*. Springer, 3rd edition, 2001.
- [49] J. B. Kruskal and M. Wish. *Multidimensional Scaling*. Sage Publications, Beverly Hills, CA, 1978.
- [50] E. Oja and S. Kaski. *Kohonen Maps*. Elsevier, Amsterdam, 1999.
- [51] D. Pelleg and A. Moore. X-means: Extending k-means with efficient estimation of the number of clusters. In *Proc. 17th International Conf. on Machine Learning*, pages 727–734. Morgan Kaufmann, San Francisco, 2000.
- [52] I. Rigoutsos, D. Platt, A. Califano, and D. Silverman. Representing and matching of small flexible molecules in large databases of 3d molecular information. In [62].
- [53] B.D. Ripley. *Pattern Recognition and Neural Networks*. Cambridge University Press, 1996.
- [54] H. Ritter, T. Martinetz, and K. Schulten. *Neural Computation and Self-Organizing Maps*. Addison-Wesley, 1992.
- [55] R. Rojas. *Neural Networks - A Systematic Introduction*. Springer, 1996.
- [56] J. W. Sammon. A nonlinear mapping for data structure analysis. *IEEE Transcations on Computers*, C-18(5):401–409, 1969.
- [57] T. Schlick and H. H. Gan (editors). *Computational Methods for Macromolecules: Challenges and Applications — Proc. of the 3rd Intern. Workshop on Algorithms for Macromolecular Modelling*, New York, 2000. Springer, 2002, In Press.
- [58] Ch. Schütte. *Conformational Dynamics: Modelling, Theory, Algorithm, and Application to Biomolecules*. Habilitation Thesis, Dept. of mathematics und computer science, Free University Berlin, 1998. Available as ZIB-Report SC-99-18 via <http://www.zib.de/bib/pub/pw/>.

- [59] Ch. Schütte, A. Fischer, W. Huisenga, and P. Deufhard. A direct approach to conformational dynamics based on hybrid Monte Carlo. *J. Comput. Phys., Special Issue on Computational Biophysics*, 151:146–168, 1999.
- [60] R. Varga. *Matrix iterative analysis*. Springer, 2nd edition, 2000.
- [61] J. Vesanto. Som-based data visualization methods. *Intelligent Data Analysis*, (3):111–126, 1999.
- [62] J. Wang, B. Shapiro, and D. Shasha. *Pattern Discovery in Biomolecular Data*. Oxford University Press, 1999.
- [63] S. Wu-Pong and Y. Rojanasakul. *Biopharmaceutical Drug Design and Development*. Humana Press, 1999.
- [64] T. Zhang, R. Ramakrishnan, and M. Livny. BIRCH: an efficient data clustering method for very large databases. In *Proc. of ACM SIGMOD Int. Conf. on Management of Data*, pages 103–114. ACM Press, 1996.

