Neural network algorithms and related models

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The NETLAB toolbox for MATLAB™ (Nabney 2002) is well established for teaching and research in the fields of pattern recognition and data analysis. To provide students and practitioners those tools also outside the Matlab framework, we have implemented an R package covering NETLAB's complete functionality. Although some tools for neural networks are already available in existing R packages, this new implementation enables consistent usage and should make it easier for existing NETLAB users to switch to R. The code is written 100% in pure R, thus making it easy to adapt models to one's own needs and ensuring platform independence. The original toolbox does not use object oriented methods, while in the R implementation S3 mechanisms were facilitated.

All tools and methods provided are theoretically well founded, with in-depth discussion in Bishop (1995). Complementary information for the toolbox - and thus implicitly also for the R counterpart - is given in Nabney (2002), where also more recent developments that are part of the toolbox are described.

The toolbox covers general purpose optimization routines, for example scaled conjugate gradient and quasi Newton methods. For density estimation, Gaussian mixture models (GMMs), Probabilistic Principle Component Analysis (PPCA), Generative Topographic Mapping (GTM) are available. The most commonly used neural network models are implemented, i.e. the multi-layer perceptron (MLP) and the radial basis function (RBF) network. Simpler models, such as K-means clustering, K-nearest-neighbor classifiers, and single layer network, are included to act as benchmarks. The Mixture Density Network (MDN) provides a general purpose model for conditional density estimation and to model multi-branched functions. For visualization, besides PCA, PPCA, SOM and the more principled alternative GTM, Neuroscale is included, which is a non-linear topographic projection that uses an underlying RBF network. The Bayesian approach to neural networks is addressed in a twofold way: the evidence procedure allows adding error bars to predictions and automatic determination of variable importance; Metropolis-Hastings and hybrid Monte Carlo methods are provided for sampling.

References

Bishop, C. M. (1996). Neural Networks for Pattern Recognition, Oxford University Press.
Nabney, I. T. (2002). Netlab: Algorithms for Pattern Recognition. Berlin, Springer.