

Inferring Hierarchical Clustering Structures by Deterministic Annealing

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Abstract

The unsupervised detection of hierarchical structures is a major topic in unsupervised learning and one of the key questions in data analysis and representation. We propose a novel algorithm for the problem of learning decision trees for data clustering and related problems. In contrast to many other methods based on successive tree growing and pruning, we propose an objective function for tree evaluation and we derive a non-greedy technique for tree growing. Applying the principles of maximum entropy and minimum cross entropy, a deterministic annealing algorithm is derived in a meanfield approximation. This technique allows us to canonically superimpose tree structures and to fit parameters to averaged or ‘fuzzified’ trees.

Introduction

Clustering is one of the fundamental problems in exploratory data analysis. Data clustering problems occur in pattern recognition, statistics, unsupervised learning, neural networks, data mining, machine learning and many other scientific fields. The wide range of applications is explained by the fact that clustering procedures are important tools for an automated or interactive detection of structure in data sets. Especially for large data sets grouping data and extracting typical prototypes is important for a compact representation and is a precondition for further symbolic processing stages. In the context of data clustering the detection of hierarchical structures is an essential goal of data analysis. In this paper we consider binary trees with stochastic transition nodes, (Breiman *et al.* 1984) applied to vector-valued data.

We will formulate data clustering as a stochastic optimization problem to be addressed in the *maximum entropy framework*. Maximum entropy methods have been introduced as a stochastic optimization method, called *simulated annealing* in a seminal paper of Kirkpatrick *et al.* (Kirkpatrick, Gelatt, &

Vecchi 1983). To overcome the computational burden of Monte Carlo sampling, efficient *deterministic annealing* variants have been derived for a number of important optimization problems (Yuille 1990; Kosowsky & Yuille 1994; Buhmann & Hofmann 1994; Gold & Rangarajan 1996), including unconstrained clustering and vector quantization. (Rose, Gurewitz, & Fox 1990; Buhmann & Kühnel 1993). Maximum entropy methods have recently been successfully applied to the case of tree-structured vector quantization in (Miller & Rose 1994; 1996). Similar methods have also been used in the context of regression (Jordan & Jacobs 1994) and for unsupervised learning problems (Dayan, Hinton, & Zemel 1995). The key idea in simulated and deterministic annealing is to reformulate a given combinatorial optimization problem as a stochastic optimization problem. A temperature parameter T is introduced to control the amplitude of the induced noise. In the zero temperature limit, $T \rightarrow 0$, the combinatorial problem is recovered, while for high temperatures the objective function is smoothed. Tracking solutions from high temperatures thus helps us to avoid unfavorable local minima.

The major novelty of our approach is an *explicit* treatment of the topology of binary trees in the maximum entropy framework, which results in a systematic and well-founded ‘fuzzification’ of binary tree topologies. At a finite computational temperature different trees are superimposed resulting in an average tree structure. An average tree is not a single tree but a tree mixture. The proposed algorithm optimizes the tree topology jointly with all other relevant parameters, e.g. data assignments to clusters and decision node parameters.

Unconstrained Data Clustering

We restrict our attention to the case of real-valued data vectors $\mathcal{X} = \{\mathbf{x}_i \in \mathbb{R}^d : 1 \leq i \leq N\}$, and a corresponding set of prototypes $\mathcal{Y} = \{\mathbf{y}_\nu \in \mathbb{R}^d : 1 \leq \nu \leq K\}$, $K \ll N$, \mathbf{y}_ν representing a group G_ν . To describe the mapping of data vectors to prototypes we introduce an indicator function representation by Boolean assignment matrices $M \in \{0, 1\}^{N \times K}$ obeying the con-

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Deterministic Annealing For Clustering Compression

Kosar, Tevfik



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Intelligent Information and Database Systems Manh Thanh Le, Jerzy Swiatek, Ngoc Thanh

Nguyen, 2010-03-05 The 2010 Asian Conference on Intelligent Information and Database Systems ACIIDS was the second event of the series of international scientific conferences for research and applications in the field of intelligent information and database systems The aim of ACIIDS 2010 was to provide an international forum for scientific research in the technologies and applications of intelligent information database systems and their applications ACIIDS 2010 was co organized by Hue University Vietnam and Wroclaw University of Technology Poland and took place in Hue city Vietnam during March 24 26 2010 We received almost 330 papers from 35 countries Each paper was peer reviewed by at least two members of the International Program Committee and International Reviewer Board Only 96 best papers were selected for oral presentation and publication in the two volumes of the ACIIDS 2010 proceedings The papers included in the proceedings cover the following topics artificial social systems case studies and reports on deployments collaborative learning collaborative systems and applications data warehousing and data mining database management technologies database models and query languages database security and integrity business e commerce e finance e learning systems information modeling and requirements engineering information retrieval systems intelligent agents and multi agent systems intelligent

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Regularized Radial Basis Function Networks Paul V. Yee, Simon Haykin, 2001-04-16 Simon Haykin is a well known author of books on neural networks An authoritative book dealing with cutting edge technology This book has no competition *Proceedings*, 2003 *Annual Meeting of the North American Fuzzy Information Processing Society--NAFIPS*. North American Fuzzy Information Processing Society. Annual Meeting, 2000 *Medical Imaging*, 2000 **Neural Networks and Learning Machines** Simon S. Haykin, 2009 For graduate level neural network courses offered in the departments of Computer Engineering Electrical Engineering and Computer Science Renowned for its thoroughness and readability this well organized and completely up to date text remains the most comprehensive treatment of neural networks from an engineering perspective Matlab codes used for the computer experiments in the text are available for download at <http://www.pearsonhighered.com/haykin> Refocused revised and renamed to reflect the duality of neural networks and learning machines this edition recognizes that the subject matter is richer when these topics are studied together Ideas drawn from neural networks and machine learning are hybridized to perform improved learning tasks beyond the capability of either independently *Oceans '04 MTS/IEEE*, 2004 **Computer Vision - ACCV ...**, 1998 **Materials of the Tutorial Lectures in Systems Sciences**, 2001 *Recurrent Neural Networks for Prediction* Danilo P. Mandic, Jonathon A. Chambers, 2001 New technologies in engineering physics and biomedicine are demanding increasingly complex methods of digital signal processing By presenting the latest research work the authors demonstrate how real time recurrent neural networks RNNs can be implemented to expand the range of traditional signal processing techniques and to help combat the problem of prediction Within this text neural networks are considered as massively interconnected nonlinear adaptive filters Analyses the relationships between RNNs and various nonlinear models and filters and introduces spatio temporal architectures together with the concepts of modularity and nesting Examines stability and relaxation within RNNs Presents on line learning algorithms for nonlinear adaptive filters and introduces new paradigms which exploit the concepts of a priori and a posteriori errors data reusing adaptation and normalisation Studies convergence and stability of on line learning algorithms based upon optimisation techniques such as contraction mapping

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