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Book of Abstracts

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Committees

Scientific

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List of Abstracts
Wild adaptive trimming for robust estimation and cluster analysis
Andrea Cerioli\textsuperscript{1}, Alessio Farcomeni\textsuperscript{2} and Marco Riani\textsuperscript{1}
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Trimming principles play an important role in robust statistics. However, their use for clustering typically requires some preliminary information about the contamination rate and the number of groups. In this talk we describe a fresh approach to trimming that does not rely on this preliminary knowledge and that proves to be particularly suited for solving problems in robust cluster analysis. Our approach replaces the original $K$-population (robust) estimation problem with $K$ distinct one-population steps, which take advantage of the good breakdown properties of trimmed estimators when the trimming level exceeds the usual bound of 0.5. In this setting we prove that exact affine equivariance is lost on one hand, but on the other hand an arbitrarily high breakdown point can be achieved by “anchoring” the robust estimator. We also support the use of adaptive trimming schemes, in order to infer the contamination rate from the data. A further bonus of our methodology is its ability to provide a reliable choice of the usually unknown number of groups.

References

Constrained maximum likelihood estimation of clusterwise linear regression models with unknown number of components
Roberto Di Mari\textsuperscript{1}, Roberto Rocci\textsuperscript{2}, and Stefano Antonio Gattone\textsuperscript{3}
\textsuperscript{1}Department of Economics and Business, University of Catania, Italy; \textsuperscript{2}Department of Economics and Finance, University of Rome Tor Vergata, Italy; \textsuperscript{3}Department of Philosophical and Social Sciences, Economics and Quantitative Methods, University G. d’Annunzio, Chieti-Pescara, Italy.

We consider an equivariant approach imposing data-driven bounds for the variances to avoid singular and spurious solutions in maximum likelihood (ML) estimation of clusterwise linear regression models. We investigate its use in the choice of the number of components and we propose a computational shortcut, which significantly reduces the computational time needed to tune the bounds on the data. In the simulation study and the two real-data applications, we show that the proposed methods guarantee a reliable assessment of the number of components compared to standard unconstrained methods, together with accurate model parameters estimation and cluster recovery.
Exploring robust Fuzzy clustering on multivariate skew data

Francesca Greselin\textsuperscript{1}, Luis Angel García-Escudero\textsuperscript{2} and Agustin Mayo-Iscar\textsuperscript{2}

\textsuperscript{1}University of Milano-Bicocca; \textsuperscript{2}University of Valladolid

With the increasing availability of multivariate datasets, asymmetric structures in the data ask for more realistic assumptions, with respect to the incredibly useful paradigm given by the Gaussian distribution. Moreover, in performing ML estimation we know that a few outliers in the data can affect the estimation, hence providing unreliable inference. Challenged by such issues, more flexible and solid tools for modeling heterogeneous skew data are needed. Our fuzzy clustering method is based on mixtures of Skew Gaussian components, endowed by the joint usage of impartial trimming and constrained estimation of scatter matrices, in a modified maximum likelihood approach. The algorithm generates a set of membership values, that are used to fuzzy partition the data set and to contribute to the robust estimates of the mixture parameters. The new methodology has been shown to be resistant to different types of contamination, by applying it on artificial data. A brief discussion on the tuning parameters has been developed, also with the help of some heuristic tools for their choice. Finally, synthetic and real dataset are analyzed, to show how intermediate membership values are estimated for observations lying at cluster overlap, while cluster cores are composed by observations that are assigned to a cluster in a crisp way.

References


Keynote Lecture 1

Model Based Clustering through copulas for high dimensional data

Dimitris Karlis
Dept of Statistics, Athens University of Economics and Business

In a recent paper Kosmidis and Karlis (2016) proposed model based clustering based on multivariate distributions defined through copulas. This approach offers a number of advantages over existing methods mainly due to the flexibility to define appropriate models in certain different circumstances. Some of the existing models can be seen as a special case of this construction. In this talk we exploit the ideas of extending the approach for higher dimensions and different types of data. The central idea is to use a Gaussian copula and implement the correlation matrix of the Gaussian copula through certain parsimonious representations giving rise to models of different complexity. To some extent this is based on existing representations in the MBC literature suitably adapted for the case of Gaussian copulas. We use two different approaches, the first makes use of factor analyzers based on the factor decomposition of the correlation matrix and the second is based on Choleski type decompositions. Application with real and simulated data will be also described.

This is joint work with Ioannis Kosmidis, University of Warwick and Fotini Panagou (AUEB)

References
Heterogeneity in large-scale data: invariance, causality and novel robustness
Peter Bühlmann
ETH Zürich

Heterogeneity in potentially large-scale data can be beneficially exploited for causal inference and novel robustness. The key idea relies on invariance and stability across different heterogeneous regimes or sub-populations (Peters et al., 2016). What we term as “anchor regression” (Rothenhäusler et al., 2018) opens up new insights and connections between causality and protection (robustness) against worst case perturbations in prediction problems. We will discuss the methodology and some applications.

References
Talk Session 2: Supervised and unsupervised classification

Unobserved Classes and Extra Variables in High-dimensional Discriminant Analysis

Michael Fop\(^1\), Pierre-Alexandre Mattei\(^2\), Thomas Brendan Murphy\(^1\) and Charles Bouveyron\(^3\)

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\(^2\)Department of Computer Science, IT University of Copenhagen, Denmark.
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In supervised classification problems, the test set may contain data points belonging to classes not observed in the learning phase. Moreover, the same units in the test data may be measured on a set of additional variables, recorded at a subsequent stage with respect to when the learning sample was collected. In this situation, the classifier built in the learning phase needs to adapt to handle potential unknown classes and the extra dimensions. We introduce a model-based discriminant approach that can detect unobserved classes and adapt to the increasing dimensionality. The method is embedded in a more general framework for adaptive variable selection and classification, developed in application to high-dimensional spectrometry data.

References


Maximizing the Usefulness of Statistical Classifiers for Two Populations

Daniel. R. Jeske

Department of Statistics University of California, Riverside

The usefulness of two-class statistical classifiers is limited when one or both of the conditional misclassification rates is unacceptably high. Incorporating a neutral zone region into the classifier provides a mechanism to refer ambiguous cases to follow-up where additional information might be obtained to clarify the classification decision. Through the use of the neutral zone region, the conditional misclassification rates can be controlled and the classifier becomes useful. An application to prostate cancer will be used to illustrate how neutral zone regions can extract utility from a potentially disappointing classifier that might otherwise be abandoned.
A multivariate characterisation of some popular cluster analysis methods

Christian Hennig
University College London

I have argued (Hennig 2015) that there are various different aims of cluster analysis, for which different clusterings may be optimal even on the same dataset. I present a collection of indexes that measure different aspects of interest in clustering (such as within-cluster homogeneity, between-cluster separation, representation of the underlying distance structure by the clustering, correspondence to high density regions, good representation of clusters by centroids etc.). There are a number of cluster validity indexes proposed in the literature (Valkidi et al. 2015). Most if not all of them attempt to give a one-dimensional assessment of the overall quality of a clustering, which does not provide insight into how the trade-off between the specific characteristics that could be potentially desirable plays out.

The proposed collection of indexes is used to give a multivariate characterisation of the behaviour of some popular clustering methods including Gaussian and skew-t mixtures based on 20 real datasets. The focus here is not on “recovering the true clusters” but rather on elaborating how the methods differ in a data analytic sense. This can help users to choose an appropriate method for a specific clustering task.

References


Model-based double hierarchical parsimonious clustering

Carlo Cavicchia, Maurizio Vichi and Giorgia Zaccaria
Department of Statistical Sciences, Sapienza University of Rome

Starting from a dissimilarity data set between \( n \) statistical units, the hierarchical classifications produced by clustering algorithms usually comprise partitions into \( K \) classes for all values of \( K \) between 1 and \( n \), being represented by dendrograms that contain \( (n - 1) \) internal nodes. Several authors noted that the complete sets of partitions and classes do not appear to be used by investigators, and can hinder interpretation. One approach for resolving this difficulty has involved the construction of parsimonious trees, which contain a limited number of internal nodes; some information is discarded in this process, but the main features of the data can be represented more clearly.

In this papers starting from the data matrix \( X \) of size \( (n \times J) \), corresponding to \( n \) statistical units and \( J \) quantitative variables, we propose a model for double hierarchical
parsimonious clustering. This is a new methodology for simultaneous hierarchical par-
simonious clustering of the units – aggregated around centroids – and of the variables
– aggregated around factors. The model is estimated by using the LS method and an
efficient coordinate descent algorithm is given. The goodness of fit of the double hierar-
chical parsimonious trees can be computed to assess the quality of the two hierarchical
partitions.
Matrix sketching is a data compression technique that has been recently developed in the computer science community. An input matrix $A$ is efficiently approximated with a smaller matrix $B$, so that $B$ preserves most of the properties of $A$ up to some guaranteed approximation ratio. In so doing numerical operations on big data sets become faster. Sketching algorithms generally use random projections to compress the original dataset and this stochastic generation process makes them amenable to statistical analysis. The statistical properties of sketched regression algorithms have been widely studied in Woodruff (2014) and in Ahfock, Astle and Richardson (2017). In this work we study the performances of sketching algorithms in the supervised classification context, both in terms of misclassification rate and of boundary approximation, as the degree of sketching increases. We also address, through sketching, the issue of unbalanced classes, which hampers most of the common classification methods.

References


Data Units as (Co-)Clustering Model Enlargement

Christophe Biernacki$^1$ and Alexandre Lourme$^2$

$^1$Inria & University of Lille & CNRS (France); $^2$University of Bordeaux (France)

Model-Based-Clustering methods [McLachlan G. and Peel D., 2000] aim at splitting unlabelled data into groups. Model-Based-Co-Clustering methods [Govaert G. and Nadif M., 2013] yields simultaneously groups of data and variables. In both cases, changing the data units may affect the estimated partition(s). But, combining several data units with scale dependent models enables to enlarge the set of competing (Co-)Clustering models since any unit change can be seen as a particular model definition [Biernacki C. and Lourme A., 2018]. Consequently, it raises the following open question: how to select a model when the number of (co-)clustering models explodes?
Robust Adaptive Eigenvalue Decomposition Discriminant Analysis: supervised learning in presence of outliers, label noise and unobserved classes

Andrea Cappozzo, Francesca Greselin\textsuperscript{1} and Thomas Brendan Murphy\textsuperscript{2}

\textsuperscript{1}Department of Statistics and Quantitative Methods, University of Milano-Bicocca, Via Bicocca degli Arcimboldi, 8 20126, Milano, Italy; \textsuperscript{2}School Of Mathematics & Statistics and Insight Research Centre, University College Dublin, Belfield, Dublin 4, Ireland

In a standard classification framework a set of trustworthy learning data are employed to build a decision rule, with the final aim of classifying unlabelled units belonging to the test set. Therefore, unreliable learning observations can strongly undermine the classifier performance, especially if the training size is small. Additionally, the test set may include classes not previously encountered in the learning phase. The present work introduces a robust adaptive model-based discriminant analysis (RAEDDA) capable of handling situations in which one or more of the following problems occur: outliers both in the training and in the test set, label noise in the training set and extra classes in the test not observed in the learning phase. An inductive EM-based procedure is employed for robust parameter estimation, making use of impartial trimming for identifying possible outliers and data with uncertain labels. Experiments on real data, artificially adulterated, are provided to underline the benefits of the proposed method.

References


A thinned-trimmed CEM algorithm for robust clustering around regression lines

Andrea Cerioli¹, Luis Angel García-escudero², Agustín Mayo-Iscar², Domenico Perrotta³ and Francesca Torti³

¹University of Parma, Italy; ²University of Valladolid, Spain; ³European Commission, Joint Research Centre

Robust techniques typically allow for a contamination rate of at most 50% and robust clustering is no exception to this rule (García-Escudero et al., 2008, and Ritter, 2014). The motivation lies in the (sometimes implicit) assumption that the “good” population should correspond to the majority of data. However, there may be instances where the relevant structure only concerns a possibly very small portion of the data, while the remaining observations do not contribute any meaningful information. In these situations robust methodologies clearly fail to unveil the relevant data structure even if they are tuned to ensure the supposedly maximum value of their breakdown point, i.e. 50% (see Cerioli et al., 2017, and the related discussions).

One way to attack the problem in a multivariate framework is to adopt robust estimation procedures based on trimming with arbitrarily high breakdown (Cerioli et al., 2018). Instead, in this work we follow a different approach which proves to be preferable when the data have a cluster-wise regression structure and the largest portion of contaminated observations can be interpreted as concentrated noise. This is precisely the context of our motivating application field: fraud detection in international trade data, where traded values and quantities are recorded. These variables are linked by a functional linear relationship and anomalous transactions often stand out as outliers from the regression clusters defined by genuine trading behaviour. Noise corresponds to the presence of a possibly very dense “small trade area”, which is often concentrated close to the origin of the coordinate axes but which can also span along one or more regression lines.

Our approach combines the usual levels of trimming (i.e., up to 50%) with thinning, a denoising procedure based on density estimation. Thinning is able to remove a very high fraction of the observations that contribute to noise, thus allowing robust cluster-wise regression methods, such as TCLUST-REG (García-Escudero et al., 2010), to work on data with “standard” (i.e., lower than 50%) contamination rates. For this purpose, we develop a modified version of the Classification EM (CEM) algorithm of García-Escudero et al. (2010), where thinning weights are computed and applied before each maximization step. An additional problem that we address is the comparison of alternative solutions arising from different random starting points of the CEM algorithm, which may be based on a different number of observations retained after thinning.

We show the potential of our method through simulated data and through applications to real anti-fraud scenarios in international trade. We also
• compare the performance of our proposal with the tandem approach developed by Cerioli and Perrotta (2014), in which denoising is performed before robust clusterwise regression and thus outside the robust CEM algorithm;

• investigate its performance under alternative attitudes towards robustness to high-leverage points, a critical issue in robust regression methods (Huber and Ronchetti, 2009 and García-Escudero et al., 2010).

References


Critical Discussions of Selected Robust Clustering Procedures and Their Applications in Economics

Przemysław Jaśko, Daniel Kosiorowski and Ewa Szlachtowska
Cracow University of Economics

In this paper we critically discusses advantages and disadvantages of the selected robust clustering methods known from literature. We among others study TCLUST algorithm proposed by García-Escudero et al. (2008) and compare it with selected model-based procedures appealing to Bayesian Clustering and Mixture Clustering.

References


Robust clustering in the presence of skewed data groups

Yana Melnykov¹, Volodymyr Melnykov¹ and Xuwen Zhu²
¹The University of Alabama; ²University of Louisville

The performance of model-based clustering depends on the presence of noise or outlying observations severely. Such observations might ruin the systematic structure of the groups leading to incorrect or misleading results. Among the most famous approaches taking into account the potential presence of outliers, there are finite mixture models with t, skew-t, or contaminated normal components. We propose an alternative to the traditional approaches that is capable of modeling skewed heavy-tailed data groups effectively. A novel approach to identifying noise observations is introduced. The procedure is illustrated on simulated and real-life data sets with good results.

References


Finite mixtures present a powerful tool for modeling complex heterogeneous data. One of their most important applications is model-based clustering. It assumes that each data group can be reasonably described by one of mixture model components. This establishes a one-to-one relationship between mixture components and clusters. In some cases, however, this relationship can be broken due to the presence of observations from the same class recorded in different ways. This effect can occur because of recording inconsistencies due to the use of different scales, operator errors, or simply various recording styles. The idea presented in this paper aims to alleviate this issue through modifications incorporated into mixture models. While the proposed methodology is applicable to a broad class of mixture models, in this paper it is illustrated on Gaussian mixtures. Several simulation studies and an application to a real-life data set are considered, yielding promising results.

References

Alimoglu, F. and Alpaydin, E. (1996). Methods of Combining Multiple Classifiers Based on Different Representations for Pen-based Handwriting Recognition. *Proceedings of the Fifth Turkish Artificial Intelligence and Artificial Neural Networks Symposium (TAINN 96).*


A model-based approach for analyzing and modeling ordinal data is presented. This model relies on the latent block model embedding a probability distribution specific to ordinal data (the so-called BOS or Binary Ordinal Search distribution). Classification, clustering and co-clustering algorithms are derived from the proposed model. Model inference relies on a Stochastic EM algorithm coupled with a Gibbs sampler, and the ICL-BIC criterion is used for selecting the number of clusters in clustering, the number of co-clusters in co-clustering, and the level of parsimony in classification. The main advantages of these ordinal dedicated models are their parsimony, the interpretability of the parameters (mode, precision) and the possibility to take into account missing data. All these algorithms are available in the ordinalClust package for R. The usefulness of the proposed algorithms are illustrated by analyzing a psychological survey on women affected by a breast tumor.

References


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**Keynote Lecture 3**

**Classification, clustering and co-clustering for ordinal data**

Julien Jacques¹, Margot Selosse¹ and Christophe Biernacki²

¹Université de Lyon, Lyon 2 ERIC EA3083; ²Université de Lille & Inria

6 Sept.
14.00–14.55
KL 3
A robust clustering method for probabilities in Wasserstein space is introduced. This new “trimmed $k$-barycenters” approach relies on recent results on barycenters in Wasserstein space that allow intensive computation, as required by clustering algorithms to be feasible. The possibility of trimming the most discrepant distributions results in a gain in stability and robustness, highly convenient in this setting. As a remarkable application, we consider a parallelized clustering setup in which each of $m$ units processes a portion of the data, producing a clustering report, encoded as $k$ probabilities. We prove that the trimmed $k$-barycenter of the $m \times k$ reports produces a consistent aggregation which we consider the result of a “wide consensus”. We also prove that a weighted version of trimmed $k$-means algorithms based on $k$-barycenters in the space of Wasserstein keeps the descending character of the concentration step, guaranteeing convergence to local minima. We illustrate the methodology with simulated and real data examples. These include clustering populations by age distributions and analysis of cytometric data.

References

Talk Session 3: Model-based clustering of complex data

Clustering for multidimensional networks via infinite mixture models

Silvia D’Angelo¹, Michael Fop² and Marco Alfò¹
¹Sapienza, University of Rome; ²University College Dublin

Network data are relational data where the presence of a given relation between any two units is expressed by an edge connecting them. When multiple relations are observed among the same group of nodes, a collection of networks is available. This collection takes the name of multidimensional network, or multiplex. Latent space models for network data describe the observed structure in the multidimensional network by means of an unobserved latent space, in which the main assumption is that units close in the latent space are more likely to be connected. In many data applications, units have the propensity to aggregate into communities. This characteristic has been modelled in the context of single and dynamic networks. We propose a clustering framework for multidimensional networks based on infinite mixtures of Gaussian distributions. The model is estimated within a hierarchical Bayesian framework. Moreover, a single latent space is employed to describe the multiplex, both for representation and computational efficiency purposes.

References


On modelling multivariate high-dimensional time series: a factorial hidden Markov model

Antonello Maruotti¹, Antonio Punzo² and Jan Bulla³
¹Libera UniversitÃ­ Maria Ss. Assunta; ²UniversitÃ­ di Catania; ³University of Bergen

We introduce multivariate models for the analysis of stock market returns. Our models are developed within the hidden Markov framework to describe the temporal evolution of the returns, whereas the marginal distribution of the returns is described by a mixture of multivariate contaminated-normal distributions. The contaminated-normal distribution represents an elliptical generalization of the Gaussian distribution allowing for automatic outlier/extreme value detection in the same natural way as observations are typically assigned to the latent states in the hidden Markov model (HMM) context (Punzo and Maruotti, 2016). The proposed HMMs account for three major dependency structures in multivariate time series data, including the correlation among multiple series,
temporal dependence, and heterogeneity. Following the HMMs literature, we assume that the hidden structure underlying the observed data is a first-order Markov chain, and that returns can be modeled as a multivariate process conditioning on the sequence of hidden states. The challenge of modeling multiple stock series and their interactions is fairly common to all analyses of high dimensional data with many variable of interest. Dimensionality-related aspects present a challenge because these series could potentially be highly correlated. Therefore, estimation and interpretation of model parameters may become nontrivial. In order to examine the interrelationships between series to perform dimensionality reduction in the variable space simultaneously (allowing for an easy interpretation of model parameters), we propose the use of a latent factor model (Maruotti et al., 2017). Accordingly, we define a general class of parsimonious HMMs by imposing a factor decomposition on state-specific covariance matrices. The loadings and noise terms of the covariance matrix may be constrained to be equal or unequal across latent states. In addition, the noise term may be subject to further restrictions, resulting in a set of eight parsimonious covariance structures (McNicholas and Murphy, 2008). This model structure allows for the accounting of dependence between series, and provides a clear interpretation of the (latent) association structure between series. Even in this relatively general framework, the parameters of the proposed parsimonious HMMs can be estimated using the method of maximum likelihood based on the Alternating Expectation Conditional Maximization (AECM) algorithm.

References


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**Clustering of spatially dependent functional data**

Vincent Vandewalle¹, Cristian Preda² and Sophie Dabo³

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Two approaches for clustering spatial functional data are presented. The first one is the model-based clustering that uses the concept of density for functional random variables and logistic weights on the prior cluster probabilities depending on spatial coordinates. The second one is the hierarchical clustering based on univariate statistics for functional data such as the functional mode or the functional mean, and includes spatial weights in the distances computation. These two approaches take into account the spatial features of the functional data: two observations that are spatially close share a common distribution of the associated random variables. The two methodologies are illustrated by an application to air quality data.
References


Talk Session 4: Developments in modeling high-dimensional data

High-dimensional clustering with Random Projections
Laura Anderlucci, Francesca Fortunato and Angela Montanari
University of Bologna

Random projections (RPs) have shown to provide promising results for high-dimensional classification. In this work, we address the issue of high-dimensional clustering by exploiting the general idea of RP ensemble to perform unsupervised classification. Specifically, we generate a set of low dimensional independent random projections and we perform a model-based clustering on each of them. The top $B_1$ projections, i.e. the ones showing the best grouping structure according to different cluster quality measures, are then selected. The final partition is obtained by aggregating, via consensus, the chosen classifiers. The performances of the method are assessed on a set of both real and simulated data.

References

Robust patients sub-typing with noisy high-dimensional gene expression data
Pietro Coretto$^1$, Angela Serra$^2$ and Roberto Tagliaferri$^1$

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One of the most important research areas in personalised medicine is the discovery of disease sub-types with relevance in clinical applications. This is usually accomplished by exploring gene expression data with unsupervised clustering methodologies. However, microarray data sampling is terribly noisy, and this undermines the possibility to reach scientific consensus on the empirical evidence. This is recognized as a crucial issue, and the research concentrated on the improvement of sampling, and data acquisition techniques. However, even modern microarrays still remain noisy. In this work we propose a new methodology under the commitment to be robust to noise in every step. The proposed
method first computes a robust and sparse correlation matrix (called RSC) of the genes, then decomposes it and projects the patient data onto the first $m$ spectral components. After that, a robust and adaptive to noise clustering algorithm (called OTRIMLE) is applied. The algorithm is set up to optimise the separation between survival curves estimated cluster-wise. The method is able to identify clusters that have different omics signatures, and statistically significant differences in survival times. The proposed method obtains a competitive performance in terms of survival separability, even if it uses a single gene expression view compared to the multi-view approach of the state-of-the-art SNF method. Finally, the method is able to find meaningful and interesting biological pathways within groups.

References


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Infinite Mixtures of Infinite Factor Analysers

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Factor-analytic Gaussian mixture models are often employed as a model-based approach to clustering high-dimensional data. Typically, the numbers of clusters and latent factors must be specified in advance of model fitting, and remain fixed. The pair which optimises some model selection criterion is then chosen. For computational reasons, models in which the number of latent factors is common across clusters are generally considered.

Here the infinite mixture of infinite factor analysers (IMIFA) model is introduced. IMIFA employs a Poisson-Dirichlet process prior to facilitate automatic inference of the number of clusters using the stick-breaking construction and a slice sampler. Furthermore, IMIFA employs shrinkage priors to allow cluster specific numbers of factors, automatically inferred via an adaptive Gibbs sampler. IMIFA is presented as the flagship of a family of factor-analytic mixture models, providing flexible approaches to clustering high-dimensional data.
Applications to the benchmark olive oil data set and a manifold learning handwritten digit example illustrate the IMIFA model and its advantageous features: IMIFA obviates the need for model selection criteria, reduces model search and the associated computational burden, improves clustering performance by allowing cluster-specific numbers of factors, and quantifies uncertainty in the numbers of clusters and cluster-specific factors.

References


Lightning Talk Session 2

Generalized Additive Cluster-Weighted Model

Stefano Barberis\textsuperscript{1}, Salvatore Ingrassia\textsuperscript{2} and Giorgio Vittadini\textsuperscript{1}

\textsuperscript{1}University of Milano Bicocca; \textsuperscript{2}University of Catania

An extension of mixture models with random covariates related to the Cluster Weighted Model (Ingrassia et al., 2012) is presented for model-based clustering applications. The Generalized Additive Cluster Weighted Model (GAM-CWM) is a very flexible model, able to capture complex relations between a response variable and a set of covariates in each mixture component. The main difference between models related to the CWM and other mixture models is that in CWM the joint probability $p(x, y)$ of a response variable $y$ and a set of explanatory variables $x$ is modelled in each mixture component rather than the conditional $p(y|x)$. Different extensions of the basic CWM have been proposed including the student-t distribution (Ingrassia et al., 2012), generalized linear mixed CWM (Ingrassia et al., 2015) and the polynomial gaussian CWM (Punzo, 2014).

The theory of Generalized Additive Model (Hastie et al., 1986) extends the generalized linear model precisely with the aim of making it more flexible introducing a sum of smooth functions of covariates in the linear predictor. In the same way the GAM-CWM extends the generalized linear CWM and the polynomial CWM defining a new powerful and very general class of models where the principles of CWM model and the GAM model are combined together.

Maximum likelihood estimates are provided via EM algorithm and model selection is carried out using Bayesian Information Criterion (BIC) and Integrated Completed Likelihood (ICL). With simulated and real data are investigated performances, limits and benefits comparing this model with other mixture models related to it.

References


In the framework of density-based clustering, regardless of the specific paradigm chosen, the first step requires to obtain an estimate of the density assumed to describe the data generating mechanism. In the parametric paradigm the estimation task is carried out using mixture models with a clear predominant position taken by Gaussian components. Operationally several models, usually having different number of components and possibly different parametrizations, are estimated and the single best one among them is chosen according to an information criterion. The final partition of the data points is then obtained exploiting the one-to-one correspondence between the groups and the components of the single chosen model. Nevertheless throwing away all the fitted models except for the best one could be sub-optimal since useful information could be lost in the process, especially if the values of the information criterion for the discarded models are close to the one of the selected model. Furthermore, from an inferential point of view, not taking into account the selection step could lead to anti-conservative statements since a source of uncertainty is disregarded. A viable solution to workaround this issue consists in appropriately weight a subset of the top estimated models, as in Bayesian Model Averaging approaches proposed by Wei and McNicholas (2015) and Russell et al (2015). In this work, taking our step from Smyth and Wolpert (1999), we adapt the ideas on which stacking is based on in an unsupervised framework. We consider a density estimator being a convex linear combination of a suitably chosen subset of the fitted models where the weights of the combination are estimated via maximum likelihood. In order to avoid weighting excessively highly parametrized models, possibly prone to overfitting the data, we follow a penalized likelihood approach and examine different penalizations. Since by averaging over different models the correspondence between groups and mixture components is lost, we discuss possible solutions, coherent with the density-based framework, to obtain partitions starting from the estimated density.

References


Subspace Clustering for the Finite Mixture of Generalized Hyperbolic Distributions

Nam-Hwui Kim, Ryan P. Browne
University of Waterloo

The finite mixture of Generalized Hyperbolic distributions is a flexible model for clustering, but its large number of parameters for estimation, especially in high dimensions, can make it computationally expensive to work with. In light of this issue, we provide an extension of the subspace clustering technique developed for finite Gaussian mixtures to that of Generalized Hyperbolic distribution. The methodology will be demonstrated with numerical experiments.

References

Learning the number of components and data clusters in Bayesian finite mixture models

Gertraud Malsiner-Walli¹, Sylvia Frühwirth-Schnatter¹ and Bettina Grün²
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Bayesian cluster analysis aims at inferring the number of data clusters present in a data set using either finite or infinite mixture models. In Bayesian finite mixture models usually a one-to-one relationship between components and data clusters is assumed. The number of components can be determined by comparing the marginal likelihoods of the potential models (Frühwirth-Schnatter, 2006) or by approximating the posterior of the number of components using different methods, e.g., reversible jump Markov chain Monte Carlo (Richardson and Green, 1997), Markov birth-and-death process sampling (Stephens, 2000) or the Jain-Neal split-merge sampler (Miller and Harrison, 2018).

We propose to explicitly distinguish between the number of data clusters and components and purposely allow for more components than data clusters. We extend the standard approach by including priors on the number of components and on the parameters of the Dirichlet distribution for the mixture weights. This allows us to approximate the posteriors of the number of components as well as data clusters using Gibbs sampling techniques. The performance of the proposed sampling technique is compared to previously proposed approaches. The additional flexibility gained by suitably selecting the parameters of the hyperpriors is highlighted and guidance for their choice provided.

References


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**Constraining kernel estimators in semiparametric copula-based mixture models**

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We present a novel algorithm for performing inference and/or clustering in semiparametric copula-based mixture models. The algorithm replaces the standard kernel density estimator by a weighted version that permits to take into account the constraints put on the underlying marginal densities. Lower misclassification error rates and better estimates are obtained on simulations. The pointwise consistency of the weighted kernel density estimator is established under an assumption on the rate of convergence of the sample maximum.

**References**


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**Gaussian Parsimonious Clustering Models with Covariates**

Keefe Murphy and T. Brendan Murphy

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In model-based clustering methods using finite Gaussian mixture models, clustering is typically implemented on response variables only and reference is not made to associated covariates until the structure of the clustering is investigated in light of information present in the covariates. It is desirable to have covariates incorporated into the clustering process and not only into the interpretation of the clustering structure and model parameters, in order to exploit clustering capabilities and provide richer insight into the type of observation which characterises each cluster.

The mixture of experts model provides one such framework: it extends the mixture model to accommodate the presence of covariates by modelling the parameters of the
mixture model as functions of fixed covariates. However, for Gaussian responses, the flexibility afforded by parsimonious parameterisations of the component covariance matrices have to date been lacking in the mixture of experts context.

We consider model-based clustering methods with constrained covariance structures that account for external information available in the presence of covariates by proposing the general MoEClust family of models; these models allow the distribution of the latent cluster membership variable and/or the distribution of the response variable to depend on covariates. This family of models address the aim of including covariates in Gaussian parsimonious clustering models or, equivalently, the aim of incorporating parsimonious covariance structures into the framework of Gaussian mixtures of experts. The MoEClust models demonstrate significant improvement from both perspectives in applications to univariate and multivariate data sets. A software implementation for the full suite of MoEClust models is also introduced.

References


Model-based Clustering with R-vine copulas

Marta Nai Ruscone¹ and Thomas Brendan Murphy²

¹LIUC Università Cattaneo; ²University College Dublin

Finite mixtures are applied to perform model-based clustering of multivariate data. Existing models are not flexible enough for modeling the dependence of multivariate data since they rely on potentially undesirable correlation restrictions to be computationally tractable. We discuss a model-based clustering method via R-vine copula to understand the complex and hidden dependence patterns in correlated multivariate data. One of the advantages of this approach is that it accounts for the tail asymmetry of the data by using blocks of asymmetric bivariate copulas. We use real datasets to illustrate the proposed procedure.

References


Keynote Lecture 5

Deep Gaussian Mixture Models

Cinzia Viroli\(^1\) and Geoffrey J. McLachlan\(^2\)

\(^1\)University of Bologna; \(^2\)University of Queensland

In the recent years, there has been an increasing interest on deep learning for classification and clustering tasks. Deep learning is a hierarchical inference method formed by subsequent multiple layers of learning able to more efficiently describe complex relationships. In this work, Deep Gaussian Mixture Models are introduced and discussed. A Deep Gaussian Mixture model is a network of multiple layers of latent variables, where, at each layer, the variables follow a mixture of Gaussian distributions. Thus, the deep mixture model consists of a set of nested mixtures of linear models, which globally provides a nonlinear model able to describe the data in a very flexible way. In order to avoid overparameterized solutions, dimension reduction by factorial models can be applied at each layer of the architecture thus resulting in deep mixtures of factor analysers.

References


It is easy to focus on methods and accuracy when designing classification and clustering algorithms, but as soon as we apply them to people, there is a range of other considerations that we need to keep in mind.

The combination of machine learning and big data has enabled us to create a new generation of artificial intelligence (AI), and now we interact with its applications daily. The strategic position occupied by AI agents within our global information infrastructure means that they are in the position to observe a large portion of our activities, learning from them, but also creates a new type of risk, including the possibility of surveillance and manipulation of user behaviour, unintended bias, lack of transparency, etc.

Based on the details of how AI has emerged from the combination of machine learning and this unified data infrastructure, we can understand recent reports that have raised concerns, from fake news to psychometric election targeting, from criminal justice applications to dynamic pricing in insurance based on social media content. By reviewing the way this technology works, we can put these reports in a context, and look ahead at forthcoming challenges. Importantly, we can plan future regulation of this strategic sector.
Talk Session 5: Issues in hidden Markov models

Consistent estimation of the filtering and smoothing probabilities in non parametric hidden Markov models

Yohann De Castro, Sylvain Le Corff and Elisabeth Gassiat
Université Paris-Sud

We consider the filtering and smoothing recursions in nonparametric finite state space hidden Markov models (HMMs) when the parameters of the model are unknown and replaced by estimators. We provide an explicit and time uniform control of the filtering and smoothing errors in total variation norm as a function of the parameter estimation errors. We prove that the risk for the filtering and smoothing errors may be uniformly upper bounded by the $L^1$-risk of the estimators. It has been proved very recently that statistical inference for finite state space nonparametric HMMs is possible. We study how the recent spectral methods developed in the parametric setting may be extended to the nonparametric framework and we give explicit upper bounds for the $L^2$-risk of the nonparametric spectral estimators. In the case where the observation space is compact, this provides explicit rates for the filtering and smoothing errors in total variation norm. The performance of the spectral method is assessed with simulated data for both the estimation of the (nonparametric) conditional distribution of the observations and the estimation of the marginal smoothing distributions.

References


We consider identification and estimation in dynamic latent variable models with state-dependent distributions from a nonparametric class.

First, we investigate general finite-state hidden Markov models and obtain nonparametric identification of the parameters as well as the order of the Markov chain if the transition probability matrices have full-rank and are ergodic, and if the state-dependent distributions are all distinct, but not necessarily linearly independent. Based on this identification result, we develop nonparametric maximum likelihood estimation theory. Numerical properties of the estimates as well as of nonparametric goodness of fit tests are investigated in a simulation study.

Second, we consider the dynamic stochastic block model as recently introduced in Matias and Miele (2017), and obtain nonparametric identification in case of binary, finitely weighted and general edge states. We formulate conditions on the true parameters which guarantee actual point identification instead of mere generic identification, and which also lead to novel conclusions in the static case. We also give numerical illustrations via the variational EM algorithm in simulation settings covered by our identification analysis.

References


optimal sequence for the number of groups and cluster subjects. The penalized likelihood is optimized through a novel Expectation-Maximization-Markov-Metropolis algorithm. The work is motivated by an analysis of the progress of well-being of nations, as measured by the three dimensions of the Human Development Index over the last 25 years. The main findings are that (i) transitions among nation clubs are scarce, and mostly linked to historical events (like dissolution of USSR or war in Syria) and (ii) there is mild evidence that the number of clubs has shrunk over time, where we have four clusters before 2005 and three afterwards. In a sense, nations are getting more and more polarized with respect to standards of well-being. Non-optimized R code for general implementation of the method, data used for the application, code and instructions for replicating the simulation studies and the real data analysis are available at https://github.com/afarcome/LMrectangular.
Lightning Talk Session 3

The analysis of high frequency financial price changes
Leopoldo Catania¹, Roberto Di Mari² and Paolo Santucci de Magistris³

¹Aarhus University and CREATEs; ²University of Catania; ³Luiss University and CREATEs

High frequency price changes of financial assets are usually assumed to follow a distribution defined over a continuous support, with time-varying parameters. However, in the real world high frequency prices, and thus their changes, are intrinsically discrete variable. We start from this empirical evidence to develop a new model able to describe the dynamic properties of a multivariate time-series of high frequency price changes. Emphasis is given to the large presence of zeroes that characterize these series. We assume the existence of two independent unobserved latent processes which determine the price changes’ dynamic properties and the zeroes occurrences. Given the probabilistic structure embedded in our modelling framework we analyze the different sources of this large amount of zeroes as for example: absence of news, same magnitude of positive and negative news, and periods of market illiquidity. Furthermore, multivariate dynamic properties driving the different sources of zeroes between several assets are analyzed.

Multi-Resolution Bagging for Ensemble Classification
Majed El Helou, Rawan Chanouha, Hazem Hajj
Faculty of Engineering and Architecture, AUB, Beirut, Lebanon

Recent years have witnessed significant advances in the performance of classification algorithms, where ensemble techniques have had their fair share of success. However, some problems are yet to be solved, one of which is known as the imbalanced dataset classification problem [1]. Another challenge for ensemble techniques is the need for richer and larger ensembles (different classifier model definitions, different training strategies etc.). In this paper, we propose a novel approach to tackle the difficulties faced with imbalanced datasets. The solution we present is inspired by the well-known bagging approach [2]. Our algorithm leverages a hierarchically-structured bagging technique on the training data, forming models that are experts on different degrees of resolution and in different subregions of the feature space. This strategy is able to solve ambiguities at different levels of scale in the feature space. It is therefore able to correctly focus on minority classes. Very importantly, the underlying architecture permits the creation of a rich set of classifiers from a single model, which can then be integrated into any large ensemble. Our approach improves classification on various datasets used in the literature [1, 3]. In addition, we compare our ensemble results to the ones obtained with our base classifier as an illustration of the ensembling capabilities.

References
Improving clustering assessment through supervised classification modeling

Mario Fordellone\textsuperscript{1} and Maurizio Vichi\textsuperscript{1}

\textsuperscript{1}Sapienza University of Rome

In the unsupervised classification techniques, clusters of homogeneous objects are detected by means of a set of features measured (observed) on a set of objects without knowing the membership of objects to clusters. In these applications the aim is to discover the heterogeneity structure of the data. Often, techniques based on separability and homogeneity criteria of the groups are used, giving \textit{a priori} the number of groups. In the unsupervised classification models the principal approaches of cluster analysis are: Connectivity-based clustering better known as hierarchical clustering, Centroid-based clustering, Distribution-based clustering, Density-based clustering, and many other parametric and non-parametric techniques.

Conversely, supervised classification is based on the idea to forecast the membership of new objects (output) based on a set of features (inputs) measured on a training set of objects for which the membership to clusters is known. Therefore, in these applications the aim is to generalize a function or mapping from inputs to outputs which can then be used speculatively to generate an output for previously unseen inputs. Usually, a sub-sample (training) that is representative of specific groups is selected and then this model is used as references for the classification of new (unobserved) other objects. Training sets are selected based on the knowledge of the user. In the supervised classification models we have Artificial neural network, Naive Bayes classifier, Nearest Neighbor Algorithm, decision trees, logistic regression, generalized linear models, and many other parametric and non-parametric techniques are included.

Now, we know that in the unsupervised classification field, we have important issues that could drastically influence results: the unknown number of clusters, the selection of variables that most contribute to clustering, the final assessment of clusters. In other words, all the taken decisions to address the study can lead different results and then, each single decision become crucial on the aim of our study and should be tested.

In this work, we propose an algorithm based on the use of supervised classification modeling. In particular, we will prove that by using of supervised classification techniques we have effective inferential tools for choosing the number of clusters, selecting the most important variables for the clustering and assessing the quality of clusters. An application on both toy data and real data will be discussed.
References


Simulating mixtures of non-normal multivariate data with fixed cluster overlap in FSDA.

Marco Riani2, Francesca Torti1 and Domenico Perrotta1

1 European Commission, Joint Research Centre 2 University of Parma, Italy

The linear combination or product of independent random variables with known distributions and characteristic functions, in general cannot be derived in closed form. Witkovsky (2018) proposes to compute the characteristic function of the combination/product through the numerical, rather than analytical, inversion of the characteristic function of the random variables. To this end, he developed the MATLAB toolbox CharFunTool. A similar library, CharFun, is also available in R (Simkova, 2017).

In the case of linear combinations of non central χ² random variables, Davies (1980) also proposed a numerical solution based on the numerical inversion of the characteristic
function. This solution was adopted by Melnykov et al. (2012) in his MixSim framework for mixtures generation, which we have ported and extended in our MATLAB FSDA toolbox (Riani et al., 2015).

We now propose to extend the current FSDA implementation of MixSim to the linear combinations of other relevant distributions through the use of the CharFunTool framework.

References


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**Parsimonious models in matrix data mixture modeling**

Shuchismita Sarkar\(^1\), Xuwen Zhu\(^2\), Volodymyr Melnykov\(^1\) and Salvatore Ingrassia\(^3\)

\(^1\)University of Alabama; \(^2\)University of Louisville; \(^3\)UniversitÃ­ di Catania

Finite mixture modeling is a popular technique for capturing heterogeneity in data. Although the vast majority of the theory developed in this area up to date deals with vector-valued data, some recent advancements have been made to expand the concept to matrix-valued data, for example, by means of matrix Gaussian mixture models (Viroli 2011; Melnykov and Zhu 2018). Unfortunately, matrix mixtures tend to suffer from the overparameterization issue due to a high number of parameters involved in the model. As a result, this may lead to problems such as overfitting and mixture order underestimation. One possible approach of addressing the overparameterization issue that has proven to be effective in the vector-valued framework is to consider various parsimonious models. One of the most popular classes of parsimonious models is based on the spectral decomposition of covariance matrices (Bandfield and Raftery 1993; Celeux and Govaert 1995). In this study, an attempt to generalize this class and make it applicable in the matrix setting is made. Estimation procedures are thoroughly discussed for all models considered. The application of the proposed methodology is illustrated on a real-life data set.
### The Delta Machine: Binary Data Classification

Zdenek Sulc\(^1\), Beibei Juan\(^2\) and Mark de Rooij\(^2\)

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The Delta Machine is a statistical tool for the supervised classification with similar aims as the logistic regression or the support vector machines. Based on (dis)similarities between profiles of the observations to profiles of a representation set consisting of prototypes, it predicts the value of a class variable. One can choose one from four similarity measures for quantitative data (the Euclidean the squared Euclidean distances, the Exponential decay and the Gaussian decay functions) and the Gower coefficient for the mixed-type data. However, when dealing with the binary data, one can only use the Gower coefficient in the \(R\) function `daisy` from the `cluster` package (Maechler et al., 2018). In order to improve the binary data analysis, 15 similarity measures for binary data, such as the Jaccard, Dice or Hamann coefficients, see, e.g., Warrens (2008), were added to the Delta Machine. They offer different ways to express the similarity between the categories. The aim is to compare the classification performance of the newly added similarity measures with the original ones in binary-coded datasets. The results are also compared with commonly used classification methods, namely, the logistic regression and support vector machines described e.g. in James et al., (2013). For the comparison, the accuracy and the ROC analysis statistics obtained by the repeated cross-validations are used. The variability of these statistics is also analyzed using box-plots. The preliminary results show that the different similarity measures perform similarly concerning the classification performance, but the numbers of the used parameters in the models differ substantially.

### References

James, G., Witten, D. Hastie, T., Tibshirani, R. (2013). *An Introduction to Statistical Learning with Applications in R*. Springer-Verlag, New York.


The peculiar characteristics of the empirical loss given default distribution (LGD) call for more flexible models. In fact, it has support $[0,1]$, exhibit an excess of zeros and ones, and it is generally multimodal on $(0,1)$. Thus, we introduce a zero-and-one inflated mixture where a three level multinomial model is considered for the membership of the LGD values to the sets $\{0\}$, $(0,1)$ and $\{1\}$, while a finite mixture of distributions is used on $(0,1)$. To allow for more flexible shapes on $(0,1)$, besides considering distributions already defined on $(0,1)$, we used distributions defined on $(-\infty, \infty)$ mapped on $(0,1)$ via the inverse-logit transformation. The models are then fitted on two real LGDs datasets, one from an European Bank and the other from the Bank of Italy, and compared according to information criteria and goodness-of-fit.

References


Schuermann, T. (2004). What do we know about Loss Given Default?.

Talk Session 6: Recent developments in clustering of matrix data

Matrix Transformation Mixture Modeling
Volodymyr Melnykov and Xuwen Zhu
University of Alabama, University of Louisville

The existing finite mixture modeling and model-based clustering literature focuses primarily on the analysis of multivariate data observed in the form of vectors, with each element representing a specific feature. In this setting, multivariate Gaussian mixture models have been the most commonly used. Due to severe modeling issues observed when normal components cannot provide adequate fit to groups, much attention has been paid to developing models capable of accounting for skewness in data. In our work, we target the problem of mixture modeling with components that can handle skewness in matrix-valued data. The proposed developments open a wide range of possible modeling capabilities, with numerous applications, as illustrated in this paper. A novel matrix mixture model is proposed. Its skewness parameters enjoy appealing interpretability. The corresponding estimation procedure and various ways of parameterization are discussed. Comprehensive simulation studies and applications to real-life datasets illustrate the efficiency of the proposed developments, supported by good results.

References

Mixtures of Matrix Variate Bilinear Factor Analyzers
Michael P. B. Gallaugher, Paul D. McNicholas
McMaster University, Ontario, Canada

Over the years data has become increasingly higher dimensional, which has prompted an increased need for dimension reduction techniques. This is perhaps especially true for clustering (unsupervised classification) as well as semi-supervised and supervised classification. Although dimension reduction in the area of clustering for multivariate data has been quite thoroughly discussed in the literature, there is relatively little work in the area of three way, or matrix variate, data. A mixture of matrix variate bilinear factor analyzers (MMVBFA) model is developed for use in clustering high-dimensional matrix variate data. This work can be considered both the first matrix variate bilinear factor analyzers model as well as the first MMVBFA model. Parameter estimation is discussed, and the MMVBFA model is illustrated using simulated and real data.
Model-based clustering of tensor data
Shuchismita Sarkar\textsuperscript{1}, Volodymyr Melnykov\textsuperscript{1} and Xuwen Zhu\textsuperscript{2}
\textsuperscript{1}The University of Alabama; \textsuperscript{2}University of Louisville

The majority of existing mixture modeling and model-based clustering techniques are designed for the analysis of multivariate data. However, there are situations when the data are presented in more complex forms such as matrices or tensors. We extend the recent work in the matrix-valued setting by developing a methodological framework for mixture modeling and model-based clustering of tensor-valued observations and illustrate it on the data set containing self-reported salaries of faculty employed in American institutions. The information is available over thirteen academic years and grouped by the faculty rank and gender. The illustrative study aims at identifying salary patterns at American universities and investigating the potential sources of the variability in salary.

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