

Classification 2016 - Abstracts of the 5th German-Japanese Symposium

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Japanese Classification Society (JCS) and the German Classification Society (GfKI)

11.09. - 13.09.2016, Schloss Reisensburg (Günzburg)

Workshop Program

Sunday, September 11, 2016

17:00-17:50	Informal Meeting
18:00-21:00	Welcome Reception and Get Together

Monday, September 12, 2016

08:50-09:00	Hans Kestler (Ulm)	Opening
09:00-10:15		Chair: B. Lausen
09:00-09:25	Tadashi Imaizumi (Tokyo)	Model Based Clustering for a Sparse Similarity Matrix
09:25-09:50	Akinori Okada, Hiroyuki Tsurumi (Tokyo, Yokohama)	Estimating Market Share of New Brand by Analyzing Brand Switching Matrix Using Asymmetric Multidimensional Scaling
09:50-10:15	Ludwig Lausser (Ulm)	Exact relabeling tests for classification
10:15-10:45		Break
10:45-12:00		Chair: T. Imaizumi
10:45-11:10	Berthold Lausen (Essex)	Ensemble methods for clustering and classification
11:10-11:35	Sadaaki Miyamoto (Tsukuba)	Ward method applied to non-positive definite matrices with a model of unstrict users
11:35-12:00	Atsuho Nakayama (Tokyo)	Analysis of Trending Topics in Consumer Web Communication Data
12:00-13:30		Lunch
13:30-14:20		Chair: C. Weihs
13:30-13:55	Fumitake Sakaori (Tokyo)	Fully Bayesian Soft Impute for Matrix Completion
13:55-14:20	Johann Kraus (Ulm)	Tuning hierarchical clustering with domain knowledge
14:20-14:50		Break
14:50-15:40		Chair: A. Wilhelm
14:50-15:15	Claus Weihs (Dortmund)	Classification on Large-Scale Data: Systematic Testing in the many-features case
15:15-15:40	Yoshiro Yamamoto, Sanetoshi Yamada (Hiratsuka)	Visualization of cross tabulation using association plot

Tuesday,	September	13,	2016
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09:00-10:15		Chair: J. Kraus
09:00-09:25	Adalbert Wilhelm (Bremen)	The imbalanced class problem revisited
09:25-09:50	Masahiro Mizuta (Sapporo)	Analysis of environmental data with SDA and FDA
09:50-10:15	Andreas Geyer-Schulz (Karlsruhe)	Do Industrial End-Consumer Product-Configurators Use Ratio- nal Pricing? A Case Study
10:15-10:45		Break
10:45-13:55		Chair: A. Okada
10:45-11:10	Hans-Hermann Bock (Aachen)	Interaction-based co-clustering - but which interactions?
11:10-11:35	Kei Kurakawa, Yasumasa Baba (Tokyo)	Tensor based relational learning for the author name disambiguation
11:35-12:00	Jun Tsuchida (Kyoto)	Majorization algorithm for dominance point model
12:00-13:30		Lunch
13:30-13:55	Hans-Joachim Mucha (Berlin)	Big Data Clustering: Is Subsampling Better than Fast Pre- clustering?
13:55-14:20	Hans Kestler (Ulm)	Closing Remarks
15:40		Departure

Synopsis

This volume comprises abstracts of talks presented at the 5th German-Japanese Symposium on Classification hosted by the Institute of Medical Systems Biology, Ulm University and the German Classification Society (GfKI) at the Reisensburg Castle in Günzburg 2016. President Prof. Dr. B. Lausen (University of Essex) and 1st Vice President Prof. Dr. H. A. Kestler (Ulm University) of the GfKI as well as President Tadashi Imaizumi (Tama University) and other members of the Japanese Classification Society (JCS) attended the symposium. The conference was supported by the GfKI as well as the German Research Foundation (DFG).

The scientific program of the symposium includes presentations covering a broad range of topics. A special emphasis is laid on research and development of tools, techniques, and strategies that address challenges of data science using computational, mathematical, statistical and data analytical methods for classification.

With half of the participants coming from outside of Germany, the symposium corroborates the spirit of international networks and cooperations.

Selected papers will be published in a special issue of the "Archives of Data Science".

Past Symposiums:

- Tokyo 2005
- Berlin 2006
- Karlsruhe 2010
- Kyoto 2012

September 2016

Hans Kestler Director, Institute of Medical Systems Biology Ulm University

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Model Based Clustering for a Sparse Similarity Matrix

Tadashi Imaizumi¹

When a given (dis)similarity matrix **S** of $n \times n$, a hierarchical clustering methods is useful for us to understand the relationship of objects in data. However, it is difficult to choose the "proper" clustering results, without prior information of the number of clusters and distance metric between clusters etc. Bock(1996) discussed on probabilistic clustering and Fraley and Raftery(2003) discussed on the model-based cluster analysis. These probabilistic model-based clustering approach will be more appropriate to find the hidden clusters in data matrix of objects \times attributes.

It is also applicable for a similarity matrix after obtaining a dimensional representation of objects(configuration). However this approach is not appropriate one as it consists of two different phases. And how to derive this configuration becomes the key point. We propose a probabilistic model-based clustering approach for a similarity matrix. The normal distribution is assumed to derive a configuration for a fixed number of clusters G. An object configuration will be obtained by a method of multi-dimensional scaling with a distributional assumption,

$$X_i \sim N(\mu_q, \Sigma_q), i = 1, 2, \cdots, n.$$
(1)

The covariance matrix of each cluster Σ_g is assumed to be decomposed as

$$\Sigma_q = \lambda_g \mathbf{D}_k \mathbf{A}_k \mathbf{D}_k^t, g = 1, 2, \cdots, G$$
⁽²⁾

where \mathbf{D}_k is the orthogonal matrix of eigenvectors. And the similarity s_{ij} between two objects i and j of same cluster are related as the distance between two corresponding points within cluster. And those between two objects of different clusters are related as the distance between two cluster means of each cluster. The configuration is updated with using the estimated covariance matrices. When a given sparse similarity matrix is one of the block-diagonal matrix, then the above procedure works well as the covariance matrix of each cluster will be identified, but, we need to pay attention when similarity matrix is more complex one. In that case, the structure of the covariance matrix will be restricted.

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Estimating Market Share of New Brand by Analyzing Brand Switching Matrix Using Asymmetric Multidimensional Scaling

Akinori Okada¹ and Hiroyuki Tsurumi²

When a new brand is introduced into market, the new brand may dominate existing brands and takes a lot of customers away from the existing brands or the new brand may not dominate the other brands and takes only small number of the customers away from the existing brands. A brand switching matrix among existing brands is analyzed by asymmetric multidimensional scaling of Okada & Tsurumi (2014) to derive configuration of existing brands. The analysis represents one configuration along each dimension, where asymmetric relationships among existing brands are represented by the outward tendency and the inward tendency. The outward tendency of a brand represents the tendency of switching from the brand to the other brands, and the inward tendency of a brand represent the tendency of switching from the other brands to the brand. The characteristics of a new brand are compared with those of the existing brands along dimensions, and the location of the new brand in the configuration is determined. The location of the new brand is used to estimate the frequency of brand switching to/from th new brand with existing brands and the market share of the new brand as well. The procedure is applied to frequent shoppers program data analyzed in Okada & Tsurumi (2014).

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Exact relabeling tests for classification

Ludwig Lausser¹, Alexander Groß¹, Hans A. Kestler¹

An object can typically be assigned to many different concepts. It is therefore not a sample for one particular class or category. This eclectic character of an object can be a hindrance for the process of supervised learning. Being not aware of the characteristic patterns of a categorization, a classifier might be diverted by the patterns of a different one.

For a chosen classification task, the suitability of a set of samples is therefore not only characterized by the classification accuracy achieved by the corresponding classifier. It is also characterized by the classification accuracy achieved for any other (possibly unknown) classification of the dataset. A relative measure of these two quality scores is needed.

In this work, we propose a relabeling strategy that allows the exhaustive evaluation of all binary labelings in the leave one out cross-validation experiments. The strategy utilizes the characteristics of k-nearest neighbor classifiers and the corresponding graph structures for fast and efficient calculation. It can be applied for the construction of an exact permutation test which relates the classification performance achieved for a chosen categorization to any other categorization. We utilize this strategy in artificial scenarios and the domain of functional genomics.

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Ensemble methods for clustering and classification

Berthold Lausen¹, Kaloyan Stoyanov², Luca Citi³, Rolando Medellin^{1,2}, Henrik Nordmark², Aris Perperoglou¹

We review methods to use ensembles of selected classifiers to achieve classification rules with increased accuracy (Gul et al. 2016, Khan et al. 2016). Feature selection methods are often used as preprocessing method. For example after preprocessing microarray data with 500 000 probes and 22125 features (probesets) which represent genes, we use a proposal to improve feature selection of microarray data based on a proportional overlapping score (Mahmoud et al. 2014).

We investigate ensemble methods for cluster analysis. Using ensemble concepts Stoyanov (2015) developed an R package to use hierarchical clustering as preprocessing for k-means clustering. In addition we discuss proposals to use nonparametric and parametric bootstrap resampling and distance based variance estimation (Felsenstein 1985; Lausen & Degens, 1987; Degens, Lausen & Vach 1990) to derive a statistical evaluation of clusters.

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Ward method applied to non-positive definite matrices with a model of unstrict users

Sadaaki Miyamoto¹

It is well-known that the Ward method can only be applied to a set of objects as points in an Euclidean space and not to a general matrix of similarity/dissimilarity. More recently, it has also been proved that the Ward method can be applied to the class of semi-positive definite matrix of similarity by applying the theory of kernels. At the same time, the Ward method cannot be applied to the case of a non-positive definite matrix of similarity which has a negative eigenvalue. In spite of this fact, the aim of this study is to show the possibility to apply the Ward method even to the case of non-positive definite matrices of similarity S with a mild condition of S(i, i) = 1 for $i = 1, \ldots, n$ and $S(i, j) \leq S(i, i)$ for all j.

It is of course impossible that the Ward method is rigorously justified in the latter case. Instead, we introduce a model of *unstrict* users. Probably most researchers will agree that users of agglomerative hierarchical clustering in applications are rather rough or unstrict: they not care much about details of used similarities or very details of the output of dendrograms. Hence we assume a model of an unstrict user as follows: he does not care about the difference of two dissimilarities of D(i, j) and D'(i, j) = D(i, j) + constant when i and j are different. He does not care about the difference of two dendrograms when they produce the same sequence of the same clusters in the same order, but the merged levels of clusters may be different. We now have the following result:

Let S be a similarity matrix produced from D by a simple transformation of S = E - D, assuming $0 \le D(i, j) \le 1$. S' = S + aE will be positive-definite for sufficiently large constant a. Then the Ward method can be justified to S'. The Ward method applied to S cannot be justified in the rigorous way, but the algorithm of the Ward method to S still works and the dendrogram applied to S is 'isomorphic' to another dendrogram applied to S' in the sense that the two dendrograms will produce the same sequence of the same clusters in the same order, but the merged levels of clusters are different. It is also easy to see that D'(i, j) = D(i, j) + constant.

To summarize, the Ward method can be applied to a non positive-definite S under the assumption of the above model of unstrict users. This result make the applicability of the Ward method much broader, e.g., to the case of network clustering without the use of a particular type of kernels.

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Analysis of Trending Topics in Consumer Web Communication Data

Atsuho Nakayama¹

In this study, we detected trending topics by classifying words into clusters based on the co-occurrence of words in web communications among consumersD We collected web communication data about certain specific theme based on their specific expressions of sentiment or interest. Because of the desire to identify market trends, the analysis of consumer web communication data has received much attention in Japan. To detect topics more easily, we tokenized each web communication data that was written in sentences or sets of words. However, one of the most difficult natural language-processing problems in Japanese is tokenization. This is referred to as the "wakachigaki" problem. In most Western languages, words are delimited by spaces and punctuation. In Japanese, words are not separated by spaces. We used morphological analyses such as tokenization, stemming, and part-of-speech tagging to separate the words. In our study, we used the Japanese morphological analyzer ChaSen to separate words in passages and to distinguish all nouns, verbs, and adjectives. ChaSen (http://chasen.naist.jp/) is a fast, customizable Japanese morphological analyzer that takes the form of a hierarchical structure. It is designed for generic use, and can be applied to a variety of languageprocessing tasks. The entry \times word matrix obtained from the web communication data was sparse and of high dimensionality, so it was necessary to perform a dimensionality reduction analysis. We classified the words extracted from web communication data using non-negative matrix factorization as a dimensionality reduction model (Lee & Seung, 2000).

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Fully Bayesian Soft Impute for Matrix Completion

Fumitake Sakaori¹, Hiroki Kurosawa¹

Matrix completion methods for an incomplete low-rank matrix have been applied in many practical situation such as collaborative filtering, image processing and analysis of gene expression array. Accordingly, various matrix completion methods have been developed and investigated theoretically. The objective of these methods are to complete a incomplete observed matrix under the assumption that the observed matrix are represented as a sum of a low-rank matrix and a noise matrix.

Mazumder *et al.* (2010) proposed Soft-Impute, a sparse modeling for an incomplete matrix, where the sparsity of singular values of the low rank matrix is achieved by regularizing the nuclear norm of the low rank matrix. Todeschini *et al.* (2013) proposed an adaptive extension of the Soft-Impute, Hierarchical Adaptive Soft-Impute and gave their bayesian representation. The effectiveness of these methods heavily rely on the choice of tuning parameters.

In this study, we propose a fully bayesian modeling of Soft-Impute which can estimate the tuning parameters simultaneously.

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Tuning hierarchical clustering with domain knowledge

Johann M. Kraus¹ and Hans A. Kestler¹

Cluster analysis presents a variety of tools from the explorative data analysis that are used for predicting an unknown structure hidden in data. Unsupervised cluster methods do not make use of domain knowledge about any possible grouping of the data. However, many partitional cluster algorithms were adapted to additionally make use of available background information either by constraining the search process or by modifying the underlying metric. Limitations in the reproducibility of clustering results in resampling experiments triggered the inclusion of domain knowledge into the hierarchical clustering process, too. Based on our previous work (Kestler et al. 2006, Kraus et al. 2007), we present a general framework for including domain knowledge into a hierarchical clustering process. Our new semi-supervised cluster strategy aims at assessing the reliability of hierarchical clustering. Reliable clusters now can be identified by searching for the most stable partitions under different clustering conditions in resampling experiments.

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Classification on Large-Scale Data: Systematic Testing in the many-features case

Claus Weihs¹, Tobias Kassner¹

In this paper we develop a systematic approach for testing the performance of classical classification methods on Large-Scale Data in the case with many more features than observations. We examine, e,g, the influence of the distance of the classes, of the covariance matrix, of the balance between the classes, and of the true error rate on the performance of the classifiers.

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Visualization of cross tabulation using association plot

Yoshiro Yamamoto¹ and Sanetoshi Yamada²

When comparing the response in a survey or medical treatments by some groups, we make the cross-tabulation tables then visualize them by such like bar plot or mosaic plot. For many questions or treatments, we want to find the item that the reaction of a particular group is different from the others. Association rule analysis are suitable for the kind of analysis. By using the coordinates by biplot of correspondence analysis it is possible to plot the relationship between items (treatments) and groups. In this visualization, correspondence analysis and association rules analysis are complement each other. Yamada and Yamamoto [1] introduce this kind of visualization with interactive by using Shiny.

For the medical treatments analysis, it is good to explain with odds ratio.

Then we introduce odds ratio criterion to our visualization method. To introduce this criterion, our interactive visualization has a meaningful reference plot.

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The imbalanced class problem revisited

Adalbert F.X. $Wilhelm^1$

The last decades have seen the invention of a number of modern classification algorithms, such as CART, AdaBoost, support vector machines, and random forests which have shown to result in improved predictions for the expense of diminished interpretability. Imbalanced classes pose a challenge for these data-driven classifiers since the majority class provides more information to fine tune the classifier and equips even naive classifiers with good accuracy performance measures. However, the minority class is typical of higher importance and hence classifiers that yield improved predictions for the minority class are desired. In this presentation, we present an overview on various methods for classifying imbalanced data which each has its own advantages and disadvantages. The evaluation of the algorithms will be illustrated by examples predicting the occurrence of military conflicts.

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Analysis of environmental data with SDA and FDA

Masahiro Mizuta¹

In our talk, we focus on an environmental dataset. Most of environmental data sets are constructed with location, time, and many factors. We utilize two approaches: Symbolic Data Analysis (SDA) [2] and Functional Data Analysis (FDA) [4]. FDA and SDA are both proposed around 1980's. They gave us new frameworks for complex structured data.

In FDA, the objects in the data sets are represented by functions or curves. When saying in other words, the individuals which were described as the points in p dimensional space in the frame work of the conventional multivariate analysis, are represented by a set of continuous functions. This representation is good for analysis of transition of the values depended on time.

In SDA, the targets objects are named as "concepts". The concepts have descriptions, e.g. interval values, distributional values, a set of them and so on. This means that SDA takes advantage of various kinds of descriptions and has the flexibility. We use the environmental data; air dose rates measured every 3 seconds by 32 route buses in Fukushima Prefecture. The records of the data include time, latitude, longitude, and air dose rate. Total number of records is 13,508,200. This data set is a kind of big data. We analyze it using FDA, SDA and Mini Data approach [4].

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Do Industrial End-Consumer Product-Configurators Use Rational Pricing? A Case Study.

Andreas Geyer-Schulz¹, Tino Fuhrmann¹, Marvin Schweizer¹

In this paper we mine an anonymized open data set with car configuration data provided by TNS Infratest. We follow the a priori segmentation of car configurations by model line and engine type used by the car manufacturer. For all these segments we identify all sets of configurations with the same configuration price. For each segment with the same we compute the attribute lattices of car configurations with the same price. With the help of utility theory we formalize tests of rationality and we identify deviations from rationality in the data set. Finally, we discuss the role of rational pricing strategies in end-consumer car configurators and suggest ways of exploiting deviations from rationality in the costumer purchase process.

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Interaction-based co-clustering - but which interactions?

Hans-Hermann Bock¹

We consider the problem of clustering simultaneously the rows and columns of a realvalued $I \times J$ data matrix $X = (x_{ij})$ by corresponding row and columns partitions $\mathcal{A} = (A_1, ..., A_m)$ and $\mathcal{B} = (B_1, ..., B_n)$, respectively, with two given numbers m and n of classes (two-way clustering, bi-clustering, co-clustering). Rows and columns may correspond, e.g., to individuals and variables in a study, or to the categories of two qualitative predictor variables which may affect the target variable x_{ij} . Various methods have been proposed for solving such bi-clustering problems, e.g., by optimizing a clustering criterion, by probabilistic co-clustering modeling, by adapting classical k-means or EM algorithms, or by empirical hierarchical or patchwork approaches. In this paper we concentrate on methods that highlight the interaction structure within or between the 'block clusters' $A_p \times B_q$ in the data matrix. When browsing through the literature, it appears that it is not at all clear which type of 'interaction' to use since there are various possible options, e.g.:

- (a) the individual interactions $\gamma_{ij} := x_{ij} \bar{x}_{i,\cdot} \bar{x}_{\cdot,j} + \bar{x}_{\cdot,\cdot}$ i.e., the individual overall deviations from additivity in X
- (b) the blockwise interactions $g_{pq} := \bar{x}_{A_p,B_q} \bar{x}_{A_p,\cdot} \bar{x}_{\cdot,B_q} + \bar{x}_{\cdot,\cdot}$, i.e., the block-specific deviations from additivity in X
- (c) the individual block-specific interactions $s_{ij} := x_{ij} \bar{x}_{i,B_q,\cdot} \bar{x}_{A_p,j} + \bar{x}_{A_p,B_q}$ for $i \in A_p, j \in B_q$, i.e., the individual cluster-specific deviations from additivity in the submatrix $X^{A_p \times B_q} = (x_{ij})_{i \in A_p, j \in B_q}$.

This paper presents various co-clustering approaches dealing with these interactions, discusses the underlying models and bi-clustering structures, and cites possible application fields.

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Tensor based relational learning for the author name disambiguation

Kei Kurakawa¹ and Yasumasa Baba²

Relational learning with tensor factorization has been attracting attention as a technique for data mining, data analysis, and data science (Kolda, 2009; Nickel, 2011). We apply tensor factorization techniques for the author name disambiguation that has been one of the most important issues of digital library research (Ferreira 2012).

In our approach, we represent author similarity matrices of bibliographic citation attributes on tensor slices, and apply tensor factorizations such as CP (CANDECOMP / PARAFAC) decomposition and Tucker decomposition to extract latent feature vectors as of author. Then, we cluster the authors represented by the feature vectors with a clustering technique, k-means to identify the group of citations for each author.

We conducted experiment of our approach with bibliographic citation data that we prepared for two author names. To process the data, we used a tensor library, *scikit-tensor* and a machine learning library, *scikit-learn* and compared effectiveness of our tensor based model to another model with latent variables, LDA.

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Majorization algorithm for dominance point model

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Asymmetric multidimensional scaling (AMDS) is a visualization method that can be applied to asymmetric (dis)similarity data. The dominance point model proposed by Okada and Imaizumi (2007) is an AMDS model. This model represents asymmetry between objects as the difference in the distances between objects and a dominance point. One of the advantages of this model is the easy interpretation of asymmetry because the coordinate vectors of dominance points constitute the parameters of asymmetry. One of the disadvantages of this model is that calculation by using this algorithm is time consuming because it is a non-linear optimization algorithm. In this presentation, we introduce a majorization-minimization algorithm for dominance point model. We decompose the objective function of the dominance point model into symmetric and asymmetric parts. We create majorizing functions of the symmetric and asymmetric parts. Then, we create the update formula. Although the majorization-minimization algorithm is an iterative algorithm, we obtain often simply and explicit update formula under each step. Because the update formula of the majorization-minimization algorithm is simple, we could also introduce a majorization-minimization algorithm for the twomode three-way dominance point model proposed by Okada and Imaizumi(2015) and Okada and Imaizumi(2015).

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Big Data Clustering: Is Subsampling Better than Fast Pre-clustering?

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Often, Big Data is seen as a synonym for a massive dataset simply within the meaning of a very large number of observations (points) N. In this paper, the focus is on preclustering of such Big Data followed by a final clustering. Concretely, we propose a fast data pre-clustering by breaking a cloud of points successively into two clouds at its centroid by a hyperplane. The computational complexity of this iterative binary binning is linear proportional in N. Pre-clustering reduces the number of observations N to a much smaller number of micro-clusters $M \ll N$, say M = 1000. Alternatively, the well-known subsampling technique can be used to select $M \ll N$ observations randomly. However, if N is very large then the subsampling rate M/N becomes much smaller than the usual rates of 0.5 to 0.95 known from simulation studies. In any case, a final clustering of the M micro-clusters or the M resampled observations, respectively, results in a partition into the desired K clusters, where usually $K \ll M \ll N$. By doing so, the computational complexity of the final clustering doesn't greatly matter with respect to N. Then the question arises: is our proposed fast pre-clustering better than subsampling? To answer this question the results of some simulation studies are presented.

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