Statistical Computing 2013

Abstracts der 45. Arbeitstagung

HA Kestler, M Schmid, F Schmid
M Maucher, JM Kraus (eds)

Ulmer Informatik-Berichte

Nr. 2013-07
June 2013
**Workshop Program**

**Sunday, June 23, 2013**

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>18:15-19:30</td>
<td>Dinner</td>
</tr>
<tr>
<td>19:30-20:30</td>
<td>Chair: H.A. Kestler (Ulm)</td>
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<td>19:30-20:30</td>
<td>Uwe Ligges (Dortmund)</td>
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<td>R-3.0.x and beyond</td>
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<td>Time</td>
<td>Activity</td>
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<tr>
<td>08:50-09:00</td>
<td>Opening of the workshop: H.A. Kestler, M. Schmid</td>
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<tr>
<td>09:00-12:00</td>
<td>Chair: U. Ligges (Dortmund)</td>
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<tr>
<td>09:00-09:30</td>
<td>Günther Sawitzki (Heidelberg)</td>
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<tr>
<td>09:30-10:00</td>
<td>Helena Kotthaus (Dortmund)</td>
</tr>
<tr>
<td>10:00-10:30</td>
<td>Florian Schmid (Ulm)</td>
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<tr>
<td>09:00-09:30</td>
<td>The In and Out of R: Byte Code, Profiling and Optimization</td>
</tr>
<tr>
<td>09:30-10:00</td>
<td>Runtime and memory consumption analyses for machine learning R programs</td>
</tr>
<tr>
<td>10:00-10:30</td>
<td>gsaTools - A toolbox for gene set enrichment analysis in R</td>
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<tr>
<td>10:30-11:00</td>
<td>Coffee break</td>
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<tr>
<td>11:00-11:30</td>
<td>Axel Fürstberger (Ulm)</td>
</tr>
<tr>
<td>11:30-12:00</td>
<td>Sebastian Behrens (Ulm)</td>
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<tr>
<td>11:00-11:30</td>
<td>Extended pairwise local alignment of wild card DNA/RNA sequences using dynamic programming</td>
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<td>11:30-12:00</td>
<td>Using VennMaster to evaluate and analyse shRNA data</td>
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<tr>
<td>12:15-14:00</td>
<td>Lunch</td>
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<tr>
<td>14:00-16:00</td>
<td>Chair: M. Maucher (Ulm)</td>
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<tr>
<td>14:00-15:00</td>
<td>Tim Beißbarth (Göttingen)</td>
</tr>
<tr>
<td>15:00-15:30</td>
<td>André Burkovski (Ulm)</td>
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<tr>
<td>15:30-16:00</td>
<td>Alfred Ultsch (Marburg)</td>
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<tr>
<td>14:00-15:00</td>
<td>Methods for the integration of biological network knowledge into classification algorithms</td>
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<tr>
<td>15:00-15:30</td>
<td>Aggregating diverse high-throughput data for the identification of common differences between young and old</td>
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<tr>
<td>15:30-16:00</td>
<td>Functional genomic and transcriptomic analysis of the human olfactory bulb</td>
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<tr>
<td>16:00-17:00</td>
<td>Poster Session</td>
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<td>17:00-18:00</td>
<td>Working groups meeting on</td>
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<td></td>
<td>Statistical Computing 2014 and other topics (all welcome)</td>
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<tr>
<td>18:15-19:30</td>
<td>Dinner</td>
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<td>Time</td>
<td>Speaker</td>
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<td>09:00-09:30</td>
<td>Anna Telaar (Dortmund)</td>
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<td>09:30-10:00</td>
<td>Benjamin Hofner (Erlangen)</td>
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<td>10:00-10:30</td>
<td>Gunnar Völkel (Ulm)</td>
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<td>11:00-11:30</td>
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<td>11:30-12:00</td>
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<td>14:00-14:30</td>
<td>Vito Baccelliere (Ulm)</td>
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<td>14:30-15:00</td>
<td>Markus Maucher (Ulm)</td>
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<tr>
<td>15:00-15:30</td>
<td>Andreas Mayr (Erlangen)</td>
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<tr>
<td>15:30-16:00</td>
<td>Michel Lang (Dortmund)</td>
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<td>16:30-17:00</td>
<td>Ludwig Lausser (Ulm)</td>
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<td>17:00-17:30</td>
<td>Werner Adler (Erlangen)</td>
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<tr>
<td>Title</td>
<td>Authors</td>
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<tr>
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</tr>
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</tr>
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</tr>
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</tr>
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<td>Functional genomic and transcriptomic analysis of the human olfactory bulb</td>
<td>Alfred Ultsch, Jörn Lötsch et al.</td>
</tr>
<tr>
<td>A generic method to find disease-associated genes in databases</td>
<td>Melanie B. Grieb, Johann M. Kraus, Karl L. Rudolph and Hans A. Kestler</td>
</tr>
<tr>
<td>A model of the crosstalk between the Wnt and the IGF signaling pathways</td>
<td>Shuang Wang, Michael Kühl and Hans A. Kestler</td>
</tr>
<tr>
<td>Investigation of Fuzzy Support Vector Machines</td>
<td>Markus Frey, Martin Schels, Michael Glodek, Sascha Meudt, Markus Kächele and Friedhelm Schwenker</td>
</tr>
<tr>
<td>A pragmatic procedure for stepwise feature selection</td>
<td>Anna Telaar and Carmen Theek</td>
</tr>
<tr>
<td>Controlling false discoveries in high dimensional situations: Boosting with stability selection</td>
<td>Benjamin Hofner and Michael Drey</td>
</tr>
</tbody>
</table>
Subscan - a cluster algorithm for identifying statistically dense subspaces with application to biomedical data
Johann M. Kraus and Hans A. Kestler 24

Power network clustering in modern protection systems
Sebastian Krey, Sebastian Brato, Uwe Ligges, Claus Weihs and Jürgen Götze 25

Reconstructing gene regulatory networks: deducing the coefficients of stochastic differential equations
Vito Baccelliere and Ulrich Stadtmüller 26

A critical noise level for learning Boolean functions
Markus Maucher and Hans A. Kestler 28

Boosting sonographic birth weight prediction
Andreas Mayr, Florian Faschingbauer, Matthias Schmid 30

Automatic model selection and configuration for high dimensional survival analysis
Michel Lang, Bernd Bischl, Claus Weihs and Jörg Rahnenführer 32

Exhaustive biomarker selection for small and medium sized datasets
Ludwig Lausser and Hans A. Kestler 34

Diversity Based Ensemble Pruning for Higher Interpretability
Werner Adler, Zardad Khan, Sergej Potapov and Berthold Lausen 35
R-3.0.x and beyond

Uwe Ligges
The In and Out of R: Byte Code, Profiling and Optimization

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Runtime and Memory Consumption Analyses for Machine Learning R Programs

Helena Kotthaus, Michel Lang, Jörg Rahnenführer and Peter Marwedel

R is a multi-paradigm language with a dynamic type system, different object systems and functional characteristics. These characteristics support the development of statistical algorithms at a high level of abstraction. Although R is commonly used in the statistics domain, a big disadvantage are its performance problems when handling computation-intensive algorithms. Especially in the domain of machine learning, for example when analyzing high-dimensional genomic data, the execution of R programs is often unacceptably slow. Morandat et al. [2] analyzed R programs from different fields of statistics and were able to show major performance issues. Our goal is to overcome these issues, particularly focusing on machine learning programs [1]. As a first step towards this goal, we used the traceR tool [2] to analyze the bottlenecks arising in this domain. Here, we measured the runtime and overall memory consumption on a well-defined set of classical machine learning applications and gained detailed insights into the performance issues of these programs. Bottlenecks we identified include: boxing of scalar values, vector allocation and copy, environment and promise creation and in particular vector subsetting. As in R every value is a vector, scalar values are boxed into single-element vectors, which results in an excessively high number of vector allocations. Variable and function symbols are stored in environments representing the interpreter state. Environments are allocated on the heap of the interpreter, which also applies to variables local to the current environment. Function calls are lazily evaluated. For each function call a promise, representing a function closure with all parameters, is allocated on the heap. Those characteristics cause high runtime and memory management overhead. In this talk we present the results of our runtime and memory consumption analyses and outline approaches to overcome the identified bottlenecks.

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References


gsaTools - A toolbox for gene set analysis in R

Florian Schmid, Johann M. Kraus and Hans A. Kestler

The measurements gained from microarray or deep sequencing experiments are often analyzed for gene set enrichment. There is a wide range of methods available for performing these analyses. The aim is to check the measured data for enrichment or overrepresentation of gene sets connected to any kind of process in a cell. The R-package gsaTools embraces these various methods in one toolbox and allows their application by using a generic pipeline which is based on the modular framework given by Ackermann and co-workers [5].

In contrast to other currently available approaches (i.e. [4,2]) this modular framework provides the user the possibility to integrate his own methods into the generic pipeline of the gsaTools package. An advantage over available web interfaces (i.e. [3]) is the complete implementation of the package in R which allows a fully automated analysis of data sets. Parts of the package apply computer intensive tests on the given data. To ensure an efficient analysis the package provides the possibility of analyzing a list of gene sets in parallel.

Gene sets which are already known and published are available in databases like the MSigDB [1]. They can be downloaded and used for analysis. If there is no gene set available for a certain pathway or process it can be of interest to create a new gene set. The information sources, such as hints from the literature, which are used to create this new gene set are highly uncertain. To handle this a robustness analysis, which is also a feature of the gsaTools package, can be applied to the gene sets. A resampling experiment is performed to quantify the included uncertainty.
References


Extended pairwise local alignment of wild card DNA/RNA-sequences with wild-type protein-sequences using dynamic programming

Axel Fürstberger and Hans A. Kestler

Sequence alignment and mutation analysis are essential tasks in modern molecular medicine. Besides finding homologies to identify a common ancestor or reconstruct evolutionary changes, genotypic resistance testing is another important area of sequence alignment analysis.

Supporting the complete IUPAC nomenclature leads to a new step within the alignment-algorithm, which performs a best case or worst case wild card analysis to calculate the optimal local alignment, depending on the intended use. Supporting the different forms of nucleotide- and amino acid-mutations as well as common and individual scoring matrices, with the genotypic resistance testing the extended pairwise local alignment tool SWAT also has an additional focus on the mutated positions of alignments.

We present an algorithm for the extended pairwise sequence alignments, which covers the problem of input-data-wild cards, offers a high flexible set of parameters and display a detailed alignment output and a compact representation of the mutated positions of the alignment.
Using VennMaster to evaluate and analyse shRNA data

Sebastian Behrens and Hans A. Kestler

VennMaster is a tool to visualise set data in area proportional Venn diagrams. Since exact solutions of this problem typically do not exist for more than three sets, VennMaster uses an error function and a heuristic particle swarm optimisation algorithm to approximate a solution. We here report the extension of VennMaster to serve as a tool for statistical analysis of set data derived from next generation sequencing experiments. New features include generic criterion adjustment to select for elements included in the graph, based on sequencing counts and an analysis of the significance of the corresponding overlaps. Given a selection criterion for elements, a resampling test is used to assess the significance of each overlap between sets. Overlap significance is then visualised within the graph via colour coding.

A data set of shRNA knockdown experiments on human cancer cell lines was analysed to identify genes playing a key role in proliferation of these cells. VennMaster was used to visualise gene set overlap for different minimal sequencing counts between technical and biological replicates as well as between different cell lines.

While originally intended for, and improved for shRNA library and sequencing data, these new VennMaster features can also be of great use in any other scenario, where overlap between multiple sets need to be visualised and statistically verified.

Additionally a parallelized implementation of the optimisation algorithm was realised, greatly speeding up the diagram generation on machines with multiple cpu-cores making VennMaster suitable for the analysis of growing amounts of next generation sequencing data.

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References


Methods for the integration of biological network knowledge into classification algorithms

Tim Beißbarth
Aggregating diverse high-throughput data for the identification of common differences between young and old

Andre Burkovski, Johann M. Kraus and Hans A. Kestler

High-throughput studies provide rankings of genes related to a study of interest, like gene activity difference in aging. It is often the case that the rankings of genes vary in each study because of differences in the experimental setup. Also use of different high-throughput technologies hinders a direct comparison of different rankings. Rank aggregation is used to infer a ranking that shows which genes are considered high ranked across all studies. In this regard, rank aggregation combines diverse information to build up a consensus ranking of differentially expressed genes. In this study we integrate several aging related studies for the identification of common differences between young and old phenotype: (i) mouse comparison between old (wildtype liver, 4 samples) and young phenotype (p53ko liver, 4 samples) (Katz et al.), (ii) mouse experiment old (TTD- liver, 6 samples) and young phenotype (TTD+ liver, 6 samples) experiments (Begus-Nahrman et al.), (iii) mouse experiment old (CMP cell type, 22 months, 8 samples) and young phenotype (CMP cell type, 3 months, 8 samples), (iv) mouse experiment from old (Crypts cell type, irradiated, 8 samples) and young phenotype (non irradiated, 8 samples), and (v) Drosophila melanogaster experiment old (gut, 3 samples) and young phenotype (gut, 3 samples). Applying rank aggregation and further analysing the consensus ranking via enrichment analysis reveals several enriched pathways common to all studies that are not reported when analysing each study individually. These pathways can be interpreted as the common difference in aging related experiments. We conclude, that aggregating results from different studies related to the research question can lead to a higher confidence in the gene signature and the discovery of new information in enrichment analysis.

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References


Functional genomic and transcriptomic analysis of the human olfactory bulb

Alfred Ultsch¹, Jörn Lötsch² et.al.

This reports the analysis of the transcriptome of the human olfactory bulb via RNA quantification intersected with the set of expressed transcriptomic genes using independently available proteomic expression data. To obtain a functional genomic perspective, this intersection was analyzed for higher-level organization of gene products into biological pathways established in the gene ontology database. We report that a fifth of genes expressed in adult human olfactory bulbs serve functions of nervous system or neuron development, half of them functionally converging to axonogenesis but no other non-neurogenetic biological processes. Other genes were expectedly involved in signal transmission and response to chemical stimuli. This provides a novel, functional genomics perspective supporting the existence of neurogenesis in the adult human olfactory bulb.

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A generic method to find disease-associated genes in databases

Melanie B. Grieb, Johann M. Kraus, Sebastian Behrens, Karl L. Rudolph and Hans A. Kestler

Background

The improvement and cheaper availability of microarray and gene sequencing technologies has led to an increasing number of studies about the association of gene mutations with diseases. Multiple databases collect different types of results of these studies. We developed a generic method that extracts a minimal set of common disease genes from any database containing mutations in genes and samples to a disease. The resulting minimal set can then be applied in enrichment analysis to predict if an arbitrary gene set is associated with the disease.

The method is based on finding a minimal set of genes that covers all samples in the database. Mathematically, the solution to this question is a set covering problem. As it is computationally infeasible to compute the exact solution, we use the greedy heuristic. It starts with the set covering the most elements and adds in each step the set covering the most still uncovered elements, breaking ties by choosing the set covering the most total elements. The algorithm traverses all remaining ties (same number of uncovered elements and same number of total covered elements), until 99% of all elements are covered.

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Results

To evaluate the validity of the approach on a biological dataset, the algorithm was applied to the Catalogue of Somatic Mutations in Cancer (COSMIC) [1]. The COSMIC has its origin in the census of human cancer genes [1]. It is a database of somatic mutations in cancer based on publications. The current COSMIC version (64) contains more than 800000 entries of mutations in more than 20000 genes for more than 180000 samples.

The algorithm found one solution containing 108 genes, resulting in one minimal set. Vogelstein et al [2] used a cancer-specific approach to identify Tumor suppressor genes and oncogenes from the COSMIC database. These Tumor suppressor genes and oncogenes were used as a positive control for our analysis. The minimal set found with our generic approach has a true positive rate of 88%, covering 72% of all tumor suppressor genes and 81% of all oncogenes from Vogelstein.

References

A model of the crosstalk between the Wnt and the IGF signaling pathways

Shuang Wang\textsuperscript{1}, Michael Kühl\textsuperscript{2} and Hans A. Kestler\textsuperscript{1}

The Wnt signaling pathway regulates various aspects of cellular processes, such as cell growth and differentiation. The IGF signaling pathway has been shown to tightly influence aging and longevity. Previous research suggests that several molecules function as regulators or downstream effectors which present in both signaling pathways. Signaling pathways are supposed to interact with each other, forming a more complex network. Thus, revealing the crosstalk between the Wnt and the IGF-1 signaling pathways can be helpful to understand aging and lifespan determination. The aim of this study is to establish mathematical multiscale models to analyze the mutual regulation of the Wnt signaling pathway and the IGF signaling pathways. Based on published results, we constructed an overview network of these two signaling pathways which showed that Yap, GSK-3b and Akt are potential nexuses for coupling the Wnt and the IGF signaling pathways. FoxO1 is a critical downstream effector of both pathways in the control of cell aging. The initial overview model can be extended by including stochastic effects, kinetics and time delays in the future.

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Investigation of Fuzzy Support Vector Machines

Markus Frey, Martin Schels, Michael Glodek, Sascha Meudt, Markus Kächele and Friedhelm Schwenker

In many pattern recognition applications, such as medical diagnosis, stress or affect recognition, the ground truth might be hidden. Labeling data sets in such scenarios is difficult, time consuming and error-prone, and therefore experts may disagree on class label of the given input data. The results are typically soft or fuzzy labels. In this study we investigate methods for handling this type of labeled data set. There are several approaches to model uncertainty in classification. Some classification methods - typically regression-based approaches - are suited to handle fuzzy or soft labeled data directly, for instance radial basis function neural networks or multi layer perceptrons. For other classifiers the standard training algorithm must be enhanced to obtain a fuzzy-input fuzzy-output behavior, for example the fuzzy Learning-Vector-Quantization classifier introduced in [1]. Here our aim is to study algorithms that are able to handle fuzzy labels in the training phase, and to compute a fuzzy label in the classification phase.

The fuzzy-input fuzzy-output support vector machine $F^2SV M$ introduced in [2] can be applied in such pattern recognition tasks, for example in [3] it is used for classification of voice qualities in spoken language. The quality of the voice refers to the timbre or coloring of a speaker’s voice, this is a typical pattern recognition task where fuzzy labels appear. As shown, in this case $F^2SM$ can outperform the standard SVM classifiers. In [4] the $F^2SM$ is investigated on different artificial datasets and the performance of the classifier is compared between fuzzy and hard input data. Furthermore, optimization in $l_1$ and $l_2$ sense is investigated to train parameters of a logistic transfer function in order to fuzzify the SVM’s output.

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References


A pragmatic procedure for stepwise feature selection

Anna Telaar and Carmen Theek

For classification studies like for example in biomarker research often high dimensional data sets are provided. The challenge is to find a small set of features out of this high dimensional setting which allows the classification of unknown samples into pre-defined groups with the greatest possible accuracy.

Many feature selection approaches exist facing this problem with different focus, but often these are very complex multivariate methods.

We propose a simple algorithm using a stepwise forward selection approach: As classification characteristics can be determined for all single features the AUC (area under curve) calculated within a ROC (receiver operating characteristic) analysis is chosen as the primary criterion for feature selection. Starting with the feature with the highest AUC, features are added successively which improve the classification within a logistic regression model. Selection is done with respect to the improvement in the AUC, and at the same time the new feature has to show a low correlation to the features selected previously.

This pragmatic procedure determines a feature set in a transparent way and does not require a complex theoretical statistical background or time consuming computational resources.

We apply our proposed approach on median fluorescence intensity data provided by the LumineX(R) xMAP technology for individual serum samples to identify biomarker candidates for stratification of diseases. This approach is compared to other feature selection techniques like $L_1$-penalized logistic regression and Random Forest. The sets of features selected and the accuracy of classification results are considered.

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Controlling false discoveries in high dimensional situations: Boosting with stability selection

Benjamin Hofner$^1$ and Michael Drey$^2$

Modern biotechnologies often result in high-dimensional data sets with much more variables than observations ($n >> p$). These data sets pose new challenges to statistical analysis: Variable selection becomes one of the most important tasks in this setting. Recently, Meinshausen and Bühlmann (2010) proposed a flexible framework for variable selection called stability selection. By the use of resampling procedures, stability selection adds a finite sample error control to high dimensional variable selection procedures such as Lasso or boosting. We consider the combination of boosting and stability selection and present results from a detailed simulation study that presents insights on the usefulness of this combination. Limitations will be discussed and guidance on the specification and tuning of stability selection will be given. The results will then be used for the analysis of an high dimensional data set. All methods are implemented in the R package mboost (Hofner et al., 2012; Hothorn et al., 2010, 2013).

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References


Information Theoretic Measures for Strategy Evaluation in Ant Colony Optimization

Gunnar Vökel\textsuperscript{1}, Markus Maucher\textsuperscript{2} and Hans A. Kestler\textsuperscript{2}

Ant Colony Optimization (ACO) is a meta-heuristic for combinatorial optimization problems. The main idea of ACO is that in each iteration a fixed number of solutions is constructed probabilistically based on a pheromone matrix which evolves between the iterations. When implementing an ACO algorithm for an optimization problem, several strategic implementation choices are left to the researcher. Those strategic choices include the decision on a pheromone update rule and the selection of parameters, e.g. the evaporation rate, the number of solutions constructed per iteration and the number of iterations. The evaluation of those choices often consists of average fitness comparisons of black box runs of the ACO algorithm on selected problem instances. We use information theoretic measures applied to the pheromone matrices of ACO algorithm runs on problem instances to evaluate strategic choices. The internal state of the ACO variants we consider consists of the pheromone matrix and the best-so-far solution. During one iteration of an ACO algorithm all probabilities for the construction choices are derived from the current pheromone matrix. Hence, the pheromone matrix corresponds to a set of random variables. We use the entropy of those random variables during the iterations as first measure of the internal state of the ACO algorithm. As a second measure we propose \( m \)-path entropy, i.e. the entropy of constructing a sequence of \( m \) solution components probabilistically. Those entropy measures indicate how much exploration is still possible in the corresponding iteration of the algorithm. This can be used to reason about the strategic choices. We compare ClassicACO and GB-ACO, two ACO variants introduced in \cite{2}, based on information theoretic measures. Furthermore, we compare the different choices for empty group punishment in GB-ACO.

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References


Subscan - a cluster algorithm for identifying statistically dense subspaces with application to biomedical data

Johann M. Kraus and Hans A. Kestler

Cluster analysis is an important technique of initial explorative data mining. Recent approaches in clustering aim at detecting groups of data points that exist in arbitrary, possibly overlapping subspaces. Generally, subspace clusters are neither exclusive nor exhaustive, i.e. subspace clusters can overlap as well as data points are not forced to participate in clusters. In this context subspace clustering supports the search for meaningful clusters by including dimensionality reduction in the clustering process. Subspace clustering can overcome drawbacks from searching groups in high-dimensional data sets, as often observed in clustering biological or medical data. In the context of microarray or next-generation sequencing data this refers to the hypothesis that only a small number of genes is responsible for different tumor subgroups.

We generalize the notion of scan statistics to multi-dimensional space and introduce a new formulation of subspace clusters as aggregated structures from dense intervals reported by single axis scans. We present a bottom-up algorithm to grow high-dimensional subspace clusters from one-dimensional statistically dense seed regions. Our approach objectifies the search for subspace clusters as the reported clusters are of statistical relevance and are not artifacts observed by chance. Our experiments demonstrate the applicability of the approach to both low-dimensional as well as high-dimensional data.
Power network clustering in modern protection systems

Sebastian Krey, Sebastian Brato, Uwe Ligges, Claus Weihs and Jürgen Götze

In modern interconnected power systems (often comprising whole continents) the protection against blackouts is a very complex task. The ongoing replacement of classical power plants with renewable energy provided by highly distributed and relatively small power stations introduces a lot of challenges to maintain the currently in Europe very high quality of the supply with electricity.

In case of an emergency the automatic protection systems in electricity networks divide the system into regions to limit the impact of a component failure to specific region. For a successful reaction it is necessary that the created regions have a balanced energy production and consumption. In times of renewable energies with a large production variation, the classical static defense plans can not always provide an acceptable solution (for example during the large European blackout in November 2006).

In this work we present methods to cluster the network graph of the electricity network into regions based on the current network topology and static information about the electrical characteristics of the network components. We will also present ideas to incorporate the results of a stability assessment of the network using dynamic measurements of voltage and frequency as well as the current power flow (energy production and consumption) into the clustering process. We will compare the results of these different methods on different test systems with each other and a manual clustering based on the expertise of an electrical engineer.

For the selection of a specific clustering result the compliance with regulatory conditions on quality and redundancy of the network is an important factor. We present the most important aspects of this question and how the presented methods perform in this regard.

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Reconstructing gene regulatory networks: deducing the coefficients of stochastic differential equations

Vito Baccelliere and Ulrich Stadtmüller

The reconstruction of the dependence structure in gene regulatory networks is one of the most challenging tasks in system biology. As shown by Gillespie (2007) and El Samad et al. (2005) randomness is a basic characteristic, when observing a small volume of reactants in a chemical reaction system, which can be described by SDEs (Stochastic Differential Equations). The modeling with SDEs captures the volatility of the system in a flexible way. But for a small sample size, which is the case for experimental datasets, the classical estimation techniques as e.g. Maximum-Likelihood are not feasible for a multi-dimensional system. In my talk I will present some stochastic modeling approaches of chemical reaction systems, motivating the use of SDEs for gene network analysis. And I will discuss some estimation methods for multivariate parametric SDEs.
References


A critical noise level for learning Boolean functions

Markus Maucher and Hans A. Kestler

The inference of gene regulatory systems from time series measurements is a challenging task to reveal the global functionality of a cell. Among several reconstruction methods Boolean networks have been successfully applied to such data. As time-resolved gene expression measurements at different stages of a cell are difficult and expensive, all reconstruction methods are faced with a relative small number of time points compared to the number of genes. In addition to this dimension problem, biological systems as well as measurement techniques are subject to noise.

In this work, we present an analysis of the reconstructability of Boolean networks in the case of noisy data. We introduce the notion of the critical noise level, a function characteristic which measures the complexity of the reconstruction of a function from noisy time series data. This measure constitutes a natural upper bound for the noise probability under which a function can still be reconstructed, but can also be incorporated into the reconstruction process to improve reconstruction results. We show how to efficiently compute the critical noise level of any given Boolean function and present experimental data that shows how it can be used to improve the best-fit extension algorithm for the reconstruction of a Boolean network from noisy time series data.

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References


Boosting sonographic birth weight prediction

Andreas Mayr¹, Florian Faschingbauer², Matthias Schmid¹

Sonographic measurements of the fetus are often used to predict birth weight as it is the most important indicator for possible complications during delivery. Statistical challenges in the modelling of these kind of prediction models include multicollinearity and variable selection. The aim of our investigation is to analyze if modern variable selection and regularization tools like component-wise boosting algorithms (Bu?hlmann and Hothorn, 2007), which can cope with both of those issues, can improve existing prediction formulas. We therefore consider boosting generalized additive models (GAM) as well as the recently proposed, more flexible gamboostLSS algorithm (Mayr et al., 2012) for boosting generalized additive models for location, scale and shape (GAMLSS). As distribution-free competitor we applied additive quantile regression boosting (Fenske et al., 2011).

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Automatic model selection and configuration for high dimensional survival analysis

Michel Lang, Bernd Bischl, Claus Weihs and Jörg Rahnenführer

Many different models for the analysis of high dimensional survival data have been developed over the past years. While some of the models and implementations come with internal parameter tuning automatisms, others require the user to accurately adjust defaults which often feels like a guessing game. Exhaustively trying out all model and parameter combinations will quickly become tedious or infeasible in high dimensional and computational intensive settings, even if parallelization is employed. Therefore, we propose to use modern algorithm configuration approaches to efficiently move through the hypothesis space. Two well-known methods for this purpose (which to our knowledge have not been applied to survival analysis before) are iterated F-racing [10] and sequential model-based optimization [6, 9]. In our presentation we will compare the different pros and cons of these two approaches for our problem at hand. In our application we study four lung cancer microarray datasets. For these, we select and configure a predictor based on four survival models in combination with six feature selection filters. As filter methods we consider: two literature based gene lists, two simple univariate scoring filters and two multivariate filters based on mRMR [4, 11] and nearest shrunken centroids [12], respectively. On the model side, we choose the cox proportional hazards model [3] on clinical covariates for reference purposes and compare to random survival forests [7, 8], boosted cox regression [1] and elastic net cox regression [5]. We optimize important hyperparameters of the filters and models with respect to their predictive performance. We parallelize our approaches with the BatchJobs R package [2]. Currently, our optimization targets each data set separately, but we also plan to configure models for multiple data sets in order to obtain predictors that perform well across the whole domain of lung cancer.
References


Exhaustive biomarker selection for small and medium sized datasets

Ludwig Lausser and Hans A. Kestler

Feature selection algorithms are essential for increasing the interpretability of a classification model. By removing distracting measurements, they reduce the search space to a subset of potentially, discriminatory features. Designed for feature spaces of high dimensionality state-of-the-art selection algorithms are based on heuristics that only evaluate a small number of feature combinations. Usually, such heuristic algorithms cannot guarantee to find a globally optimal feature set.

We present a feature selection algorithm based on the cross-validation accuracy of a $k$-Nearest Neighbor classifier. By taking advantage of the structure of this classifier, we can evaluate the quality of different feature sets in a highly efficient way. This allows for an exhaustive evaluation of all feature subsets of datasets of small or medium dimensionality in a reasonable time span. The current implementation of the algorithm can evaluate approximately 1,100,000 feature sets per minute in $10 \times 10$ cross-validations on a dataset of 100 samples (CPU: 3.2 GHz).

The method can be seen as a prototype of a fast exhaustive feature selection algorithm suitable for a variety of distances. By indexing all subspaces in an appropriate order, the scheme can be parallelized easily.

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Diversity Based Ensemble Pruning for Higher Interpretability.

Werner Adler¹, Zardad Khan², Sergej Potapov¹ and Berthold Lausen²

Bootstrap aggregated ensembles of classification trees often show improved classification performance compared to single trees (Breiman, 1996). This comes at the cost of less interpretability which is an important aspect e.g. in medical applications, where decisions regarding future treatment of patients have to be justified. Several methods exist to combine both, improved performance and larger interpretability. For example Node Harvest proposed by Meinshausen (2010) is characterized by its interpretability and competitive performance in various situations.

A high diversity between individual base classifiers is deemed to be important in the performance of an ensemble (Kuncheva & Whitaker, 2003). It is our aim to reduce the number of trees without reducing the diversity in the ensemble, resulting in higher interpretability with comparable performance. To obtain this goal, we examine several strategies to build sparse ensembles based on several diversity measurements. We report and discuss the results obtained using simulated data as well as example data.
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<table>
<thead>
<tr>
<th></th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>91-01</td>
<td>Ker-I Ko, P. Orponen, U. Schöning, O. Watanabe</td>
<td>Instance Complexity</td>
</tr>
<tr>
<td>91-02*</td>
<td>K. Gladitz, H. Fassbender, H. Vogler</td>
<td>Compiler-Based Implementation of Syntax-Directed Functional Programming</td>
</tr>
<tr>
<td>91-03*</td>
<td>Alfons Geser</td>
<td>Relative Termination</td>
</tr>
<tr>
<td>91-04*</td>
<td>J. Köbler, U. Schöning, J. Toran</td>
<td>Graph Isomorphism is low for PP</td>
</tr>
<tr>
<td>91-05</td>
<td>Johannes Köbler, Thomas Thierauf</td>
<td>Complexity Restricted Advice Functions</td>
</tr>
<tr>
<td>91-06*</td>
<td>Uwe Schöning</td>
<td>Recent Highlights in Structural Complexity Theory</td>
</tr>
<tr>
<td>91-07*</td>
<td>F. Green, J. Köbler, J. Toran</td>
<td>The Power of Middle Bit</td>
</tr>
<tr>
<td>91-08*</td>
<td>V. Arvind, Y. Han, L. Hamachandra, J. Köbler, A. Lozano, M. Mundhenk, A. Ogiwara, U. Schöning, R. Silvestri, T. Thierauf</td>
<td>Reductions for Sets of Low Information Content</td>
</tr>
<tr>
<td>92-01*</td>
<td>Vikraman Arvind, Johannes Köbler, Martin Mundhenk</td>
<td>On Bounded Truth-Table and Conjunctive Reductions to Sparse and Tally Sets</td>
</tr>
<tr>
<td>92-02*</td>
<td>Thomas Noll, Heiko Vogler</td>
<td>Top-down Parsing with Simulataneous Evaluation of Noncircular Attribute Grammars</td>
</tr>
<tr>
<td>92-03</td>
<td>Fakultät für Informatik</td>
<td>17. Workshop über Komplexitätstheorie, effiziente Algorithmen und Datenstrukturen</td>
</tr>
<tr>
<td>92-04*</td>
<td>V. Arvind, J. Köbler, M. Mundhenk</td>
<td>Lowness and the Complexity of Sparse and Tally Descriptions</td>
</tr>
<tr>
<td>92-05*</td>
<td>Johannes Köbler</td>
<td>Locating P/poly Optimally in the Extended Low Hierarchy</td>
</tr>
<tr>
<td>92-06*</td>
<td>Armin Kühnemann, Heiko Vogler</td>
<td>Synthesized and inherited functions -a new computational model for syntax-directed semantics</td>
</tr>
<tr>
<td>92-07*</td>
<td>Heinz Fassbender, Heiko Vogler</td>
<td>A Universal Unification Algorithm Based on Unification-Driven Leftmost Outermost Narrowing</td>
</tr>
</tbody>
</table>
92-08* Uwe Schöning
On Random Reductions from Sparse Sets to Tally Sets

92-09* Hermann von Hasseln, Laura Martignon
Consistency in Stochastic Network

92-10 Michael Schmitt
A Slightly Improved Upper Bound on the Size of Weights Sufficient to Represent Any Linearly Separable Boolean Function

92-11 Johannes Köbler, Seinosuke Toda
On the Power of Generalized MOD-Classes

92-12 V. Arvind, J. Köbler, M. Mundhenk
Reliable Reductions, High Sets and Low Sets

92-13 Alfons Geser
On a monotonic semantic path ordering

92-14* Joost Engelfriet, Heiko Vogler
The Translation Power of Top-Down Tree-To-Graph Transducers

93-01 Alfred Lupper, Konrad Froitzheim
AppleTalk Link Access Protocol basierend auf dem Abstract Personal Communications Manager

The COCOON Object Model

93-03 Thomas Thierauf, Seinosuke Toda, Osamu Watanabe
On Sets Bounded Truth-Table Reducible to P-selective Sets

93-04 Jin-Yi Cai, Frederic Green, Thomas Thierauf
On the Correlation of Symmetric Functions

93-05 K.Kuhn, M.Reichert, M. Nathe, T. Beuter, C. Heinlein, P. Dadam
A Conceptual Approach to an Open Hospital Information System

93-06 Klaus Gaßner
Rechnerunterstützung für die konzeptuelle Modellierung

93-07 Ullrich Keßler, Peter Dadam
Towards Customizable, Flexible Storage Structures for Complex Objects

94-01 Michael Schmitt
On the Complexity of Consistency Problems for Neurons with Binary Weights

94-02 Armin Kühnemann, Heiko Vogler
A Pumping Lemma for Output Languages of Attributed Tree Transducers

94-03 Harry Buhrman, Jim Kadin, Thomas Thierauf
On Functions Computable with Nonadaptive Queries to NP

94-04 Heinz Faßbender, Heiko Vogler, Andrea Wedel
Implementation of a Deterministic Partial E-Unification Algorithm for Macro Tree Transducers
94-05  V. Arvind, J. Köbler, R. Schuler  
On Helping and Interactive Proof Systems

94-06  Christian Kalus, Peter Dadam  
Incorporating record subtyping into a relational data model

94-07  Markus Tresch, Marc H. Scholl  
A Classification of Multi-Database Languages

94-08  Friedrich von Henke, Harald Rueß  
Arbeitstreffen Typtheorie: Zusammenfassung der Beiträge

Construction and Deduction Methods for the Formal Development of Software

94-10  Axel Dold  
Formalisierung schematischer Algorithmen

94-11  Johannes Köbler, Osamu Watanabe  
New Collapse Consequences of NP Having Small Circuits

94-12  Rainer Schuler  
On Average Polynomial Time

94-13  Rainer Schuler, Osamu Watanabe  
Towards Average-Case Complexity Analysis of NP Optimization Problems

94-14  Wolfram Schulte, Ton Vullinghs  
Linking Reactive Software to the X-Window System

94-15  Alfred Lupper  
Namensverwaltung und Adressierung in Distributed Shared Memory-Systemen

94-16  Robert Regn  
Verteilte Unix-Betriebssysteme

94-17  Helmuth Partsch  
Again on Recognition and Parsing of Context-Free Grammars: Two Exercises in Transformational Programming

94-18  Helmuth Partsch  
Transformational Development of Data-Parallel Algorithms: an Example

95-01  Oleg Verbitsky  
On the Largest Common Subgraph Problem

95-02  Uwe Schöning  
Complexity of Presburger Arithmetic with Fixed Quantifier Dimension

95-03  Harry Buhrman, Thomas Thierauf  
The Complexity of Generating and Checking Proofs of Membership

95-04  Rainer Schuler, Tomoyuki Yamakami  
Structural Average Case Complexity

95-05  Klaus Achatz, Wolfram Schulte  
Architecture Independent Massive Parallelization of Divide-And-Conquer Algorithms
95-06 Christoph Karg, Rainer Schuler
Structure in Average Case Complexity

95-07 P. Dadam, K. Kuhn, M. Reichert, T. Beuter, M. Nathe
ADEPT: Ein integrierender Ansatz zur Entwicklung flexibler, zuverlässiger kooperierender Assistsysteme in klinischen Anwendungsumgebungen

95-08 Jürgen Kehrer, Peter Schultess
Aufbereitung von gescannten Röntgenbildern zur filmlosen Diagnostik

95-09 Hans-Jörg Burtschick, Wolfgang Lindner
On Sets Turing Reducible to P-Selective Sets

95-10 Boris Hartmann
Berücksichtigung lokaler Randbedingung bei globaler Zieloptimierung mit neuronalen Netzen am Beispiel Truck Backer-Upper

95-11 Thomas Beuter, Peter Dadam:
Prinzipien der Replikationskontrolle in verteilten Systemen

95-12 Klaus Achatz, Wolfram Schulte
Massive Parallelization of Divide-and-Conquer Algorithms over Powerlists

95-13 Andrea Mößle, Heiko Vogler
Efficient Call-by-value Evaluation Strategy of Primitive Recursive Program Schemes

95-14 Axel Dold, Friedrich W. von Henke, Holger Pfeifer, Harald Rueß
A Generic Specification for Verifying Peephole Optimizations

96-01 Ercüment Canver, Jan-Tecker Gayen, Adam Moik
Formale Entwicklung der Steuerungssoftware für eine elektrisch ortsbediente Weiche mit VSE

96-02 Bernhard Nebel
Solving Hard Qualitative Temporal Reasoning Problems: Evaluating the Efficiency of Using the ORD-Horn Class

96-03 Ton Vullinghs, Wolfram Schulte, Thilo Schwinn
An Introduction to TkGofer

96-04 Thomas Beuter, Peter Dadam
Anwendungsspezifische Anforderungen an Workflow Management-Systeme am Beispiel der Domäne Concurrent-Engineering

96-05 Gerhard Schellhorn, Wolfgang Ahrendt
Verification of a Prolog Compiler - First Steps with KIV

96-06 Manindra Agrawal, Thomas Thierauf
Satisfiability Problems

96-07 Vikraman Arvind, Jacobo Torán
A nonadaptive NC Checker for Permutation Group Intersection

96-08 David Cyrluk, Oliver Möller, Harald Rueß
An Efficient Decision Procedure for a Theory of Fix-Sized Bitvectors with Composition and Extraction
Erfahrungen bei der Modellierung eingebetteter Systeme mit verschiedenen SA/RT-Ansätzen

Falk Bartels, Axel Dold, Friedrich W. von Henke, Holger Pfeifer, Harald Rueß
Formalizing Fixed-Point Theory in PVS

Axel Dold, Friedrich W. von Henke, Holger Pfeifer, Harald Rueß
Mechanized Semantics of Simple Imperative Programming Constructs

Axel Dold, Friedrich W. von Henke, Holger Pfeifer, Harald Rueß
Generic Compilation Schemes for Simple Programming Constructs

Klaus Achatz, Helmut Partsch
From Descriptive Specifications to Operational ones: A Powerful Transformation Rule, its Applications and Variants

Jochen Messner
Pattern Matching in Trace Monoids

Wolfgang Lindner, Rainer Schuler
A Small Span Theorem within P

Thomas Bauer, Peter Dadam
A Distributed Execution Environment for Large-Scale Workflow Management Systems with Subnets and Server Migration

Christian Heinlein, Peter Dadam
Interaction Expressions - A Powerful Formalism for Describing Inter-Workflow Dependencies

Vikraman Arvind, Johannes Köbler
On Pseudorandomness and Resource-Bounded Measure

Gerhard Partsch
Punkt-zu-Punkt- und Mehrpunkt-basierende LAN-Integrationsstrategien für den digitalen Mobilfunkstandard DECT

Manfred Reichert, Peter Dadam
ADEPT flex - Supporting Dynamic Changes of Workflows Without Loosing Control

Hans Braxmeier, Dietmar Ernst, Andrea Mößle, Heiko Vogler
The Project NoName - A functional programming language with its development environment

Christian Heinlein
Grundlagen von Interaktionsausdrücken

Christian Heinlein
Graphische Repräsentation von Interaktionsausdrücken

Christian Heinlein
Sprachtheoretische Semantik von Interaktionsausdrücken
97-12 Gerhard Schellhorn, Wolfgang Reif
Proving Properties of Finite Enumerations: A Problem Set for Automated Theorem Provers

97-13 Dietmar Ernst, Frank Houdek, Wolfram Schulte, Thilo Schwinn
Experimenteller Vergleich statischer und dynamischer Softwareprüfung für eingebettete Systeme

97-14 Wolfgang Reif, Gerhard Schellhorn
Theorem Proving in Large Theories

97-15 Thomas Wennekers
Asymptotik rekurrenter neuronaler Netze mit zufälligen Kopplungen

97-16 Peter Dadam, Klaus Kuhn, Manfred Reichert
Clinical Workflows - The Killer Application for Process-oriented Information Systems?

97-17 Mohammad Ali Livani, Jörg Kaiser
EDF Consensus on CAN Bus Access in Dynamic Real-Time Applications

97-18 Johannes Köbler, Rainer Schuler
Using Efficient Average-Case Algorithms to Collapse Worst-Case Complexity Classes

98-01 Daniela Damm, Lutz Claes, Friedrich W. von Henke, Alexander Seitz, Adelinde Uhrmacher, Steffen Wolf
Ein fallbasiertes System für die Interpretation von Literatur zur Knochenheilung

98-02 Thomas Bauer, Peter Dadam
Architekturen für skalierbare Workflow-Management-Systeme - Klassifikation und Analyse

98-03 Marko Luther, Martin Strecker
A guided tour through Typelab

98-04 Heiko Neumann, Luiz Pessoa
Visual Filling-in and Surface Property Reconstruction

98-05 Ercüment Canver
Formal Verification of a Coordinated Atomic Action Based Design

98-06 Andreas Küchler
On the Correspondence between Neural Folding Architectures and Tree Automata

98-07 Heiko Neumann, Thorsten Hansen, Luiz Pessoa
Interaction of ON and OFF Pathways for Visual Contrast Measurement

98-08 Thomas Wennekers
Synfire Graphs: From Spike Patterns to Automata of Spiking Neurons

98-09 Thomas Bauer, Peter Dadam
Variable Migration von Workflows in ADEPT

98-10 Heiko Neumann, Wolfgang Sepp
Recurrent V1 – V2 Interaction in Early Visual Boundary Processing
Frank Houdek, Dietmar Ernst, Thilo Schwinn
Prüfen von C–Code und Statmate/Matlab–Spezifikationen: Ein Experiment

Gerhard Schellhorn
Proving Properties of Directed Graphs: A Problem Set for Automated Theorem Provers

Gerhard Schellhorn, Wolfgang Reif
Theorems from Compiler Verification: A Problem Set for Automated Theorem Provers

Mohammad Ali Livani
SHARE: A Transparent Mechanism for Reliable Broadcast Delivery in CAN

Mohammad Ali Livani, Jörg Kaiser
Predictable Atomic Multicast in the Controller Area Network (CAN)

Susanne Boll, Wolfgang Klas, Utz Westermann
A Comparison of Multimedia Document Models Concerning Advanced Requirements

Thomas Bauer, Peter Dadam
Verteilungsmodelle für Workflow-Management-Systeme - Klassifikation und Simulation

Uwe Schöning
On the Complexity of Constraint Satisfaction

Ercument Canver
Model-Checking zur Analyse von Message Sequence Charts über Statecharts

Johannes Köbler, Wolfgang Lindner, Rainer Schuler
Derandomizing RP if Boolean Circuits are not Learnable

Utz Westermann, Wolfgang Klas
Architecture of a DataBlade Module for the Integrated Management of Multimedia Assets

Peter Dadam, Manfred Reichert

Vikraman Arvind, Johannes Köbler
Graph Isomorphism is Low for ZPP^{NP} and other Lowness results

Thomas Bauer, Peter Dadam
Efficient Distributed Workflow Management Based on Variable Server Assignments

Thomas Bauer, Peter Dadam
Variable Serverzuordnungen und komplexe Bearbeiterzuordnungen im Workflow-Management-System ADEPT

Gregory Baratoff, Christian Toepfer, Heiko Neumann
Combined space-variant maps for optical flow based navigation
<table>
<thead>
<tr>
<th>Year</th>
<th>Title</th>
<th>Authors</th>
</tr>
</thead>
<tbody>
<tr>
<td>2000-04</td>
<td>Ein Rahmenwerk zur Einführung von Leistungspunktsystemen</td>
<td>Wolfgang Gehring</td>
</tr>
<tr>
<td>2000-05</td>
<td>Intelligent Prefetching and Buffering for Interactive Streaming of MPEG Videos</td>
<td>Susanne Boll, Christian Heinlein, Wolfgang Klas, Jochen Wandel</td>
</tr>
<tr>
<td>2000-06</td>
<td>Fehlersuche in Formalen Spezifikationen</td>
<td>Wolfgang Reif, Gerhard Schellhorn, Andreas Thums</td>
</tr>
<tr>
<td>2000-08</td>
<td>Effiziente Durchführung von Prozessmigrationen in verteilten Workflow-Management-Systemen</td>
<td>Thomas Bauer, Manfred Reichert, Peter Dadam</td>
</tr>
<tr>
<td>2000-09</td>
<td>Vermeidung von Überlastsituationen durch Replikation von Workflow-Servern in ADEPT</td>
<td>Thomas Bauer, Peter Dadam</td>
</tr>
<tr>
<td>2000-10</td>
<td>Adaptives und verteiltes Workflow-Management</td>
<td>Thomas Bauer, Manfred Reichert, Peter Dadam</td>
</tr>
<tr>
<td>2000-11</td>
<td>Workflow and Process Synchronization with Interaction Expressions and Graphs</td>
<td>Christian Heinlein</td>
</tr>
<tr>
<td>2001-01</td>
<td>DNA-based parallel computation of simple arithmetic</td>
<td>Hubert Hug, Rainer Schuler</td>
</tr>
<tr>
<td>2001-02</td>
<td>3-D Visual Object Classification with Hierarchical Radial Basis Function Networks</td>
<td>Friedhelm Schwenker, Hans A. Kestler, Günther Palm</td>
</tr>
<tr>
<td>2001-03</td>
<td>RBF network classification of ECGs as a potential marker for sudden cardiac death</td>
<td>Hans A. Kestler, Friedhelm Schwenker, Günther Palm</td>
</tr>
<tr>
<td>2001-04</td>
<td>Classification of Bioacoustic Time Series Utilizing Pulse Detection, Time and Frequency Features and Data Fusion</td>
<td>Christian Dietrich, Friedhelm Schwenker, Klaus Riede, Günther Palm</td>
</tr>
<tr>
<td>2002-01</td>
<td>Effiziente Verträglichkeitsprüfung und automatische Migration von Workflow-Instanzen bei der Evolution von Workflow-Schemata</td>
<td>Stefanie Rinderle, Manfred Reichert, Peter Dadam</td>
</tr>
<tr>
<td>2002-02</td>
<td>Deriving an Applicative Heapsort Algorithm</td>
<td>Walter Guttmann</td>
</tr>
<tr>
<td>2003-01</td>
<td>A Formal Framework for Workflow Type and Instance Changes Under Correctness Checks</td>
<td>Manfred Reichert, Stefanie Rinderle, Peter Dadam</td>
</tr>
<tr>
<td>2003-02</td>
<td>Supporting Workflow Schema Evolution By Efficient Compliance Checks</td>
<td>Stefanie Rinderle, Manfred Reichert, Peter Dadam</td>
</tr>
<tr>
<td>Year</td>
<td>Authors</td>
<td>Title</td>
</tr>
<tr>
<td>-------</td>
<td>----------------------------------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>2003-03</td>
<td>Christian Heinlein</td>
<td>Safely Extending Procedure Types to Allow Nested Procedures as Values</td>
</tr>
<tr>
<td>2003-05</td>
<td>Christian Heinlein</td>
<td>Dynamic Class Methods in Java</td>
</tr>
<tr>
<td>2003-06</td>
<td>Christian Heinlein</td>
<td>Vertical, Horizontal, and Behavioural Extensibility of Software Systems</td>
</tr>
<tr>
<td>2003-07</td>
<td>Christian Heinlein</td>
<td>Safely Extending Procedure Types to Allow Nested Procedures as Values  (Corrected Version)</td>
</tr>
<tr>
<td>2003-08</td>
<td>Changling Liu, Jörg Kaiser</td>
<td>Survey of Mobile Ad Hoc Network Routing Protocols</td>
</tr>
<tr>
<td>2004-01</td>
<td>Thom Frühwirth, Marc Meister (eds.)</td>
<td>First Workshop on Constraint Handling Rules</td>
</tr>
<tr>
<td>2004-03</td>
<td>Susanne Biundo, Thom Frühwirth, Günther Palm (eds.)</td>
<td>Poster Proceedings of the 27th Annual German Conference on Artificial Intelligence</td>
</tr>
<tr>
<td>2005-01</td>
<td>Armin Wolf, Thom Frühwirth, Marc Meister (eds.)</td>
<td>19th Workshop on (Constraint) Logic Programming</td>
</tr>
<tr>
<td>2005-02</td>
<td>Wolfgang Lindner (Hg.), Universität Ulm, Christopher Wolf (Hg.) KU Leuven</td>
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