Selected Parallel and Scalable Methods for Scientific Big Data Analytics

Dr.-Ing. Morris Riedel et al.
Research Group Leader, Juelich Supercomputing Centre
Adjunct Associated Professor, University of Iceland

ZIH Kolloquium, 21th May 2015
Technical University of Dresden
## Research Centre Juelich

### JUELICH in Numbers

- **Area:** 2.2 km²
- **Staff:** 5236
  - Scientists: 1658
  - Technical staff: 1662
  - Trainees: 303
- **Budget:** 557 Mio. €
  - incl. 172 Mio. € third party funding

**Located in Germany, Koeln – Aachen Area**

### Institutes at JUELICH

- Institute of Complex Systems
- Institute for Advanced Simulation
- Juelich Supercomputing Center
- Juelich Center for Neutron Science
- Peter-Grünberg Institute
- Institute for Neuroscience and Medicine
- Institute for Nuclear Physics
- Institute for Bio and Geosciences
- Institute for Energy and Climate Research
- Central Institute for Engineering, Electronics, and Analytics

### Research for generic key technologies of the next generation

**Scientific & Engineering Application-driven Problem Solving**

Contact: m.riedel@fz-juelich.de
University of Iceland

Schools of the University
- School of Education
- School of Humanities
- School of Engineering and Natural Sciences
- School of Social Sciences
- School of Health Sciences
- Interdisciplinary Studies

Faculties of the School
- Civil and Environmental Engineering
- Earth Sciences
- Electrical and Computer Engineering
- Industrial Engineering
- Mechanical Engineering
- Computer Science
- Life and Environmental Sciences
- Physical Sciences

Full programmes taught in English
Staff: ~1259
Students: ~14,000
Located in Reykjavik Capital Center, Iceland

Teaching of key technologies in engineering & sciences

University Courses: Statistical Data Mining & HPC-A/B
Outline
Outline

- Data Analytics @ Juelich
  - Driven by Scientific & Engineering Demands
  - Understanding of Terms & Key Focus
- Scalable & Parallel Tools
  - Clustering – DBSCAN
  - Classification – SVM
  - Scientific Applications in Context
- Recent Research Directions
  - ‘Brain Analytics‘
  - Deep Learning
- Conclusions
  - References & Backup Slides
Data Analytics @ Juelich
Data Analytics – Context JSC

- Research data-intensive science and engineering applications
- Explore computing that is more intertwined with data analysis

- Tackle Inverse Problems
- Sharing, re-use, towards reproducibility
‘Data Analytics’ is an ‘interesting mix’ of different approaches

- Analytics: Whole methodology; Analysis: data investigation process itself
- ‘Big’ requires scalable processing methods and underlying infrastructure

Concrete ‘big data’: large medical data

Concrete ‘big data’: large earth science data

- Regression++
- Classification++
- Clustering++
- Parallel Data Analytics
- Data Mining Methods
- Scientific Community Applications
- Generic Data Methods
- Machine Learning Algorithms
- Data Analysis Tools
- Data Science

JSC: Data Analytics: m.riedel@fz-juelich.de
Data Analytics – Research Key Focus

Scientific Computing

Scientific Applications using ‘Big Data’
- Traditional Scientific Computing Methods
- HPC and HTC Paradigms & Parallelization
- Emerging Data Analytics Approaches
- Optimized Data Access & Management
- Statistical Data Mining & Machine Learning
- Inverse Problems & their Research Questions

‘Big Data’ Methods

Scientific Applications

‘(Big) Data from various data science applications’

Systematic & Automated Analytics guided by CRISP – DM

Classification++
Clustering++
Regression++
Data Analytics – Selected Research Group Activities

John von Neumann Institute for Computing (NIC)
- Peer-review of scientific big data analytics (SBDA) proposals
- Jointly work with SBDA users (first projects starting, prototyping process)

Research Data Alliance (RDA)
- Chairing activities of the Big Data Analytics Interest Group
- Collaboration with a variety of EU and US partners
- Geoffrey Fox, UoIndiana (map-reduce), Kuo Kwo-Sen (NASA, SciDB)

Smart Data Innovation Lab (SDIL)
- Driving activities in the personalised medicine community (with Bayer)
- Collaboration with partners from industry (e.g. IBM, SAP, Siemens, etc.)
Data Analytics – Selected Research Expertise

Key expertise making algorithms parallel & scalable for ‘big data’

- Driven by scientific and engineering cases, e.g. understanding the human brain, remote sensing applications, marine measurements analysis, …
- Automate and/or support the data analysis process
- Example codes: Density-based Spatial Clustering of Applications with Noise (DBSCAN), Support Vector Machines (SVMs),

Parallel & Scalable DBSCAN clustering tool
Parallel & Scalable SVM classification tool

Problem: Automatic outlier detection for data quality
- Tailor solution for community
- Scalability towards Big Data
- Design and improve automatic data analytics approaches

Problem: Classification of buildings from multi-spectral images
- Enable smooth transition from ‘manual Matlab SVM scripts’
- Research on parallel SVM methods (map-reduce, HPC)


JSC: Data Analytics: m.riedel@fz-juelich.de
Scalable & Parallel Tools: Clustering
Learning From Data – Clustering Technique

**Classification**
- Groups of data exist
- New data classified to existing groups

**Clustering**
- No groups of data exist
- Create groups from data close to each other

**Regression**
- Identify a line with a certain slope describing the data
Selected Clustering Methods

K-Means Clustering – Centroid based clustering
- Partitions a data set into K distinct clusters (centroids can be artificial)

K-Medoids Clustering – Centroid based clustering (variation)
- Partitions a data set into K distinct clusters (centroids are actual points)

Sequential Agglomerative hierarchic nonoverlapping (SAHN)
- Hierarchical Clustering (create tree-like data structure → ‘dendrogram’)

Clustering Using Representatives (CURE)
- Select representative points / cluster; as far from one another as possible

Density-based spatial clustering of applications + noise (DBSCAN)
- Reasoning: density similarity measure helpful in our driving applications
- Assumes clusters of similar density or areas of higher density in dataset
## Technology Review of Open & Available Tools

<table>
<thead>
<tr>
<th>Technology</th>
<th>Platform</th>
<th>Approach</th>
<th>Analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>HPDBSCAN (authors implementation)</td>
<td>C; MPI; OpenMP</td>
<td>Parallel, hybrid, DBSCAN</td>
<td></td>
</tr>
<tr>
<td>Apache Mahout</td>
<td>Java; Hadoop</td>
<td>K-means variants, spectral, no DBSCAN</td>
<td></td>
</tr>
<tr>
<td>Apache Spark/MLlib</td>
<td>Java; Spark</td>
<td>Only k-means clustering, No DBSCAN</td>
<td></td>
</tr>
<tr>
<td>scikit-learn</td>
<td>Python</td>
<td>No parallelization strategy for DBSCAN</td>
<td></td>
</tr>
<tr>
<td>Northwestern University PDSDBSCAN-D</td>
<td>C++; MPI; OpenMP</td>
<td>Parallel DBSCAN</td>
<td></td>
</tr>
</tbody>
</table>

*M. Goetz, M. Riedel et al., 6th Workshop on Data Mining in Earth System Science, International Conference of Computational Science (ICCS), Reykjavik, to be published*
Parallel & Scalable DBSCAN MPI/OpenMP Tool (1)

DBSCAN Algorithm

- Groups number of similar points into clusters of data
- Similarity is defined by a distance measure (e.g. euclidean distance)

Distinct Algorithm Features

- Clusters a variable number of clusters
- Forms arbitrarily shaped clusters
- Identifies outliers/noise

Understanding Parameters for MPI/OpenMP tool

- Looks for a similar points within a given search radius → Parameter *epsilon*
- A cluster consist of a given minimum number of points → Parameter *minPoints*

Parallel & Scalable DBSCAN MPI/OpenMP Tool (2)

Parallelization Strategy
- Smart ‘Big Data‘ Preprocessing into Spatial Cells
- OpenMP standalone
- MPI (+ optional OpenMP hybrid)

Preprocessing Step
- Spatial indexing and redistribution according to the point localities
- Data density based chunking of computations

Computational Optimizations
- Caching of point neighborhood searches
- Cluster merging based on comparisons instead of zone reclustering

Performance Comparisons

- With another open-source parallel DBSCAN implementation (aka ‘NWU’)
- 3,705,635 data points (2 dimensions)
- Use of Hierarchical Data Format (HDF) v.5 for scalable input/output of ‘big data’

Parallel & Scalable DBSCAN MPI/OpenMP Tool (4)

Selected ‘Big Data‘ Applications

- London twitter data (goal: find density centers of tweets)
- Bremen thermo point cloud data (goal: noise reduction)
- PANGAEA earth science datasets (goal: automated outlier detection)

<table>
<thead>
<tr>
<th>Computation time</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
<th>32</th>
</tr>
</thead>
<tbody>
<tr>
<td>JSC-HPDBSCAN</td>
<td>117,18 s</td>
<td>59,64 s</td>
<td>30,68 s</td>
<td>16,25 s</td>
<td>10,86 s</td>
<td>9,39 s</td>
</tr>
<tr>
<td>NWU-PDSDBSCAN</td>
<td>288,35 s</td>
<td>162,47 s</td>
<td>105,94 s</td>
<td>89,87 s</td>
<td>85,37 s</td>
<td>88,42 s</td>
</tr>
<tr>
<td>Speed-Up</td>
<td>1,00 x</td>
<td>1,96 x</td>
<td>3,82 x</td>
<td>7,21 x</td>
<td>10,79 x</td>
<td>12,48 x</td>
</tr>
<tr>
<td>Memory</td>
<td>251,064 MB</td>
<td>345,276 MB</td>
<td>433,340 MB</td>
<td>678,248 MB</td>
<td>1,101 GB</td>
<td>2,111 GB</td>
</tr>
<tr>
<td></td>
<td>500,512 MB</td>
<td>725,104 MB</td>
<td>1,370 GB</td>
<td>4,954 GB</td>
<td>19,724 GB</td>
<td>59,685 GB</td>
</tr>
</tbody>
</table>
Parallel & Scalable DBSCAN MPI/OpenMP Tool (5)

Free tool available
- Public bitbucket account – open-source
- Tool Website with more information
- Maintained on best effort basis

Usage via simple jobscripts

Usage
- module load hdf5/1.8.13
- mpiexec -np 1 ./dbscan -e 300 -m 100 -t 12 bremenSmall.h5

Parameter
- epsilon
- minPoints


3D Point Cloud of Bremen/Germany
Parallel & Scalable DBSCAN MPI/OpenMP Tool (6)

Usage via jobs script

- Using MOAB job scheduler
- Important: module load hdf5/1.8.13
- Important: library gcc-4.9.2/lib64
- np = number of processors
- t = number of threads

```bash
mriedel@judge:/home/zam/analytic/bigdata/hpdbscan/jsc_mpi/mriruns> more datajobscript.sh
#!/bin/bash
#MSUB -N HPDBSCAN_BremenSmall_1_12
#MSUB -l nodes=1:ppn=12:gpus=0:performance
#MSUB -l walltime=00:03:00
#MSUB -M m.riedel@fz-juelich.de
#MSUB -m abe
#MSUB -v tpt=12
#MSUB -v vmem=64gb
#MSUB -q devel

module load hdf5/1.8.13
export LD_LIBRARY_PATH=/home/zam/analytic/bigdata/hpdbscan/gcc-4.9.2/lib64:$LD_LIBRARY_PATH
DBSCAN=/home/zam/analytic/bigdata/hpdbscan/jsc_mpi/dbscan
SMALLBREMEMDATA=/home/zam/analytic/bigdata/hpdbscan/jsc_mpi/mriruns/bremenSmall.h5

cd /home/zam/analytic/bigdata/hpdbscan/jsc_mpi/mriruns
mpilexec -np 1 $DBSCAN -e 300 -m 100 -t 12 $SMALLBREMEMDATA
```
Parallel & Scalable DBSCAN MPI/OpenMP Tool (7)

Output with various information

- Run-times of different stages
- Clustering task information (e.g. number of identified clusters)
- Noise identification
- Data volume (small Bremen): ~72 MB
- Data volume (large Bremen): ~1.9 GB

```
mriedel@judge:/home/zam/analytic/bigdata/hpdbscan/jsc_mpi/mriruns> more HPDBSCAN_BremenSmall_1_12.0220066
Calculating Cell Space...
  Computing Dimensions... [OK] in 0.011853
  Computing Cells... [OK] in 0.073445
  Sorting Points... [OK] in 0.124476
  Distributing Points... [OK] in 0.060060

DBSCAN...
  Local Scan... I am ready 0
  in 90.006330 [OK] in 90.006364
  Merging Neighbors... [OK] in 0.000000
  Adjust Labels... [OK] in 0.004972
  Rec. Init. Order... [OK] in 1.255420
  Writing File... [OK] in 0.019120

Result...
  65 Clusters
  2973821 Cluster Points
  26179 Noise Points
  2953129 Core Points

Took: 92.214843s
```

Output results written in same input data:
cluster number & noise label (depends on parameters)
Visualization Example

- Using Point Cloud Library (PDL) toolset
- Transformation of Data to PCD format (python script on the right)

Usage

- python H5toPCD.py bremenSmall.h5
- pcl_viewer bremenClustered.pcd
Earth Science Application
‘Automated outlier detection in time series’

- Collaboration with MARUM, Bremen (work in progress)
- Example: water quality data of Koljoefjords
- Connected underwater device
- Measurements: oxygen, temperature, salinity, ...

Use of HPBSCAN algorithm

- Detect outliers and anomalies/events
- Compare with manually annotated data by domain-scientist
- Needs automation
Neuroscience Application

‘Cell nuclei detection and tissue clustering’
- Scientific Case: Detect various layers (colored)
- Layers seem to have different density distribution of cells
- Extract cell nuclei into 2D/3D point cloud
- Cluster different brain areas by cell density

Use of HPBSCAN algorithm
- First 2d results detect various clusters
- Work in progress, not very good results
- Approach: Several iterations (with 3D) with potentially different parameter values
- Investigate other methods (e.g. OPTICS)

➢ Research activities jointly with T. Dickscheid et al. (Juelich Institute of Neuroscience & Medicine)
Parallel & Scalable DBSCAN MPI/OpenMP Tool (11)

Neuroscience Application – Work in progress (e.g. 3120x3288)  
‘Cell nuclei detection and tissue clustering’ – varying parameters

Research activities jointly with T. Dickscheid et al. (Juelich Institute of Neuroscience & Medicine)
Scalable & Parallel Tools: Classification
Learning From Data – Classification Technique

Classification
- Groups of data exist
- New data classified to existing groups

Clustering
- No groups of data exist
- Create groups from data close to each other

Regression
- Identify a line with a certain slope describing the data
Selected Classification Methods

Perceptron Learning Algorithm – simple linear classification
- Enables binary classification with ‘a line’ between classes of separable data

Support Vector Machines (SVMs) – non-linear (‘kernel‘) classification
- Enables non-linear classification with maximum margin (best ‘out-of-the-box’)
  
  Reasoning: achieves often better results than other methods in remote sensing application

Decision Trees & Ensemble Methods – tree-based classification
- Grows trees for class decisions, ensemble methods average n trees

Artificial Neural Networks (ANNs) – brain-inspired classification
- Combine multiple linear perceptrons to a strong network for non-linear tasks

Naive Bayes Classifier – probabilistic classification
- Use of the Bayes theorem with strong/naive independence between features
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<tr>
<td>Apache Spark/MLlib</td>
<td>Java; Spark</td>
<td>Parallel linear SVMs (no multi-class)</td>
<td></td>
</tr>
<tr>
<td>Twister/ParallelSVM</td>
<td>Java; Twister; Hadoop 1.0</td>
<td>Parallel SVMs, open source; developer version 0.9 beta</td>
<td></td>
</tr>
<tr>
<td>scikit-learn</td>
<td>Python</td>
<td>No parallelization strategy for SVMs</td>
<td></td>
</tr>
<tr>
<td>piSVM 1.2 &amp; piSVM 1.3</td>
<td>C; MPI</td>
<td>Parallel SVMs; stable; not fully scalable</td>
<td></td>
</tr>
<tr>
<td>GPU LibSVM</td>
<td>CUDA</td>
<td>Parallel SVMs; hard to programs, early versions</td>
<td></td>
</tr>
<tr>
<td>pSVM</td>
<td>C; MPI</td>
<td>Parallel SVMs; unstable; beta version</td>
<td></td>
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*M. Goetz, M. Riedel et al., 6th Workshop on Data Mining in Earth System Science, International Conference of Computational Science (ICCS), Reykjavik, to be published*
SVM Algorithm Approach

- Introduced 1995 by C. Cortes & V. Vapnik et al.
- Creates a ‘maximal margin classifier‘ to get future points (‘more often‘) right
- Uses quadratic programming & Lagrangian method with $N \times N$

\[ \min_{w,\xi,b} \left\{ \frac{1}{2} \|w\|^2 + C \sum_i \xi_i \right\} \]
\[ y_i (w \cdot x_i - b) \geq 1 - \xi_i, \quad \xi_i \geq 0 \]

(maximizing hyperplane turned into optimization problem, minimization, dual problem)

(kernel trick, quadratic coefficients – Computational Complexity & Big Data Impact)
Parallel & Scalable SVM MPI Tool (2)

- True Support Vector Machines are Support Vector Classifiers combined with a non-linear kernel
- Non-linear kernels exist - mostly known are polynomial & Radial Basis Function (RBF) kernels

Understanding the MPI tool parameters
- Selecting non-linear kernel function K type as RBF \( \rightarrow \) parameter \(-t 2\)
- Setting RBF Kernel configuration parameter \( \gamma \) \( \rightarrow \) e.g. parameter \(-g 16\)
- Setting SVM allowed errors parameter \( \rightarrow \) e.g. parameter \(-c 10000\)

Major benefit of Kernels: Computing done in original space
- Linear Kernel
  \[ K(x_i, x_i') = \sum_{j=1}^{p} x_{ij}x_{i'j} \] (linear in features)
- Polynomial Kernel
  \[ K(x_i, x_i') = (1 + \sum_{j=1}^{p} x_{ij}x_{i'j})^d \] (polynomial of degree \(d\))
- RBF Kernel
  \[ K(x_i, x_i') = \exp(-\gamma \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2) \] (large distance, small impact)
Parallel & Scalable SVM MPI Tool (3)

Original parallel piSVM tool 1.2
- Open-source and based on libSVM library, C, 2011
- Message Passing Interface (MPI)
- New version appeared 2014-10 v. 1.3 (no major improvements)
- Lack of ‘big data‘ support (memory, layout, etc.)

Tuned scalable parallel piSVM tool 1.2.1
- Open-source (repository to be created)
- Based on piSVM tool 1.2
- Optimizations: load balancing; MPI collectives
- Contact: m.richerzhagen@fz-juelich.de

Parallel & Scalable SVM MPI Tool (4)

Sattelite Data (Quickbird)
Parallel Support Vector Machines (SVM)
HPC / MPI

Classification Study of Land Cover Types

<table>
<thead>
<tr>
<th>Class</th>
<th>Training</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>Buildings</td>
<td>18126</td>
<td>163129</td>
</tr>
<tr>
<td>Blocks</td>
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<td>98834</td>
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<td>81792</td>
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<tr>
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<td>73144</td>
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<tr>
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<td>13551</td>
</tr>
<tr>
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<td>43124</td>
</tr>
<tr>
<td>Total</td>
<td>77542</td>
<td>697859</td>
</tr>
</tbody>
</table>

"Reference Data Analytics“ for reusability & learning

CRISP-DM Report
Openly Shared Datasets
Running Analytics Code

[10] Rome Image dataset
Parallel & Scalable SVM MPI Tool (5)

Example dataset: Geographical location: Image of Rome, Italy

- Remote sensor data obtained by Quickbird satellite

High-resolution (0.6m) panchromatic image

Pansharpened (UDWT) low-resolution (2.4m) multispectral images
Labelled data available for train/test data

- Groundtruth data of 9 different land-cover classes available

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Data preparation

- We generated a set of training samples by randomly selecting 10% of the reference samples (with labelled data)
- Generated set of test samples from the remaining labels (labelled data, 90% of reference samples)
Based on ‘LibSVM data format’ (using feature extraction method)

- Add ‘Self-Dual Attribute Profile (SDAP) on Area’ on all images training file

```
Class Feature
1 1:0.105882 2:0.109804 3:0.101961 ........ 54:0.121569 55:0.130952
2 1:0.364706 2:0.360784 3:0.356863 ........ 54:0.356863 55:0.349206
6 1:0.152941 2:0.34902 3:0.454902 ........ 54:0.466667 55:0.460317
........
........
........
........
9 1:0.247059 2:0.247059 3:0.227451 ........ 54:0.227451 55:0.218254
7 1:0.411765 2:0.411765 3:0.415686 ........ 54:0.415686 55:0.40873
```

Each line is a training vector with gray levels

Number Feature
Class
Gray Level

Area
Std Dev
Moment of Inertia

[10] Rome Image dataset

Usage via jobscript

- Using MOAB job scheduler
- \( np \) = number of processors; o/q partitioning

```bash
#!/bin/bash
#MOAB -N Train-tune-rec06-4-16-32
#MOAB -l nodes=4:ppn=16:performance
#MOAB -l walltime=03:00:00
#MOAB -M m.riedel@fz-juelich.de
#MOAB -m abc
#MOAB -W x=naccesspolicy:singlejob
#MOAB -v tpt=2
#MOAB -q devo1

### jobscript
cd $PBS_O_WORKDIR
echo "workdir: $PBS_O_WORKDIR"

NSLOTS=32
echo "running on $NSLOTS cpus..."

### location
PISVM=/home/m/riedel/pisvm-1.2/pisvm-1.2/pisvm-train

TRAINDATA=/home/m/riedel/bigdata/86-rome06/sdap_area_all_training.sl

### submit
mpiexec -np $NSLOTS $PISVM -o 1024 -q 512 -e 10000 -g 16 -t 2 -m
1024 -a 0 $TRAINDATA
```

→ Usage via simple jobscripts

SVM Parameters

[12] Rome Analytics Results & job scripts
Training speed-up is possible when number of features is ‘high’

- Serial Matlab: ~1277 sec (~21 minutes)
- Parallel (16) Analytics: 220 sec (3:40 minutes)
- Accuracy remains

Training vector
- 77542 samples
Another more challenging dataset: high number of classes

- Parallelization challenges: unbalanced class representations

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<td>number</td>
<td>name</td>
<td>training</td>
<td>test</td>
</tr>
<tr>
<td>1</td>
<td>Buildings</td>
<td>1720</td>
<td>15475</td>
</tr>
<tr>
<td>2</td>
<td>Corn</td>
<td>1778</td>
<td>16005</td>
</tr>
<tr>
<td>3</td>
<td>Corn?</td>
<td>16</td>
<td>142</td>
</tr>
<tr>
<td>4</td>
<td>Corn-EW</td>
<td>51</td>
<td>463</td>
</tr>
<tr>
<td>5</td>
<td>Corn-NS</td>
<td>236</td>
<td>2120</td>
</tr>
<tr>
<td>6</td>
<td>Corn-CleanTill</td>
<td>1240</td>
<td>11164</td>
</tr>
<tr>
<td>7</td>
<td>Corn-CleanTill-EW</td>
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<td>14</td>
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<td>26</td>
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</table>

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[20] Indian pines dataset, processed and raw
Parallel & Scalable SVM MPI Tool (11)

Another example dataset: high number of classes

- Parallelization benefits: major speed-ups, ~interactive (<1 min) possible

![Graphs showing processing time vs. number of cores for different scenarios.]

<table>
<thead>
<tr>
<th>manual &amp; serial activities (in minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>k pca</td>
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<tr>
<td>-------</td>
</tr>
<tr>
<td>(1) Scenario</td>
</tr>
<tr>
<td>(2) Scenario</td>
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</table>

‘big data’ is not always better data

<table>
<thead>
<tr>
<th>Number of features</th>
<th>(1) Scenario</th>
<th>(2) Scenario</th>
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<tbody>
<tr>
<td>Overall Accuracy (%)</td>
<td>40.68</td>
<td>77.96</td>
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</table>

Can we automate feature extraction mechanism to some degree?

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[21] Analytics Results (raw)
[22] Analytics Results (processed)

Manual WORK: Trade-off between raw data processing and using feature extraction methods
Parallel & Scalable SVM MPI Tool (12)

2x benefits of parallelization (shown in n-fold cross validation)

- Evaluation between Matlab (aka serial) and parallel piSVM
- 10x cross-validation (RBF kernel parameter and C, gridsearch)

<table>
<thead>
<tr>
<th>γ / C</th>
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<th>10</th>
<th>100</th>
<th>1000</th>
<th>10000</th>
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<tbody>
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<td>34.59 (124.46)</td>
<td>39.05 (107.85)</td>
<td>37.38 (116.29)</td>
<td>37.20 (121.51)</td>
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<tr>
<td>4</td>
<td>29.24 (98.18)</td>
<td>37.75 (85.31)</td>
<td>38.91 (113.87)</td>
<td>38.36 (119.12)</td>
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<td>8</td>
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<td>39.68 (118.28)</td>
<td>39.06 (112.99)</td>
<td>39.06 (190.72)</td>
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<td>39.46 (171.11)</td>
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<td>34.61 (179.04)</td>
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<td>38.37 (231.10)</td>
<td>38.37 (240.50)</td>
<td>38.37 (278.02)</td>
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<table>
<thead>
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<th>γ / C</th>
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<th>10</th>
<th>100</th>
<th>1000</th>
<th>10000</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>48.90 (18.81)</td>
<td>65.01 (19.57)</td>
<td>73.21 (20.11)</td>
<td>75.55 (22.53)</td>
<td>74.42 (21.21)</td>
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<td>70.74 (13.94)</td>
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<td>64.18 (18.30)</td>
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<td>76.51 (20.69)</td>
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<td>74.72 (19.66)</td>
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<tr>
<td>32</td>
<td>70.17 (34.45)</td>
<td>75.48 (34.76)</td>
<td>74.88 (34.05)</td>
<td>74.08 (34.03)</td>
<td>73.84 (38.78)</td>
</tr>
</tbody>
</table>

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[23] Analytics 10 fold cross-validation Results (raw)
[24] Analytics 10 fold cross-validation Results (processed)
Recent Research Directions
Recent Research Directions – Brain Data Classification

- Build ‘reconstructed brain (one 3d volume) that matches with sections & block images
- Understanding the ‘sectioning of the brain’ and support automation of reconstruction

1. Some ‘pattern’ exists
   - Image content classification (e.g. SVMs, RandomForst, etc.)

2. No exact mathematical formula exists
   - No precise formula for ‘contour of the brain’

3. Dataset (next: 5 brains, >100.000 pixels, 2PB raw)
   - Block face images (of frozen brain tissue)
   - Every 20 micron (cut size), resolution: 3272 x 2469
   - ~ 14 MB / RGB image
   - ~ 8 MB / corresponding mask image (‘groundtruth’)
   - ~ 700 images → ~40 GB dataset

Research activities jointly with T. Dickscheid et al. (Juelich Institute of Neuroscience & Medicine)
Recent Research Directions – Deep Learning

1. Some ‘pattern’ exists
   - Image content classification & clustering

2. No exact mathematical formula exists
   - No precise formula for ‘brain layers’

3. Dataset – raw images exist
   - Needs to be properly prepared
   - Generate labeled data to learn from (manual tool supporting scientists)
   - Use Deep Learning (deep convolutional neural network, GPGPUs) to classify cell nuclei
   - Extract cell nuclei into 2D/3D point cloud
   - Cluster different brain areas by cell density (parallel DBSCAN)

- Investigate a pipeline for cell nuclei detection and tissue clustering

- Research activities jointly with T. Dickscheid et al. (Juelich Institute of Neuroscience & Medicine)
Conclusions

Scientific Peer Review is essential to progress in the field

- Work in the field needs to be guided & steered by communities
- NIC Scientific Big Data Analytics (SBDA) first step (learn from HPC)
- Towards enabling reproducability by uploading runs and datasets

Selected SBDA benefit from parallelization

- Statistical data mining techniques able to reduce ‘big data‘ (e.g. PCA, etc.)
- Benefits in n-fold cross-validation & raw data, less on preprocessed data
- Two codes available to use and maintained @JSC: HPDBSCAN, piSVM

Number of Data Analytics et al. Technologies incredible high

- Thorough analysis and evaluation hard (needs different infrastructures)
- (Less) open source & working versions available, often paper studies
- Still evaluating approaches: HPC, map-reduce, Spark, SciDB, MaTex, …
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[10] B2SHARE data collection Rome Dataset, online: http://hdl.handle.net/11304/4615928c-e1a5-11e3-8cd7-14feb57d12b9


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Mohammad Shahbaz Memon
Markus Goetz
Christian Bodenstein
Philipp Glock
Matthias Richerzhagen
Thanks

Slides available at http://www.morrisriedel.de/talks
Selected Backup Slides for Discussions
Distributed Large-scale Data Management

UNICORE

[14] UNICORE.eu

PRACE

XSEDE

Extreme Science and Engineering Discovery Environment

Portal e.g. GridSphere
UCC command-line client
URC Eclipse-based Rich client
HiLA Programming API

Gateway
Service Registry
Workflow Engine
Service Orchestrator

Gateway – Site 1
UNICORE Atomic Services
OGSA-
XNJS – Site 1
XAC/ML entity
KUDDB

Target System Interface – Site 1
Local RMS (e.g. Torque, LL, LSF, etc.)

External Storage
U Space

Gateway – Site 2
UNICORE Atomic Services
OGSA-
XNJS – Site 2
XAC/ML entity
KUDDB

Target System Interface – Site 2
Local RMS (e.g. Torque, LL, LSF, etc.)

U Space

JSC: Data Analytics: m.riedel@fz-juelich.de
In-Situ Analytics for HPC & Exascale

Exascale computer with access to exascale storage/archives

- **In-situ correlations**
- **Data reduction**

**Analytics part**
- Key-value pair DB
- Scalable I/O
- Distributed archive
- In-memory

**Visualization part**
- Interactive

**Computational simulation part**

**In-situ statistical data mining**
- E.g. clustering, classification

**In-situ correlations & data reduction**
- E.g. map-reduce jobs, R-MPI

**Scientific visualization & ‘beyond steering’**

**Exascale application**

[15] Inspired by ASCAC DOE report
Tools for Large-scale Distributed Data Management

- Useful tools for data-driven scientists & HPC users

Need for Sharing & Reproducability in HPC – Example

- Sharing different datasets is key
- One tends to lose the overview of which data is stored on which platform
- How do we gain trust to delete data when duplicates on different systems exist

- Research & PhD thesis activities & papers, and...
- Bachelor thesis activities, e.g. improving code (same data)
- Teach class with good AND bad examples!

**B2SHARE** Store and Share Research Data

- Professor
- PhD Student
- Bachelor thesis Student
- Student Classes
- Another collaborator
Smart Data Analytics Process

Big Data Analytics

- Simple Data Preprocessing
- Automated Parallel Data Analytics
- Data Postprocessing

Traditional Data Analysis

- Manual Feature Reduction
- Manual Feature Extraction
- Manual Feature Selection

Combine both: Smart Data Analytics

Concrete Datasets (& source/sensor)
(parallel) Algorithms & Methods

Technologies & Ressources

Scientific Data Applications

Choose choose choose

"Reference Data Analytics" for reusability & learning

Report for joint usage
Openly Shared Datasets
Running Analytics Code


JSC: Data Analytics: m.riedel@fz-juelich.de
Selected Research Data Alliance (RDA) Activities

- Big Data Analytics Interest Group – Establish something like UCI machine learning repository, but for big data analytics…


Satellite Data (Quickbird)
Parallel Support Vector Machines (SVM)
HPC & MPI

Classification Study of Land Cover Types

Classification++

‘Best Practices’

JUDGE system @ JSC

Reference Data Analytics“ for reusability & learning

CRISP-DM Report
Openly Shared Datasets
Running Analytics Code

➢ Research activities with Gabriele Cavallaro (PhD thesis, UoIceland) on Self Dual Attribute Profile
Reproducability Example in Data-driven Science (1)

- Having this tool available on the Web helps tremendously to save time for no research tasks
- Using the tool enables to focus better on the research tasks
Reproducability Example in Data-driven Science (2)

- Sharing pre-processed data
- LibSVM format
- Training and Testing Datasets
- Different setups for analysis (SDAP on All or SDAP on Panchromatic)
Simple download from http using the wget command

```
mriedel@judge:~/bigdata> ls -al
total 640
drwxrwxrwx 21 mriedel zam 32768 2014-09-17 22:20 ..
drwxr-xr-x  19 mriedel zam 32768 2014-09-18 11:49 .
drwxr-xr-x   2 mriedel zam 32768 2014-06-19 07:17 102-salinasindian
drwxr-xr-x   2 mriedel zam 32768 2014-06-19 20:11 107-salinasrescaled
...
```

- **Simple Download** from http using wget
- **Well defined directory structures**

...other open B2SHARE datasets

...before adopting B2SHARE regularly
Reproducability Example in Data-driven Science (4)

Make a short note in your directory linking back to B2SHARE

- Enables the trust to delete data if necessary (working against big data)
- Link back to B2SHARE for quick checks and file that links back fosters trust

```bash
mriedel@judge:~/.bigdata> cd 86-romeok/
mriedel@judge:~/.bigdata/86-romeok> ls -al
```

```
total 580320
  drwxr-xr-x  2 mriedel zam       512 2014-07-09 11:03 .
  drwxrwxrwx 21 mriedel zam       32768 2014-06-17 22:20 ..
-rw-r--r--  1 mriedel zam       35 2014-07-09 11:01 b2share.txt
-rw-r--r--  1 mriedel zam   410074972 2014-05-22 13:26 sdap_area_all_test.el
-rw-r--r--  1 mriedel zam  46652874 2014-05-22 13:36 sdap_area_all_training.el
-rw-r--r--  1 mriedel zam 114763982 2014-05-22 13:36 sdap_area_panch_test.el
-rw-r--r--  1 mriedel zam 12745692 2014-05-22 13:36 sdap_area_panch_training.el
mriedel@judge:~/.bigdata/86-romeok> more b2share.txt
https://b2share.eudat.eu/record/86
mriedel@judge:~/.bigdata/86-romeok> ```
Reproducability Example in Data-driven Science (5)

True reproducability needs: (1) datasets; (2) technique parameters (here for SVM); and (3) correct versions of algorithm code.
Classical Machine Learning

Dealing with Big Data in traditional Machine Learning
- Define Features to learn from ?!
- Transform data into supported format ?!
- How to reduce dimensions ?!
- How to parallelize ?!
Deep Learning

Dealing with Big Data in Deep Learning

- Define Features to learn from
  - Automatically learn how to define features
- Transform data into supported format
  - Adopt the model to your data
- How to reduce dimensions
  - Automatically reduce dimensions in every hidden layer
- How to parallelize
  - Naturally the brain is parallel, so Artificial Neural Networks are!

A. Ng, Google Brain
Deep Learning in Computational Biomedicine

Genome Analysis
- Find high level features on low level –omics data

Medical Image Analysis
- Use 2D (or 3D) structure of the data for classification

Unstructured Data Analysis
- Use DL for text analysis to classify patient data, drug recommendations by users, …

Etc…
Deep Learning Packages

There exist several frameworks for deep neural networks:

- **Pylearn2**
  - Python tool on the top of the Theano python library
  - Easy configuration of data, model, learning via YAML files
  - CUDA support for accelerated calculations
  - Jobman for parallel cross validation

- **Caffe**
  - C++ implementation with python & matlab wrappers
  - CUDA acceleration

- **DL4J**
  - Java implementation of Deep Learning
  - CUDA + Hadoop support
Chances and Pitfalls for ‘Scientific Big Data Analytics’

~2009 – H1N1 Virus Made Headlines
- Nature paper from Google employees
- Explains how Google is able to predict fast winter flu
- Not only on national scale, but down to regions
- Possible via logged big data – ‘search queries’

~2014 – The Parable of Google Flu
- Large errors in flu prediction & lessons learned
  (1) Dataset: Transparency & replicability impossible
  (2) Study the algorithm since they keep changing
  (3) It’s not just about size of the data

- Big data is not always better data – Think about difference of causality vs. correlation


Location-based Social Network-based Health Analytics

Scientific Domain Area
- Smart Cities approaches combined with Health Analytics Research

Scientific Outcome
- Traffic density estimation
- Network emission model

Location-based Social Networks (LBSN) Data
- Open data sources: Twitter & Foursquare
- Plan: Validation with real measurements in cities

Research activities with Markus Goetz (PhD thesis) – Juelich Supercomputing Centre, UoIceland