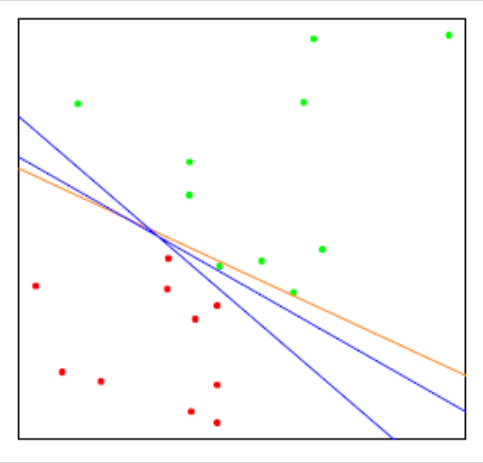

Big Data Analytics

Basic concepts of analyzing very large amounts of data

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LECTURE BDA5

Tools and Techniques

2014-02-08 (v2)
Online Material

UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING, MECHANICAL ENGINEERING AND COMPUTER SCIENCE

JÜLICH
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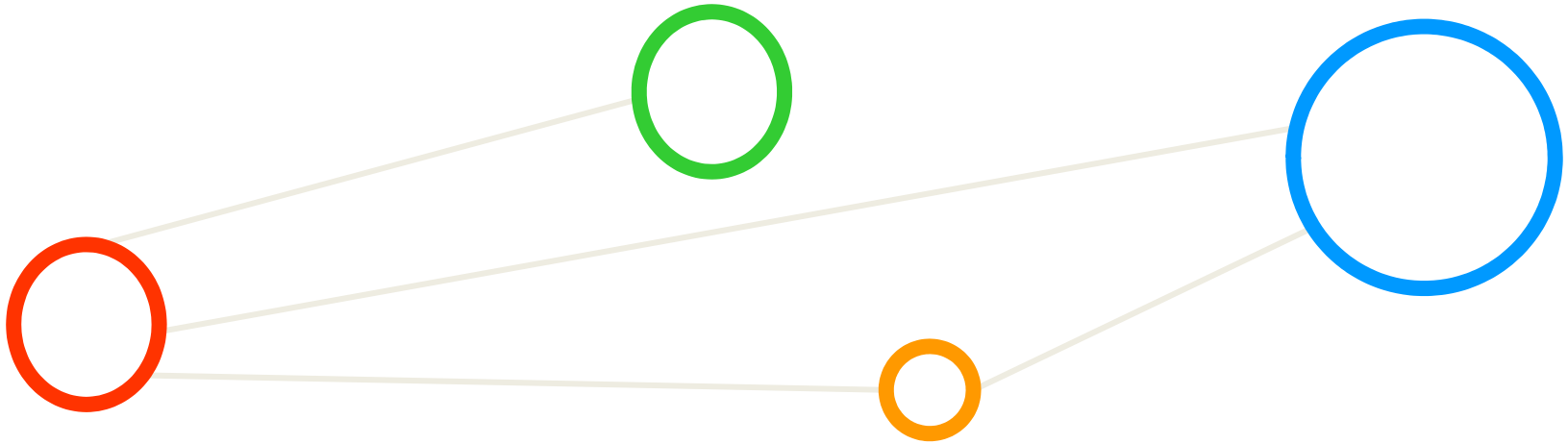
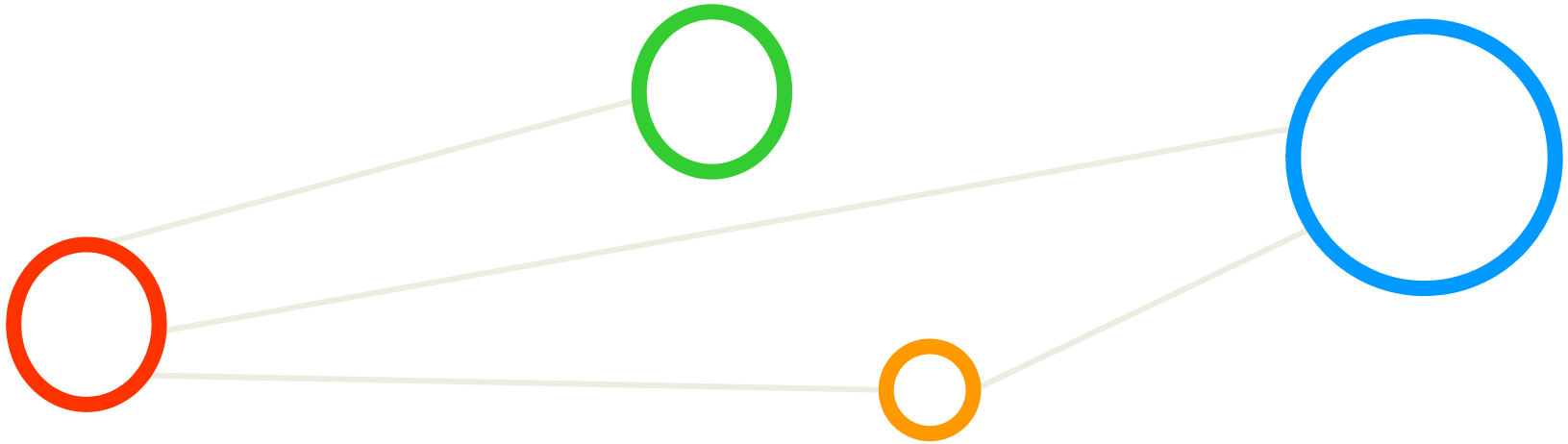
Outline



Outline

- Tools Overview and Selected Use Cases
  - RMPI – R interface to MPI
- Methods
  - Statistical Techniques
  - Data Mining
  - Machine Learning
  - Evolutionary Optimization

RMPI



RMPI – Overview

- **The tool R is a free software environment for statistical computing and graphics**
- **RMPI is an R package and an interface (wrapper) to the Message Passing Interface (MPI)**
- **MPI is a standardized and portable parallel programming model implemented via libraries**

- RMPI ports low level MPI functions into R so that users do not have to know C or Fortran
- MPI libraries supported:
  - LAM-MPI, MPICH(2), and OpenMPI
- Write R programs using certain RMPI functions:
  - Startup and Shutdow: e.g. mpi.spawn.Rslaves([nslaves=#])
  - Cluster Information: e.g. mpi.comm.rank()
  - Use sending/receiving data/functions to send an R object like a number, string, or a list between different slaves or to all slaves (e.g. mpi.bcast.Robj2slave(object))

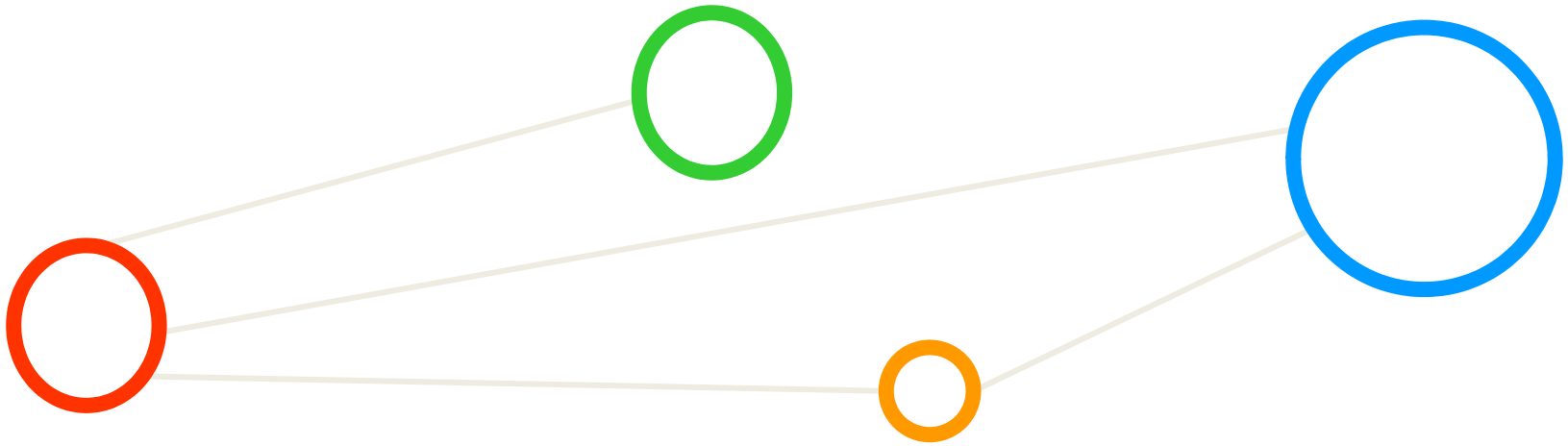
[2] RMPI Web Page

- **Enables inter process communication**

RMPI – Selected Use Cases

- ‘Precision Medicine‘ *[1] Bottomly et al., 2013*
  - Simulations and calculation of P-values and False Discovery Rate (FDR)
  - Parallel computed on Beowulf-style cluster using RMPI R-2.15.1
  - Use of parallel random number generation using L‘Ecuyer‘s method (R rlecuyer package)
  - Plotting and summaries for the simulations with ggplot2 on R-3.0.1

Methods



Statistical Techniques

- **The main task of statistical techniques is to test the likelihood of a given hypothesis**

- Limits
  - Impossible to identify new relationships in data
  - Discovery of new relationships is a very important chance to realize additional unexpected benefits from the large amounts of data
  - Example: data available from High Throughput Experimentation (HTE)

[3] Ohrenberg et al., 2005

Data Mining Techniques

- **Data mining stands for algorithms and techniques which transfer data into information**

- Provides methods that extract rules, patterns, or other structural information from data
- Identify in the data new relationships that were previously undiscovered
- Typical data-mining techniques
  - Clustering, separation methods, decision trees, association rules, etc.
- Limits
  - Data mining does not assess the validity of extracted rules
  - Making data-mining results reliable, it is essential to apply different approaches and check the resulting rules for mutual compatibility

[3] Ohrenberg et al., 2005

Machine Learning Techniques

- **Machine learning techniques are able to learn from data and train a system (model)**

- Wide variety of machine learning algorithms exist
  - Artificial Neural Networks, Support Vector Machines, etc.
- Artificial Neural Networks (ANN)
  - A kind of extremely powerful regression model (rough perspective)
  - Input-output relationships can be generated by ANN as black box model
  - Black box model: function cannot be interpreted physically – the parameters in the ANN have generally no explicit physical meaning
  - ANN need less data then other black-box methods to generate an input – output relationship of comparible quality
    (given a wide range of conditions)

[3] Ohrenberg et al., 2005

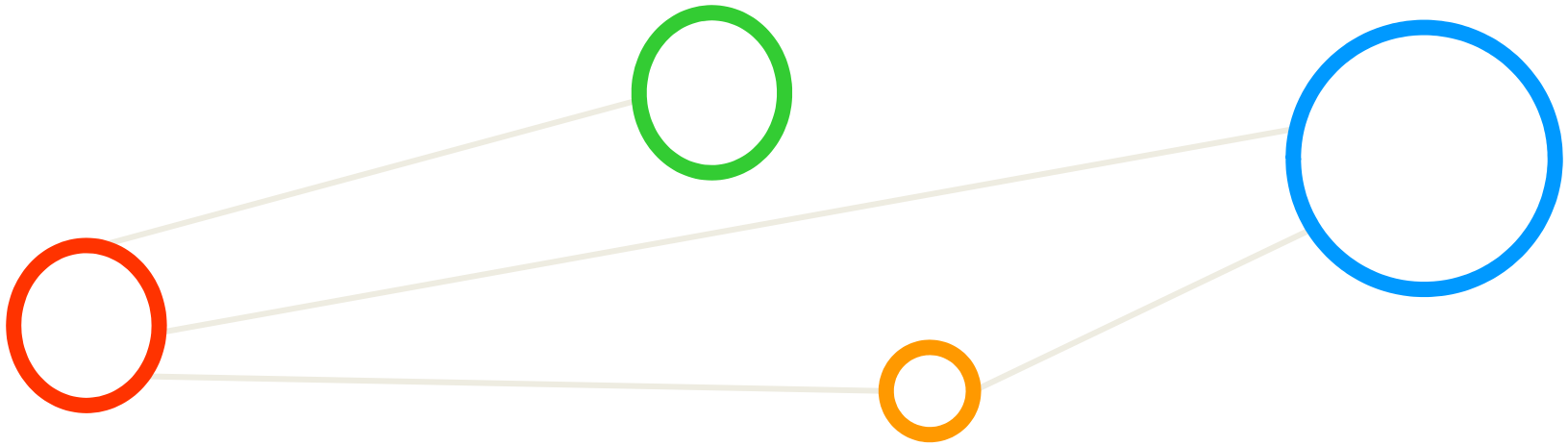
Evolutionary Optimization

- **Evolutionary optimization techniques are characterized by a stochastic approach**

- Advantages
  - Compared to statistical experiment design, evolutionary algorithms are very flexible and adaptable
- Limits
  - In most cases the optimization speed is rather slow

[3] Ohrenberg et al., 2005

Lecture Bibliography



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- [1] Bottomly et al.: Comparison of methods to identify aberrant expression patterns in individual patients: augmenting our toolkit for precision medicine. Genome Medicine 2013 5:103., Online: http://genomemedicine.com/content/pdf/gm509.pdf
- [2] RMPI Web Page, Online: http://www.stats.uwo.ca/faculty/yu/Rmpi/
- [3] Ohrenberg, Arne, et al. "Application of Data Mining and Evolutionary Optimization in Catalyst Discovery and High-Throughput Experimentation–Techniques, Strategies, and Software." *QSAR & Combinatorial Science* 24.1 (2005): 29-37.


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