Statistics Environment R

Introduction, Overview, Applications

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What is R?

R is "a language and environment for statistical computing and graphics". R

- R is Free Software under the terms of the GNU General Public License (GPL).
- R Foundation of Statistical Computing
- As an integrated suite for data analysis it includes:
 - well-developed high-level programming language.
 - extensible through packages and C/C++/Fortran codes
 - effective data handling and storage facilities,
 - large, integrated collection of tools for data analysis
 - graphical facilities for statistical (and other) plots
 - elaborate help system (text, PDF, HTML, LaTeX, ...)





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- ... CRAN ... R-Forge ... RStudio ... Rcpp ...
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Personal Relations with R

- R user since 2001 on Windows, Mac OSX, Linux ... systems
- Answering questions on the R-help mailing list since 2001
- Several packages on R-Forge and CRAN ('pracma', 'numbers', 'adagio', 'nloptwrap', 'specfun', 'LowRankQP', 'linprog')
- Maintainer of the "Numerical Math"task view on CRAN
- Mentor of two R-GSoC 'Google Summer of Code' projects ("RMaxima"2012, "rHanso"2013)
- Reviewer (and author) for the Journal of Statistical Software (JSS) special issue on "Optimization with R"(2014)
- Contributor to a book on "Using R for Numerical Analysis", to appear in 2014, Chapman & Hall/CRC Press



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R Resources

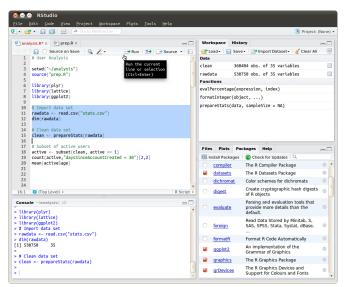
- R home and download pages (95 mirrors worldwide) http://www.r-project.org, cran.r-project.org
- Contributed packages (sorted by name or date of publication) cran.r-project.org/web/packages/
- Mailing lists (searchable)
 https://stat.ethz.ch/pipermail/r-help/,
 stackoverflow.com/questions/tagged/r/
- Task Views cran.r-project.org/web/views/
- R Journal and the Journal of Statistical Software journal.r-project.org/, www.jstatsoft.org/
- Books related to R (a.o., Springer UseR Series, CRC R Series) www.R-project.org/doc/bib/R-books.html



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Graphical User Interface: RStudio



Reproducible Research

- "Combine technical report, data analysis, and experimental data s.t. research can be recreated, better understood and verified."
- RStudio supports document preparation by
 - Markup languages: Markdown (HTML) or LaTeX (PDF)
 - knitr: literate programming
 Presentation + analysis + executable code
 - Unix-like shell programs, e.g., GNU make, pandoc
 - Storing data, code and text on Git/Github repositories
- Minimal requirements for reproducible research: fingerprinting of data, reproducing random numbers, identification of R and package versions, reproducing system settings, etc., are not covered in this framework!

Help System

- Getting help for functions and operators
 ?lm, ?"[[", ??solve, help.start()
- Extended/-able help system for package authors
 - structured help templates (Rd format)
 - automatic tests for correctness, checking examples
 - formatted inline help
 - automatic conversion to other formats: HTML, LaTeX, ...
 - generation of package manual in PDF format
- User and reference manuals easily available
- Web-based online help
 Search facilities for package manuals and mailing lists
 Online documentation: http://www.Rdocumentation.org/

Object Orientation

"Everything in R is an object."

S3 classes

'informal classes', using method dispatching on polymorphic functions e.g., generic functions summary or plot: methods(plot)

- S4 classes newer, fully object-oriented system [seldom used]
- OO in packages prototype-based: proto, R.OO; multiple inheritance: mutatr
- Reference Classes (Chambers) mutable objects, message-passing mechanism (↔ C++)

Integrating Fortran / C / C++

- Dynamically linked Fortran / C / C++ code can be directly used in R and is fully supported by package management and CRAN facilities
- 'Rcpp' provides an interface for seamlessly accessing, extending or modifying R objects at the C++ level 'Rinline': use uncompiled C++ code in R programs



- Other languages:
 - 'rJava': low-level R to Java interface
 - 'rPython': permits calls form R to Python
 - 'R.matlab': TCP/IP interface with the Matlab process

Package Management

- Packages are 'bundles' of functions, data files, help files, source files (Fortran, C, C++), vignettes, and additional information such as DESCRIPTION, NAMESPACE, NEWS
- R builds and checks packages with 50(!) different checks
- Source files are compiled and added as dynamically linked libraries
- User-contributed packages are stored on CRAN (> 5000) and are installed and updated from there: install.packages("pracma") ... update.packages() library(pracma)
- Packages can be stored and checked on R-Forge (subversion repository)

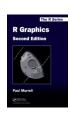
Data Sources

- Reading in data files: Text, CSV files (URL addresses) read.table(<file>, header=TRUE, sep='\t', ...)
- Data files from other systems: *.mat (Matlab), Excel, ODS, SAS, SPSS, Stata, Systat, IDL(?), ...
- Database connections: DBI, ODBC, JDBC Oracle, MySQL, PostgreSQL, SQLite (non-SQL:) MongoDB, ArangoDB
- Internet data sources: Statistical databases, data archives
 Finance, economics, ecological, census data, geographic,
 demographic, weather, medical, forensic, genomic/sequencing, ...
- Example:



Statistical Graphs

- Statistical Graphs are completely customized scatter plots, function graphs, density diagrams, pie charts, histograms, box and mosaic plots, spine/spinograms, ... advanced: grid graphics, 'pairs', 'coplots'
- Dynamic graphics: 'animation' package, 'rgobi'
- Importing and exporting graphics formats
- 'ggplot2' (Grammar of Graphics) for professional plots
- Missing Links: high-quality 3D-Graphs, interactive graphs
- Building Graphical User Interfaces Packages: 'gWidgets', 'RGtk2', 'qtbase', 'tkltk'





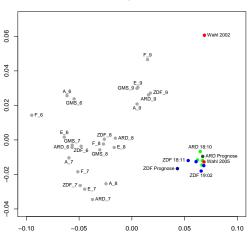
Computational Statistics

- Classical univariate Statistics:
 Distributions, summaries, random data, robust methods, density estimation, hypotheses testing, ...
- Linear regression, generalized/additive linear models Formula language for linear models: y~x1+x2-1
- Nonlinear and smooth regression
- Multivariate Statistics: cluster/factor/discriminant analysis, classification visualization methods: PCA, MDS, SOM, ICA, etc.
- Tree-based methods, random and mixed effects
- Time series, survival analysis, spatial analysis



Example: Multidimensional Scaling

Bundestagswahl 2005



Multi-Dimensional Scaling (MDS)



Example: R code for MDS

```
umf <- read.table("umfragen.txt", sep="\t", header=T, row.names=1)
umf <- umf[.-6]
dumf <- dist(umf)</pre>
cumf <- cmdscale(dumf)</pre>
# plotting
clrs <- c(rep("darkgray", 24), "darkgreen", rep("green", 4),</pre>
          "darkblue", rep("blue", 4), rep("red", 2))
plot(cumf, pch=19, col=clrs,
     xlim=c(-0.10,0.10), ylim=c(-0.04,0.07),
     xlab=, ylab=,
     main="Bundestagswahl 2005",
     sub="Multi-Dimensional Scaling (MDS)")
identify(cumf[,1], cumf[,2], labels=rownames(umf), cex=0.75)
```

Time Series

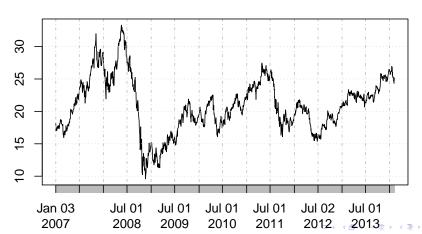
- Reading time series from different sources
 - text files, spreadsheets
 - Internet time series databases
 - PostgreSQL time series ('TSdbi')
 - Handling of time and date
- Forecasting and Modeling
 Decomposition, seasonal trends, ARMA/ARIMA
 spectral analysis, state space identification
- 'signal' package, but no 'control' package
- Time Series Data Mining
 - Clustering and classification
 - Dynamic time warping
 - Functional Data Analysis (FDA)



Example: Financial Time Series

library(quantmod); getSymbols("ABB"); plot(ABB)

ABB



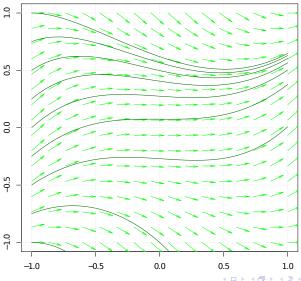
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Differential Equations

- Several packages offer to solve differential equations, e.g. 'deSolve' or 'bvpSolve', mostly by integrating known free solvers written in C or Fortran:
 - Ordinary differential equations (ODEs)
 - Partial differential equations (PDEs)
 - Boundary value problems, e.g. reactive transport equations
 - Differential algebraic equations (DAEs)
 - Delay differential equations (DDEs)



Example: Vectorfield



Statistical Learning

- Linear regression and classification
- Kernel smoothing methods (e.g., radial basis functions)
- CART, Decision Trees, MARS, Earth
- Neural Networks, Kohonen maps
- Support Vector Machines (classification, regression)
- Random Forests, ensemble learning
- Graphical models [, Bayesian networks]
- Boosting, AdaBoost, JackKnife methods
- Model assessment and selection

T. Hastie, R. Tibshirani, J. Freedman: *The Elements of Statistical Learning* James, Witten, Hastie & Tibshirani: *An Introduction to Statistical Learning – With Applications in R.*

Cousera Course on "Statistical Learning" online since Jan 21, 2014



2013-02-11

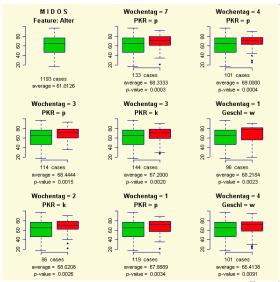
Data Mining with R

Database Mining...Data Mining...Predictive Analytics...Big Data...Data Science

- Packages providing Data Mining functionality:
 - Weka: open source machine learning software
 - Decision trees: Cubist, C5.0 (Quinlan) [GritBot ?]
 - Random Forest (Breiman): ensemble learning
 - FactorMineR: sequence analysis
- Rattle: graphical user interface for data mining in R
- RODM: interface to Oracle Data Mining
- Vikamine: open source Subgroup Discovery
- Integration of R in Data Mining environments (free) Weka, KNIME, RapidMiner; (comm.) SAS Enterprise Miner



Example: MIDOS Graph



Optimization with R (I)

- Optimization in Base R
 optim(par, fn, gr, lower, upper,
 method="Nelder-Mead", "BFGS", "CG", "L-BFGS-B", "SANN")
- (Nonlinear) Least-Squares optimzation: 'nls', 'nnls', 'minpack.lm', ...
- Derivative-free optimization: 'dfoptim'
- (Mixed-integer) Linear Programming: 'lpSolve', 'Rglpk', 'Rsymphony', 'rneos' (NEOS server)
- Nonlinear Optimization: 'nloptr' (NLopt library)
- Constraint Optimization: 'alabama', 'Rsolnp' (using "augmented Lagrangian")



Optimization with R (II)

- Global Optimization: 'GenSA', 'PSO', 'soma', 'cmaes'
 'DEoptim', 'RcppDE', 'DEoptimR' (differential evolution)
- Convex Optimization: 'Rcsdp' (semi-definite programming)
 CVX ?? ("disciplined convex programming") [Matlab toolbox]
- QP-QC (w/ quadratic constraints) ?? MIQP ??
- Non-smooth Optimization: ?? (e.g., minimax problems)
- Discrete Optimization: 'knapsack', 'TSP'
- Modeling language ?? [MathProg, AMPL, GAMS, ZIMPL]
- Recommendations: See the "Optimization" task view !, or Special Issue "Optimization in R", J. of Stat. Software, 2014



Application Areas / Related Projects

- Econometrics / Financial Engineering: Rmetrics
 "Financial Market Analysis w/ R" https://www.rmetrics.org/
- Bioinformatics: Bioconductor <www.bioconductor.org/> "Analysis and comprehension of high-throughput genomic data"
- Spatial Statistics: Rgeo <www.R-project.org/Rgeo>
- Robust Statistics: <www.statistik.tuwien.ac.at/rsr/>
- Social Network Analysis: 'igraph', 'sna'
- Optimization "community"
- See the 'R task View's <cran.r-project.org/web/views/>



High Performance / Parallel Computing

High Performance Computing
 'Rcpp' family of packages, e.g., RcppArmadillo, RcppEigen
 'RcppOctave' – interface to Octave and Matlab

Parallel Computing

- Message Passing Interface (MPI)
- Packages for explicit / implicit parallelism
- Grid computing, GPUs
- Apache Hadoop framework (HDFS, MapReduce)
- Cloud Computing, e.g., Amazon Web / EC2 services
- Large memory / big data support / profiling tools



Matlab Advantages

Matlab als Umgebung für techn.-wissenschaftl. Rechnen

- Graphische Bedienoberfläche
- Mathematische Operationen / Funktionen
- Eigene Programmiersprache
- 'Just-In-Time' (JIT) compiler
- Toolboxen, z.B. die 'Symbolic' Toolbox
- 2- und 3-dimensionale Visualisierungen
- Integration mit MS Office Paketen
- Erzeugung graphischer Benutzerschnittstellen
- Simulink: Simulation dynamischer Systeme
- C/C++ Compiler bzw. .NET Integration

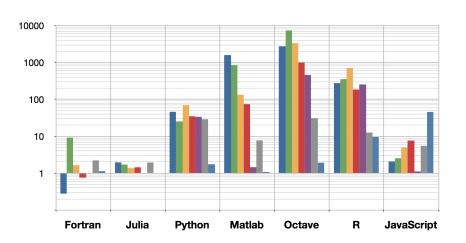


Gang of Forty

Matlab Maple Mathematica SciPy SciLab IDL R
Octave S-PLUS SAS J APL Maxima Mathcad
Axiom Sage Lush Ch LabView O-Matrix PV-WAVE
Igor Pro OriginLab FreeMat Yorick GAUSS MuPad
Genius SciRuby Ox Stata JLab Magma Euler Rlab
Speakeasy GDL Nickle gretl ana Torch7



Obligatory Performance Slide



Execution time relative to C++



Some Examples of R and Matlab Syntax

Matlab

```
x = [1, 3, 5, 7, 9]
y = A(:, 2)
% defined in 'myfun.m'
function [a,b] = myfun(x,y,z)
. . .
end
if x == 1
    v = 0
else
    v = x
end
```

R

```
x \leftarrow c(1, 3, 5, 7, 9)
y < -A[, 2]
# defined interactively
myfun <- function(x,y,z=1e-0.7) {
}
if (x == 1) {
   y <- 0
} else {
   y <- x
```

Conclusions?

