Methods for unstructured data

Lecture 1: Tools for Scientific Programming

Helge Liebert

What is this lecture about?

- Most research in economics now involves scientific programming.
- Introduce tools and ideas that may make daily research tasks easier.
- Many of these have been developed by other scientists or IT professionals. Some are decades old, others are novel.
- Focus on data processing and reproducible research.
- Text processing is a common task in research and industry.
- Working with text data requires understanding of some practical techniques.

Contents

Economics and computation

Economics and computer science

- Technical aspects rarely part of the economics curriculum.
- Data management is not taught in introductory econometrics.
- The days of entering data in spreadsheets are largely gone.
- Even before the recent advent of “big data”.
- Scientific programming common in other sciences before it gained a more prominent role in economics.

Economics and computer science

- Computer science often involves processing data.
- Most problems you are likely to encounter have been solved.
- Tools and concepts that economists can profit from.
  - Remote servers, databases, version control, acessing APIs for data, text processing and analysis, geospatial analysis, OCR, automation, …
  - Time complexity of algorithms, computational cost, databases, …

Survey

- Operating systems - Windows, MacOS, Linux?
- Scientific programming - Stata, R, Python, Matlab/Octave, Julia, ...?
- General purpose programming languages?
- Servers, shell scripting, CLI?
- (Relational) databases - SQL?
- Version control - Git?

Topics

- General points about scientific programming and working with computers.
- Superficial and incomplete. A stand-alone course on Programming Practices for Research could be devoted to these topics.
- Brief intro to get you going and help identify appropriate tools for a problem.
- Point you towards resources and explain their general concepts.
- Leave you marginally more computer literate.

- Languages, tools, version control.
- Unix shell and the command line.
- Regular expressions.

Programming languages

Which language to choose?

- *It depends*. Choice is use-case- and taste-specific.
- *Anything* can be done in *any* language. Convenience varies.
- Concepts and toolkits transfer easily most of the time.
- Trade-off: Prior knowledge vs. task suitability.
- Languages which are great for specific scientific purposes may not be well-suited for other tasks.
- Ease of exploratory analysis vs. ease of deployment in production.
- Never re-invent the wheel.

Possible options

- Specialized languages: R, MATLAB/Octave, Stata, Gauss, Julia, ...
- General-purpose languages: Python, Perl, Ruby, C, ...
- Choose a high-level, dynamic, interpreted language unless you are sure you require the extra speed of a compiled language.
- Ideally free and open source. Popular is typically better.
- Research ex ante which libraries are mature and best for solving your specific problem.

R

- R is the major statistical programming language.
- It is free, used in many sciences and in industry. Good documentation.
- New models are frequently published and implemented first in R.
- Having data processing and analysis in the same language is nice.
- Good library support for common tools (e.g. databases, regular expressions).
- Specific tasks for which high-level wrapper functions are not available may be very cumbersome.
- In recent years, R development has been very active and libraries exist for almost anything.

Python

- General-purpose programming language, supports object-oriented programming.
- Reads like english. Explicit and clear. Whitespace matters, no braces. (*"There should be one obvious way to do it"*.)
- Used extensively in industry and sciences. Good documentation.
- Libraries for almost anything.
- Many science-related libraries exist for other languages, but rarely are they as mature.
- Good and growing support for statistical modeling.
- A bit less suited for interactive data work (but more so for deployment in production).

This lecture

- The lab sessions utilize R.
- Any task covered by this lecture can be accomplished using R or Python (augmented by shell programs).
- R, Python, SQL and knowing your way around a terminal are highly valued skills on the job market.
- Rule-of-thumb recommendation:
    - Simple data analysis/small text corpora:
      Stick with R. Augment with other tools where required.
    - More involved data processing/larger text corpora:
      Go with Python. You can still analyze data in R.
    - ... and whatever program your colleagues are using.

Why not Stata, Matlab, Gauss or similar?

- Advantage: Many domain-specific models supported.
- Less support for almost anything else.
- Much less flexible for anything not to do with data analysis or numerics.
- Difficult to deploy on a server. Often tied to a GUI.
- Less popular, smaller userbase. Proprietary and expensive.
- You can still rely on them for estimation after your data is clean.

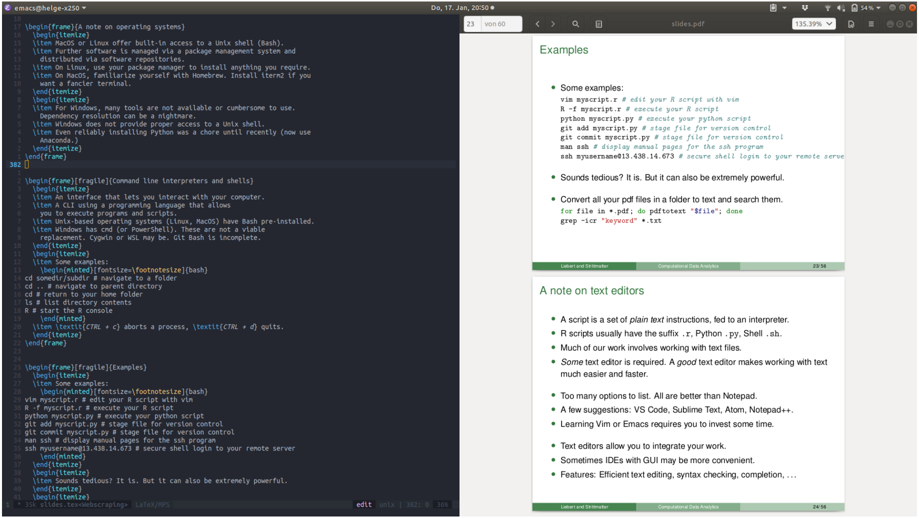
A note on text editing

- A script is a set of *plain text* instructions, fed to an interpreter.
- Editing is independent from running code.
- R scripts usually have the suffix `.r`, Python `.py`, Shell `.sh`.
- Proficiency in a text editor makes working with text easier and faster.

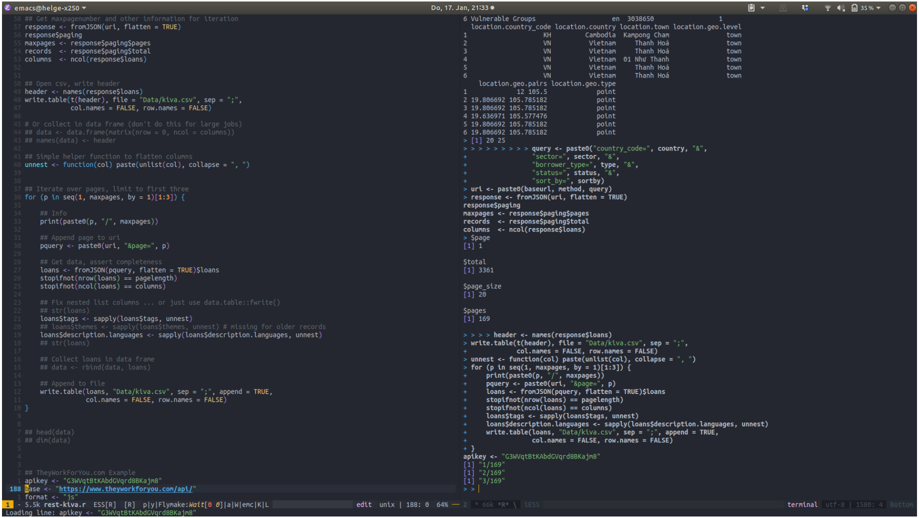
- Too many options to list. All are better than Notepad.
- A few options: VS Code, Sublime Text, Atom, Notepad++, …
- Learning Vim or Emacs requires you to invest some time.

- Text editors allow you to integrate your work and edit text efficiently.
- Sometimes IDEs with GUI may be more convenient (e.g. Rstudio, PyCharm).
- Features: Regex search and replace, grep search, diff, syntax checking, formatting, completion, persistent undo, documentation lookup …

A possible setup



… that is universal



… that is universal

```
each school-track, classroom formation is conditionally ignorable with respect to SN
status, as students from different primary school districts are mixed and their SN status
is not observed by secondary school administrators.\footnote{Using PISA data from
secondary schools in Switzerland, \citet{Vardardottir2015} shows that track-by-school
fixed effects render peer group composition conditionally uncorrelated with a large set
of students' characteristics, while track fixed effects and school fixed effects do not.}
Neither primary schools nor the SPS share information with secondary schools for equity
reasons and to avoid stigma when transitioning between schools.

% NEU: BEu bitte lesen
% changed some small things. ok for me.
Beyond this anecdotal evidence, we formally test the validity of the identification
strategy with four balancing tests, which are presented and discussed extensively in
Appendix B. First, we examine whether the proportion of SN peers predicts individual
baseline characteristics (gender, native speaker, and age). The aim of this test is to
detect potential selection into classrooms. We also conduct this test separately for SN
and non-SN students. None of the baseline characteristics are statistically significant
at conventional levels, either considered individually or jointly. Second, we regress the
indicator for SN status on class fixed effects, which should be jointly insignificant if
assignment to classrooms is ignorable with respect to SN status \citep{chettyEtal2011}.
We also conduct this test to check for ignorable assignment of SN students to teachers.
We find no evidence for systematic assignment of SN students to either classes or
teachers. Third, we conduct a simulation exercise in the spirit of \citet{carrell2010}.
We re-sample classes and thereby assign SN students randomly to classrooms, and test
whether the observed distribution of SN students differs from the simulated one. In
addition, we compute the interquartile range of the proportion SN students across classes
for each simulation, and compare these simulated interquartile ranges with the one we
observe in the data. Neither simulation procedure uncovers any worrisome pattern in the
assignment of SN students to classes. Fourth, we decompose the variation in the fraction
of SN peers across and within schools. To do so, we examine the residual variation in the
proportion of SN peers after partialling out the school-track-year fixed effects. We find
that the residual distribution in the proportion of  SN peers is consistent with
variation from a random process. Overall, the balancing tests we performed indicate that
the key identification assumption of (conditionally) ignorable assignment of SN students
to classes is plausible.

Our identification relies on variation between classes within school-track-years.
Although families can potentially choose their district of residence and thereby
influence schooling options for their children, possible selection into schools does not
confound our results.\footnote{Endogenous class formation could still occur if parents
request to transfer their children to a class with a lower SN fraction. To investigate
this potential threat, we acquired the official education statistics from the Swiss
Federal Statistical Office (SDL, \textit{Statistik der Lernenden} in German) for the
years 2012-2015. Importantly, the SDL has a classroom ID which allows us to reconstruct
the classes within each school-year-track. For the state of St.\ Gallen, we find that on
```

```
A:  104k  xSource/manuscript_R1_v3.tex  ??:0 37%    LF UTF-8  LaTeX/FPS
```

```
different education tracks, and classes are strictly separated between tracks. Within
each school-track, classroom formation is conditionally ignorable with respect to SN
status, as students from different primary school districts are mixed and their SN status
is not observed by secondary school administrators.\footnote{Using PISA data from
secondary schools in Switzerland, \citet{Vardardottir2015} shows that track-by-school
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the classes within each school-year-track. For the state of St.\ Gallen, we find that on
```
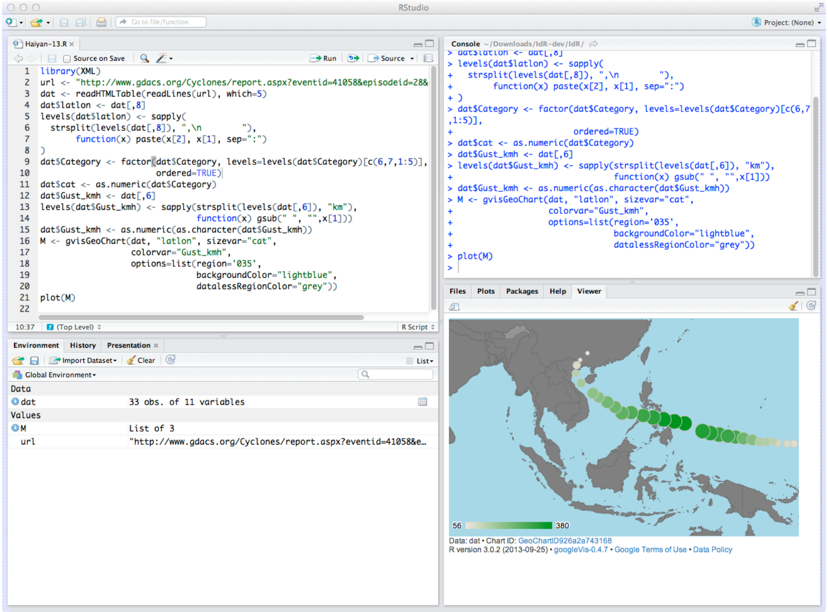
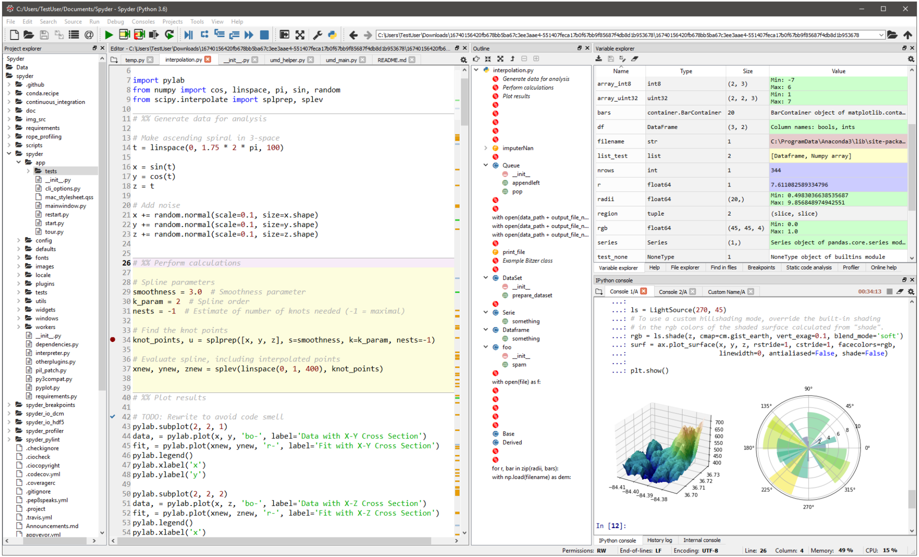

```
B:  104k  xOld/manuscript_R1_v2.tex  ??:0 37%    LF UTF-8  LaTeX/FPS
Type ? for help
-- *Ediff Control Panel*   diff 4 of 15        Quick Help
Auto-refining is ON
```

Rstudio


RStudio
Haiyan-13.R
Source on Save
Run
Source
library(XML)
url <- "http://www.gdacs.org/Cyclones/report.aspx?eventid=41058&episodeid=28&
dat <- readHTMLTable(readLines(url), which=5)
dat$latlon <- dat[,8]
levels(dat$latlon) <- sapply(
strsplit(levels(dat[,8]), ",\n "),
function(x) paste(x[2], x[1], sep=":")
)
dat$Category <- factor(dat$Category, levels=levels(dat$Category)[c(6,7,1:5)],
ordered=TRUE)
dat$cat <- as.numeric(dat$Category)
dat$Gust_kmh <- dat[,6]
levels(dat$Gust_kmh) <- sapply(strsplit(levels(dat[,6]), "km"),
function(x) gsub(" ", "",x[1]))
dat$Gust_kmh <- as.numeric(as.character(dat$Gust_kmh))
M <- gvisGeoChart(dat, "latlon", sizevar="cat",
colorvar="Gust_kmh",
options=list(region='035',
backgroundColor="lightblue",
datalessRegionColor="grey"))
plot(M)
Console ~/Downloads/IdR-dev/IdR/
Files Plots Packages Help Viewer
Environment History Presentation
Import Dataset
Clear
List
Global Environment
Data
dat 33 obs. of 11 variables
Values
M List of 3
url "http://www.gdacs.org/Cyclones/report.aspx?eventid=41058&e...
56
380
Data: dat • Chart ID: GeoChartID926a2a743168
R version 3.0.2 (2013-09-25) • googleVis-0.4.7 • Google Terms of Use • Data Policy

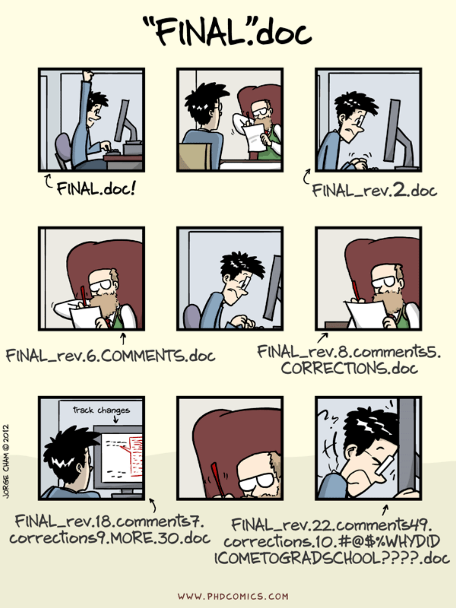
Spyder



C:/Users/TestUser/Documents/Spyder - Spyder (Python 3.6)
File Edit Search Source Run Debug Consoles Projects Tools View Help
Project explorer
Editor
Outline
Variable explorer
IPython console
import pylab
from numpy import cos, linspace, pi, sin, random
from scipy.interpolate import splprep, splev
# %% Generate data for analysis
# Make ascending spiral in 3-space
t = linspace(0, 1.75 * 2 * pi, 100)
x = sin(t)
y = cos(t)
z = t
# Add noise
x += random.normal(scale=0.1, size=x.shape)
y += random.normal(scale=0.1, size=y.shape)
z += random.normal(scale=0.1, size=z.shape)
# %% Perform calculations
# Spline parameters
smoothness = 3.0 # Smoothness parameter
k_param = 2 # Spline order
nests = -1 # Estimate of number of knots needed (-1 = maximal)
# Find the knot points
knot_points, u = splprep([x, y, z], s=smoothness, k=k_param, nests=-1)
Evaluate spline, including interpolated points
xnew, ynew, znew = splev(linspace(0, 1, 400), knot_points)
# %% Plot results
# TODO: Rewrite to avoid code smell
pylab.subplot(2, 2, 1)
data, = pylab.plot(x, y, 'bo-', label='Data with X-Y Cross Section')
fit, = pylab.plot(xnew, ynew, 'r-', label='Fit with X-Y Cross Section')
pylab.legend()
pylab.xlabel('x')
pylab.ylabel('y')
pylab.subplot(2, 2, 2)
data, = pylab.plot(x, z, 'bo-', label='Data with X-Z Cross Section')
fit, = pylab.plot(xnew, znew, 'r-', label='Fit with X-Z Cross Section')
pylab.legend()
pylab.xlabel('x')

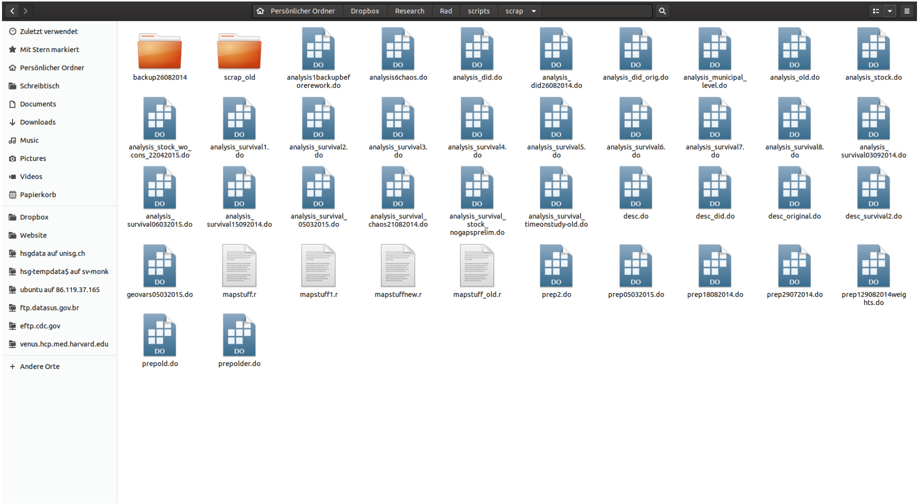
Version control

Familiar?

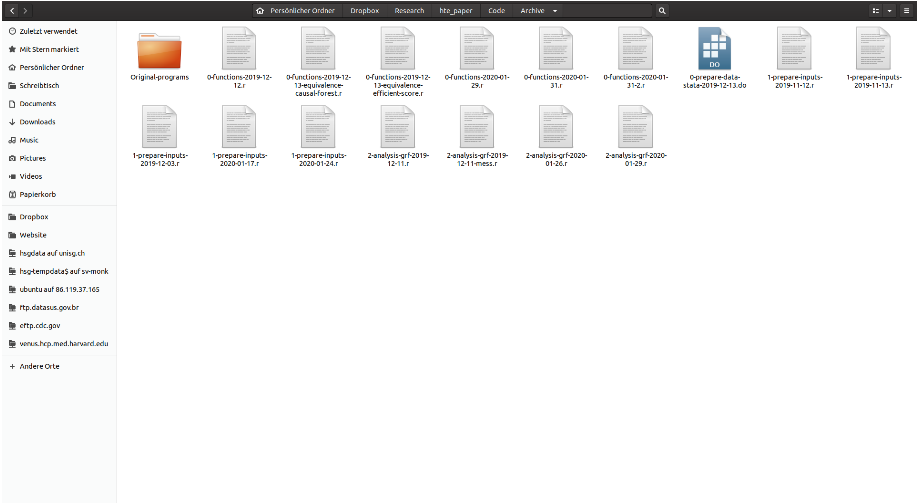


"FINAL".doc
FINAL.doc!
FINAL_rev.2.doc
FINAL_rev.6.COMMENTS.doc
FINAL_rev.8.comments5.
CORRECTIONS.doc
track changes
FINAL_rev.18.comments7.
corrections9.MORE.30.doc
FINAL_rev.22.comments49.
corrections.10.#@$%WHYDID
ICOMETOGRADSCHOOL????.doc
JORGE CHAM © 2012
WWW.PHDCOMICS.COM

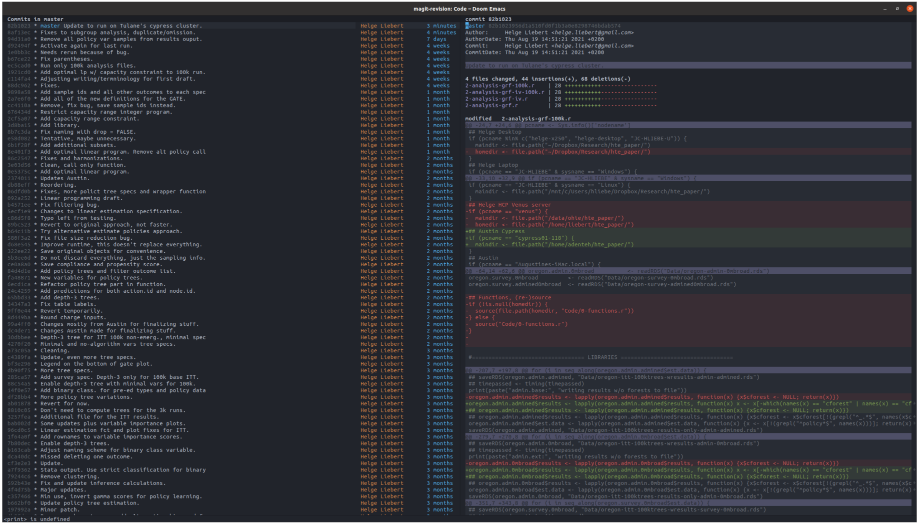
Familiar?


Persönlicher Ordner
Dropbox
Research
Rad
scripts
scrap
Zuletzt verwendet
Mit Stern markiert
Persönlicher Ordner
Schreibtisch
Documents
Downloads
Music
Pictures
Videos
Papierkorb
Dropbox
Website
hsgdata auf unisg.ch
hsg-tempdata$ auf sv-monk
ubuntu auf 86.119.37.165
ftp.datasus.gov.br
eftp.cdc.gov
venus.hcp.med.harvard.edu
Andere Orte
backup26082014
scrap_old
analysis1backupbeforerework.do
analysis6chaos.do
analysis_did.do
analysis_did26082014.do
analysis_did_orig.do
analysis_municipal_level.do
analysis_old.do
analysis_stock.do
analysis_stock_wo_cons_22042015.do
analysis_survival1.do
analysis_survival2.do
analysis_survival3.do
analysis_survival4.do
analysis_survival5.do
analysis_survival6.do
analysis_survival7.do
analysis_survival8.do
analysis_survival03092014.do
analysis_survival06032015.do
analysis_survival15092014.do
analysis_survival_05032015.do
analysis_survival_chaos21082014.do
analysis_survival_stock_nogapsprelim.do
analysis_survival_timeonstudy-old.do
desc.do
desc_did.do
desc_original.do
desc_survival2.do
geovars05032015.do
mapstuff.r
mapstuff1.r
mapstuffnew.r
mapstuff_old.r
prep2.do
prep05032015.do
prep18082014.do
prep29072014.do
prep129082014weights.do
prepold.do
prepolder.do

Familiar?


Persönlicher Ordner
Dropbox
Research
hte_paper
Code
Archive
Zuletzt verwendet
Mit Stern markiert
Persönlicher Ordner
Schreibtisch
Documents
Downloads
Music
Pictures
Videos
Papierkorb
Dropbox
Website
hsgdata auf unisg.ch
hsg-tempdata$ auf sv-monk
ubuntu auf 86.119.37.165
ftp.datasus.gov.br
eftp.cdc.gov
venus.hcp.med.harvard.edu
Andere Orte
Original-programs
0-functions-2019-12-12.r
0-functions-2019-12-13-equivalence-causal-forest.r
0-functions-2019-12-13-equivalence-efficient-score.r
0-functions-2020-01-29.r
0-functions-2020-01-31.r
0-functions-2020-01-31-2.r
0-prepare-data-stata-2019-12-13.do
1-prepare-inputs-2019-11-12.r
1-prepare-inputs-2019-11-13.r
1-prepare-inputs-2019-12-03.r
1-prepare-inputs-2020-01-17.r
1-prepare-inputs-2020-01-24.r
2-analysis-grf-2019-12-11.r
2-analysis-grf-2019-12-11-mess.r
2-analysis-grf-2020-01-26.r
2-analysis-grf-2020-01-29.r

Familiar?

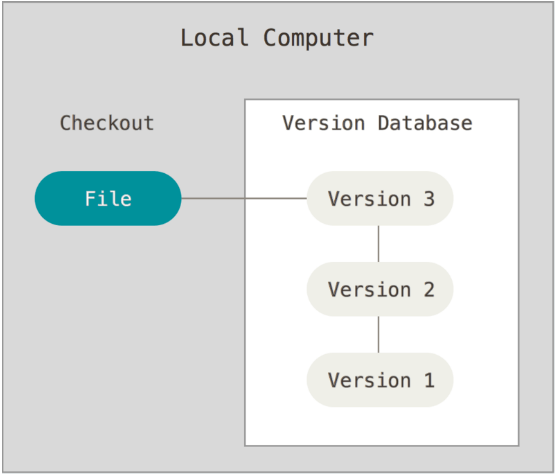


magit-revision: Code – Doom Emacs
Commits in master
82b1023 * master Update to run on Tulane's cypress cluster.
8af13ec * Fixes to subgroup analysis, duplicate/omission.
94d31a0 * Remove all policy var samples from results ouput.
d92494f * Activate again for last run.
1e0bb3c * Needs rerun because of bug.
b67ce22 * Fix parentheses.
ec5cad0 * Run only 100k analysis files.
1921cd0 * Add optimal lp w/ capacity constraint to 100k run.
c114fa4 * Adjusting writing/terminology for first draft.
88dc962 * Fixes.
9898a58 * Add sample ids and all other outcomes to each spec
2a7e6f0 * Add all of the new definitions for the GATE.
cc4110a * Remove, fix bug, save sample ids instead.
676434d * Restrict capacity range integer program.
2cf5a07 * Add capacity range constraint.
3d8ba15 * Add library.
8b7c3da * Fix naming with drop = FALSE.
e58d082 * Tentative, maybe unnecessary.
6b1f28f * Add additional subsets.
8e401f3 * Add optimal linear program. Remove alt policy call
86c2547 * Fixes and harmonizations.
3e03d56 * Clean, call only function.
0e5375c * Add optimal linear program.
2374011 * Updates Austin.
db88eff * Reordering.
06dfd0b * Fixes, more polict tree specs and wrapper function
092a252 * Linear programming draft.
b4571ee * Fix filtering bug.
5ecf1e9 * Changes to linear estimation specification.
c86d5f8 * Typo left from testing.
89bc523 * Revert to original approach, not faster.
b64c11b * Try alternative estimate policies approach.
580f3a2 * Fix file size reduction bug.
d68e545 * Improve runtime, this doesn't replace everything.
322ee22 * Save original objects for convenience.
5b3ee6d * Do not discard everything, just the sampling info.
ce0a8a0 * Save compliance and propensity score.
84d4d1e * Add policy trees and filter outcome list.
fa48871 * New variables for policy trees.
6ecd1ca * Refactor policy tree part in function.
24c4259 * Add predictions for both action.id and node.id.
65bbd33 * Add depth-3 trees.
34347a3 * Fix table labels.
9ff0e44 * Revert temporarily.
8d449ba * Round charge inputs.
99a4ff0 * Changes mostly from Austin for finalizing stuff.
dc4de71 * Changes Austin made for finalizing stuff.
30dbbee * Depth-3 tree for ITT 100k non-emerg., minimal spec
4270f20 * Minimal and no-algorithm vars tree specs.
a73c05a * Cleaning.
c4389fa * Update, even more tree specs.
bf3e296 * Legend on the bottom of gate plot.
db90f75 * More tree specs.
285ca57 * Add survey spec. Depth-3 only for 100k base ITT.
88c54a5 * Enable depth-3 tree with minimal vars for 100k.
14f0e57 * Add binary class. for pre-ed types and policy data
df28bb4 * More policy tree variations.
ab01878 * Revert for now.
8810c05 * Don't need to compute trees for the 3k runs.
3257fea * Additional file for the ITT results.
bab002d * Some updates plus variable importance plots.
96cd0c5 * Linear estimation fct and plot fixes for ITT.
1f64a0f * Add rownames to variable importance scores.
7b80dec * Enable depth-3 trees.
b163cab * Adjust naming scheme for binary class variable.
dca40dc * Missed deleting one outcome.
cf3e2e3 * Update.
a7f9362 * Stata output. Use strict classification for binary
79244c6 * Remove clustering.
592b43e * Fix and update inference calculations.
4f4d75b * Major updates.
c357466 * Min use, invert gamma scores for policy learning.
b662bf0 * Update policy tree estimation.
197992a * Minor patch.
commit 82b1023
Author: Helge Liebert <helge.liebert@gmail.com>
AuthorDate: Thu Aug 19 14:51:21 2021 +0200
Commit: Helge Liebert <helge.liebert@gmail.com>
CommitDate: Thu Aug 19 14:51:21 2021 +0200
Update to run on Tulane's cypress cluster.
4 files changed, 44 insertions(+), 68 deletions(-)
2-analysis-grf-100k.r | 28
2-analysis-grf-iv-100k.r | 28
2-analysis-grf-iv.r | 28
2-analysis-grf.r | 28
modified 2-analysis-grf-100k.r
Helge Desktop
Helge Laptop
-## Helge HCP Venus server
+## Austin Cypress
Austin
-## Functions, (re-)source
#================================= LIBRARIES =================================
<print> is undefined

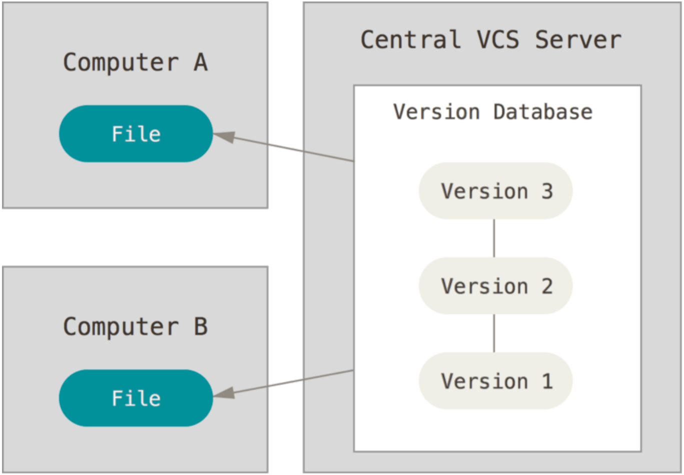
Tracking different versions

- Different options:
  - Don't keep track.
  - Keep file copies. Adhere to a versioning format. Write a changelog. Diff files.
  - Formal version control.
- Formal version control:
  - Ubiquitous in software development, extremely useful for many purposes.
  - Less established for statistical data management and analysis.
  - Workflow in data analysis differs. More effort to use properly.
  - Viewpoints on usefulness for data analysis vary.

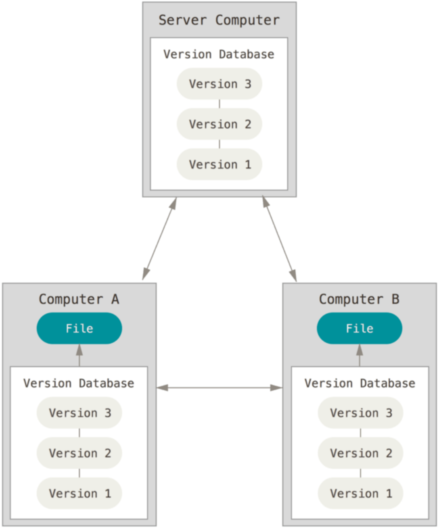
Local version control



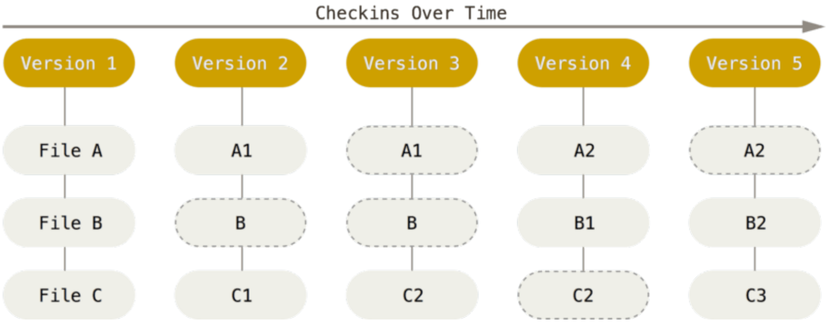
Centralized version control



Distributed version control



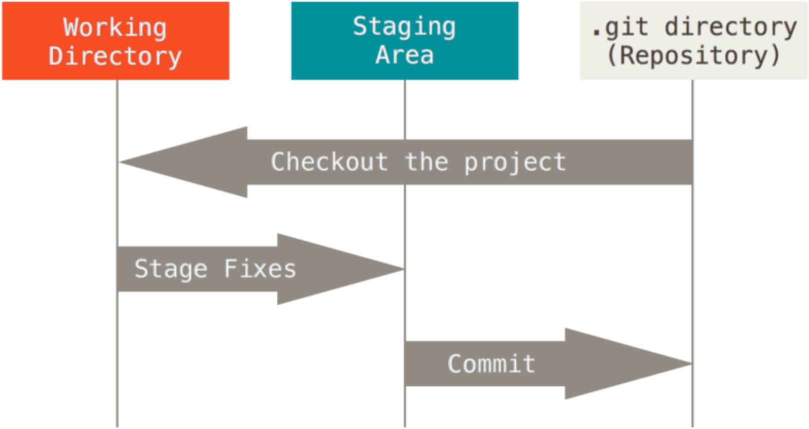
Distributed version control - snapshots



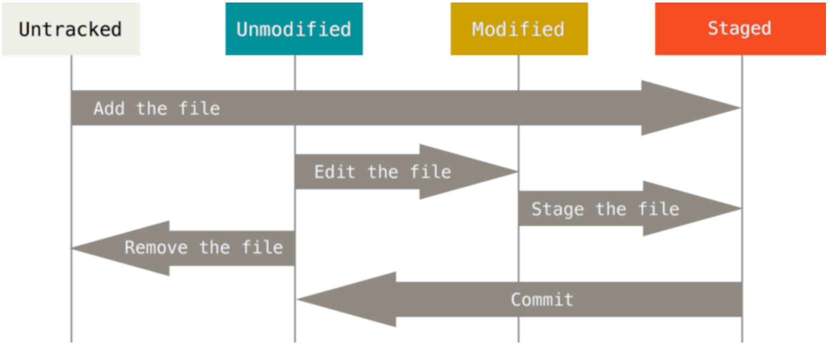
Git

- Git is the dominant *distributed* version control system today.
- Developed by Linus Torvalds, the creator of the Linux kernel.
- Can be used on the command line. GUIs/editor plugins available. Integrated into RStudio.
- Fast, good support for non-linear development (thousands of parallel branches).
- Tracks any content (but mostly plain text files).
  - Source code, manuscripts, websites, presentations, …
  - As a rule, do not version control data.

Workflow: Areas



Workflow: File lifecycle



Git

- Git stores the complete history of files and all changes you or others made to them in a local repository on your computer.
- You can have different ‘branches’ with different features, switch between them or merge them.
- You can keep a ‘remote’ copy of the repository on a server, but this is not required.
- You can ‘clone’ repositories from others and ‘push’ back changes you made to them.
- Public repositories facilitate collaboration and development.

Advantages and disadvantages

- Easy to track changes over time (from multiple people) and simple to revert them.
- Helps structure thoughts and makes you write cleaner code.
- Reproducible. Eases outside contributions and helps hunting down bugs.

- Requires work (to learn and to use), especially in the short term.
- More so if you have to convince your colleagues.
- Integrates less well with iterative back-and-forth workflow.

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➥ Useful for many projects.

➥ Good to understand the basics, even if you do not use it. Lots of programs are hosted on public git repositories, ubiquitous in industry.

Resources

- ProGit is a good and free resource. Skim the first few chapters.
- Software carpentry has a good introductory course. Many more resources online.
- Github is a site for online storage of Git repositories (Git $\neq$ Github!). You can create a remote repository there and push code to it. Public repositories are free.
- Github also offers student and educator accounts including free private repositories.
- Some editors offer *persistent undo* with branching, which can be very helpful (as long as you are aware of its limits—it is not a replacement for version control).

Command line interface

Command line interfaces

- A *command-line interface* (CLI) processes commands to a computer program in the form of lines of text.
- Different from *graphical user interfaces* (GUIs).
- The program which handles the interface is called a *command-line interpreter* or *shell*.
- A shell provides interactive or programmatic access to operating system functions and other services.
- CLI shells became the primary access to computer terminals starting in the mid-1960s. Also used by mainstream personal computers (Unix, MS-DOS, ...).

Terminals

Terminals

```
helge@helge-x250: ~
helge@helge-x250:~$ ssh -X liebert@venus.hcp.med.harvard.edu
liebert@venus.hcp.med.harvard.edu's password:
Last login: Fri Feb 14 12:33:14 2020 from 10.0.34.90
venus:/home/liebert$ ll
insgesamt 13
drwxr-xr-x+ 3 liebert users    3  8. Apr 2019  ado
drwx------+ 2 liebert users    5  5. Mär 2019  Desktop
drwx------+ 4 liebert users    4  4. Feb 15:10 hte_paper
drwx------+ 3 liebert users   10 11. Dez 06:26 iqr-simulation
drwx------+ 2 liebert users    7 11. Feb 10:38 Mortality
drwx------+ 4 liebert users    5  2. Dez 15:56 Physicians
drwx------+ 3 liebert users    3  2. Jul 2019  R
-rwx------+ 1 liebert users 1714 15. Jan 2019  Trash Bin.lnk
venus:/home/liebert$ cd Physicians/
venus:/home/liebert/Physicians$ xstata
venus:/home/liebert/Physicians$ logout
Connection to venus.hcp.med.harvard.edu closed.
helge@helge-x250:~$
```

Operating system shells

- Still in use today. Unix shells most relevant.
- Unix shells are used in Unix-derived systems (Linux, MacOS).
- Common operating system shells: `sh` (Unix), `cmd` (Windows); `bash`, `zsh` (Linux, MacOS), ...
- Unix-based operating systems (Linux, MacOS) have Bash/zsh pre-installed. Just start `Terminal`.
- On Linux, all system maintenance and software installation can be done via the shell.

Why does this matter?

- In 2019, 100% of the world's TOP500 supercomputers run on Linux.
- 96.3% of the world's top 1 million servers run on Linux.
- 90% of all cloud infrastructure operates on Linux.

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- sciCORE runs on Linux and uses CLI access.
- Switch engines provides Linux instances with CLI access.
- Amazon web services (AWS) provide Linux-based computing resources.
- So do Swisscom dynamic computing services.

➥ Much of the computing infrastructure you are likely to use will run Linux.

sciCORE

```
helge@helge-x250:~$ ssh -X cyfiwa67@login.scicore.unibas.ch
cyfiwa67@login.scicore.unibas.ch's password:
Last login: Fri Feb 14 18:49:10 2020 from vpn_pat.med.harvard.edu
            _  ____ ___  ____  _____
   ___  ___(_)/ ___/ _ \|  _ \| ____|
  / __|/ __| | |  | | | | |_) |  _|
  \__ \ (__| | |__| |_| |  _ <| |___
  |___/\___|_|\____\___/|_| \_\_____|


###################################################
    OS:               CentOS 7.5.1804
    Queing System:    Slurm
    support contact: scicore-admin@unibas.ch
###################################################

Check the cluster documentation in these links:
https://wiki.biozentrum.unibas.ch/display/scicore/sciCORE+user+guide
https://wiki.biozentrum.unibas.ch/display/scicore/Slurm+user+guide+at+sciCORE

Try "module av" or "module spider"  to see the list
of available software in the cluster.

For details about software management:
https://wiki.biozentrum.unibas.ch/display/scicore/sciCORE+user+guide#sciCOREuserguide-Software
https://lmod.readthedocs.io/en/latest/

[cyfiwa67@login10 ~]$ ll
insgesamt 0
[cyfiwa67@login10 ~]$ exit
Abgemeldet
Connection to login.scicore.unibas.ch closed.
helge@helge-x250:~$
```

A note on operating systems

- MacOS or Linux offer built-in access to a Unix shell (Bash or zsh).
- Further software is managed via a package management system and distributed via software repositories.
- On Linux, use your package manager to install anything you require.
- On MacOS, familiarize yourself with Homebrew. Install iterm2 if you want a fancier terminal.

- Windows does not provide proper access to a Unix shell out-of-the-box.
- Many common tools are not available or cumbersome to use.
- Windows has cmd (or PowerShell). These are not Unix shells and not a viable replacement for most use cases.
- Dependency resolution can be a nightmare. Package managers for Windows like scoop (or chocolatey) help.

What is a package manager?

"A package manager or package-management system is a collection of software tools that automates the process of installing, upgrading, configuring, and removing computer programs for a computer's operating system in a consistent manner."

- Software is installed and updated from official software repositories.
- System-level package managers: `apt, dnf, pacman, yum, homebrew, chocolatey, scoop, ...`
- Application-level package managers: `pip, conda, ...`
- Typically used via the command line.

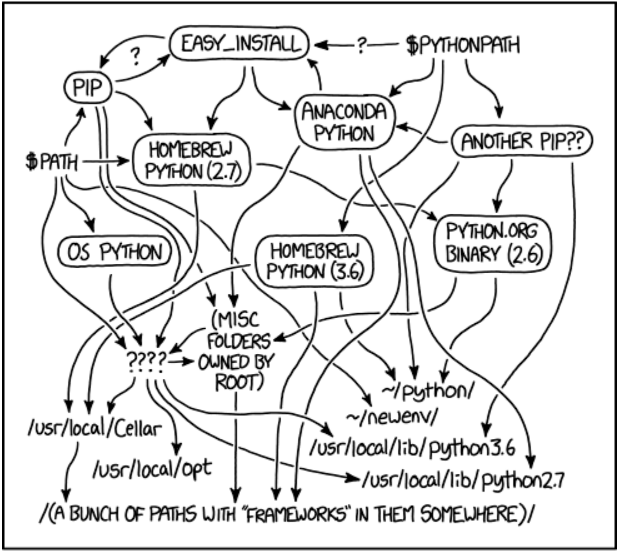
Reproducible research

- Often researchers write code and then leave it unused for a while.
- Software gets updated over time.
- Breaking changes may be introduced.
- Packages may be unmaintained and fail to work.
- Code you wrote years ago may not produce the same results any more, or fail to run at all.
- Preventing this is crucial for reproducible research.

Virtual environments

- If your projects rely on software from your global system environment, they will be prone to breakage and software rot.
- Virtual environment can help prevent this.
- Tool to keep dependencies required by different projects separate by creating isolated virtual environments for them.
- Environments can be exported/shared/saved.
- Exact dependencies incl. version numbers are specified in environment files.
- For Python: `venv`, `pipenv`, `conda env`, ...
- For R: `renv`, `conda env`.
- Most R libraries are now hosted on conda-forge (also easy to add).

Try to stick with one solution



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

More on reproducibility

- For setting up a reproducible project workflow, look into `snakemake`.
- Allows specifying all parts of a project (e.g. data management, analysis, input and output files of each step taken).
- If you want to set up a fully self-contained replication environment, look into `docker`.
- The Rocker project provides docker container images for R.
- Docker containers are also used to deploy models in production as they bundle their own dependencies and configuration and are relatively lightweight.
- The Turing Way Handbook is a great resource to get a broad overview over different options.

Simple CLI usage

- *Return* executes a command, *CTRL + c* aborts a process, *CTRL + d* quits.
- Multiple commands can be run as scripts (suffix `.sh`).
- Comment character is #.
- Some examples:

```
sudo apt install vlc # install vlc video player
cd somedir/subdir # Navigate to a folder, (c)hange (d)irectory
cd .. # Navigate to parent directory
cd # Return to your home folder
ls # List directory contents
mv file subdir/file # Move a file
cp file ../file # Copy a file
rm myscript.ch # Delete a file
R # Start the R console
man ssh # Display manual pages for the ssh program
shutdown -h +20 # Shut off computer in 20 minutes
```

Resources

- Basic knowledge often sufficient. Examples cover some ground.
- Google and O'Reilly/No Starch books and pocket references are handy.
- Software carpentry has an introductory course.
- (Brief) Introduction to the Bash Command Line
- Advanced Bash-Scripting Guide

More examples

```
# Secure shell login to remote server
ssh myusername@13.438.14.673

# Edit your R script with vim
vim myscript.r
# Search for file and open it
vim $(find -name somefile.txt)

# Execute your R script
R -f myscript.r
# Execute your Python script
python myscript.py
# Execute a shell script
sh myscript.sh

# Stage file for version control
git add myscript.py
# Commit file to version control tree
git commit myscript.py
```

Searching and filtering

- Great capabilities for pattern matching.

```
# Rename files by pattern, e.g. 'data_file1.csv' -> 'file1.csv'
rename data_ '' data_*.csv
```

- Searching/filtering of text is a very popular application.
- Popular unix filters
  - cat, head, tail, tee, wc, ...
  - cut, paste
  - find
  - sort, uniq
  - diff, comm, cmp
  - grep (or ag, ripgrep), sed, awk
  - (perl, python, ...)

Searching and filtering

- Sounds tedious? It can be. But it can also be extremely powerful.
- `grep` is a popular command line utility for searching plain text files.

```
# Search for keyword in filename
grep "keyword" filename
# Search for keyword, (i)gnore case, (r)ecursively, all files
grep -ir "keyword" *
# Print matching line and line (n)umber to output-file
grep -n "keyword" *.txt > output-file
```

Search patterns

- Convert all pdf files in a folder to text and search them.

```
for file in *.pdf; do pdftotext "$file"; done
grep -ir "keyword" *.txt
```

- Searching can be more complex than just keywords.
- Suppose you need to find all documents with sentences expressing proficiency in Spanish or Italian, but not English.

```
grep -ir
"(fluent|proficient)(?!.*?english)[^\.]*?(spanish|italian).*?\."
*.txt
```

Regular expressions

Regular expressions

- Working with text requires understanding regular expressions.
- `grep`: **g**lobally search a **r**egular **e**xpression and **p**rint.
- A regular expression is a character sequence that describes a set of strings.
- Regular expressions are constructed analogously to arithmetic expressions, by using various operators to combine smaller expressions.
- Usually used for find/replace operations on strings, or for validation.
- Pervasive in Unix text processing programs (`grep` was originally written by Ken Thompson).
- Language-independent concept. Not limited to command line search tools.

Regular expressions

- *Pattern matching*: Find one of a specified set of strings in text.
- Examples:
  - Diagnoses in medical records.
  - Addresses or zip codes in concatenated admin records.
  - Sequences within a genome, e.g. a virus signature.
  - Validate data-entry fields (URL, date, email, credit card #).
  - Example using a regex tester.

Obligatory xkcd

Examples

AHVN 13:	`756\.[0-9]{4}\.[0-9]{4}\.[0-9]{4}\.[0-9]{2}`
Matches:	`756.1234.5678.90`
Does not match:	`123.45.678.675`
US-SSN:	`[0-9]{3}-[0-9]{2}-[0-9]{4}`
Matches:	`166-11-4433`
Does not match:	`11-55555555`
Email addresses:	`[a-z]+@([a-z]+\.)+(ch|edu|com)`
Matches:	`someone@unibas.ch`
Does not match:	`someone@invalid.domain`

Screening job candidates

```
“ [First name]! and pre/2 [last name] w/7
  bush or gore or republican! or democrat! or charg!
  or accus! or criticiz! or blam! or defend! or iran contra
  or clinton or spotted owl or florida recount or sex!
  or controvers! or fraud! or investigat! or bankrupt!
  or layoff! or downsiz! or PNTR or NAFTA or outsourc!
  or indict! or enron or kerry or iraq or wmd! or arrest!
  or intox! or fired or racis! or intox! or slur!
  or controvers! or abortion! or gay! or homosexual!
  or gun! or firearm! ”
```

— *LexisNexis search string used by Monica Goodling to illegally screen candidates for DOJ positions*

LexisNexis™

http://www.justice.gov/oig/special/s0807/final.pdf

Regular expressions

- Characters in a regular expression are either regular characters (literal meaning) or metacharacters (special meaning).
- Generally, letters and numbers match themselves.
- Normally case sensitive, but can be set to ignore case.
- Careful with puntuation, most of it has special meanings.
- To match metacharacters literally, they need to be *escaped*, i.e. preceded by a backslash `\`.

Matching string literals

Regular expression	Input string
`input`	`This input string is short.`
`15`	`The due date is 15.12.`

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`15`	`The due date is 15.12.`
`15.12`	`The due date is 15.12.`
but:	
`15.12`	`The due date is 15712.`
match `.` literal:	
`15\.12`	`The due date is 15712.`
`15\.12`	`The due date is 15.12.`

Regex basics

Operation	Regular expression	Input string
concatenation	`foobar`	`Matches foobar but not foo or bar.`
disjunction	`this|that`	`Matches this or that.`
closure	`like.* apples`	`I like apples, Peter likes apples.` `Mary also likesALKFHEDL apples.`
	`like. apples`	`Mary also likesALKFHEDL apples.`
parentheses	`(He|She) likes`	`She likes apples. He likes apples.`
	`(He|She).*(very )*much\.`	`She likes apples very very much.`

- More complicated patterns can be expressed via concatenation, disjunction, repetition and scope.
- Precedence in descending order.

Quantifiers

Character	Matches
`*`	0 or more instances of preceding char
`+`	1 or more instances of preceding char
`?`	0 or one instance of preceding char
`{m}`	exactly `m` instances of preceding char
`{m,n}`	`m` through `n` instances of preceding char
`{m,}`	`m` or more instances of preceding char
`{,n}`	up to `n` instances of preceding char
`?`	add to a quantifier to match ungreedy

- Quantifiers match greedily by default (i.e. the longest string possible).

  Ex: `^begin.*end` will match 'begin bla bla end bla end'.
  `^begin.*?end` will match 'begin bla bla end bla end'.

Groups, ranges and character classes

Character	Matches	Example RE	Matches
`.`	Any character, except `\n`	`like.`	`likes like! like  like`
`(a|b)`	a or b	`(you|me)`	`you or me`
`[ab]`	Character range	`202[01]`	`2019 2020 2021 2022`
`[a-z]`	Character range	`[A-Z][a-z]*`	Capitalized words
`[0-9]`	Digit range	`20[0-9]{2}`	Years in the 21st century
`[^ab]`	Any character but (negation)	`20[^0][01]`	`2000 2010 2020 2025 2031`

- Quantifiers, ranges and other shortcuts improve expressiveness.
  Ex: `[A-E]+` is shorthand for `(A|B|C|D|E)(A|B|C|D|E)*`.
- More character classes (sometimes) available.
  Ex: `\w` for words (`[A-Za-z0-9_]`), or `\d` for digits (`[0-9]`), `\a`, `\s`, ...

Anchors and other special characters

Character	Matches	Example RE	Matches
`^`	Beginning of a string	`^New`	New research in this field
`$`	End of a string	`[A-Za-z]+!$`	A breakthrough! Finally!
`\n`	Newline		
`\t`	Tab		
…	…		

- Strings can stretch multiple lines.
- Character encodings can sometimes cause problems. Stick to UTF-8.

Regex syntaxes

- More elaborate regex syntaxes also support positive and negative lookahead/lookbehind, conditionals and group references.
  Ex: `^(?!.*word).*$` matches lines not containing a word.
- Different syntaxes (basic, extended, perl, vim, ...) mostly similar with regard to basic features.
- Perl-compatible regular expressions (PCRE) is the de-facto standard.
- Most regex implementations feature switches to invert the search pattern, to ignore case, and more.

Example: Valid RFC-822 email addresses

http://www.ex-parrot.com/ pdw/Mail-RFC822-Address.html

Remarks

- Writing a regular expression is like writing a program.
- Requires understanding the programming model.
- Can be easier to write than read.
- Can be difficult to debug.

➥ Break up problems into smaller pieces. Try not to do everything in one large regex. Comment liberally.

Resources

- Pin a cheat sheet to your office wall.
- Regular expression tools help (e.g. regex101.com).
- Simple interactive tutorial: regexone.com. Also learn regex the easy way.
- For regular expression syntax specific to R, look up this short tutorial.
- This guide also provides a more detailed overview of working with strings in R.

Remarks

- Regexes are a powerful tool.
- Easy to grasp, complex to master.

- Using them in applications can be complex and error-prone.
- Regular expressions are not parsers.

> *"Some people, when confronted with a problem, think 'I know, I'll use regular expressions.' Now they have two problems."*
>
> *Emacs newsgroup*

Next lecture: Web scraping basics

References

References

- Barrett, D. J. (2016). *Linux Pocket Guide*. Third edition. Beijing ; Boston: O'Reilly.
- Chacon, S. and B. Straub (2014). *Pro Git*. Apress.
- Fitzgerald, M. (2012). *Introducing Regular Expressions: Unraveling Regular Expressions, Step-by-Step*. 1. ed. Beijing: O'Reilly.
- Matloff, N. (2011). *The Art of R Programming: A Tour of Statistical Software Design*. No Starch Press.
- Robbins, A. (2000). *Sed & Awk Pocket Reference*. 1st ed. Beijing ; Sebastopol, CA: O'Reilly & Associates.
- Robbins, A. (2010). *Bash Pocket Reference*. 1st ed. Beijing ; Sebastopol, CA: O'Reilly.
- Shotts, W. E. (2019). *The Linux Command Line: A Complete Introduction*. Second edition. San Francisco: No Starch Press.