Best Practices for Reproducible Research

Arnaud Legrand

SyncFree Meeting, Paris, May 2014

Outline

1. Reproducible Research
   - Looks familiar?
   - A few Tools for Experiment Setup and Management
   - Many Different Alternatives for Reproducible Analysis
2. R Crash Course
   - General Introduction
   - Reproducible Documents: knitR
   - Introduction to R
   - Needful Packages by Hadley Wickam
3. Setting up a Laboratory Notebook
   - Emacs Demo of How to Keep Things Tidy

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As a Reviewer

This may be an interesting contribution but:

- This average value must hide something
- As usual, there is no confidence interval, I wonder about the variability and whether the difference is significant or not
- That can't be true, I'm sure they removed some points
- Why is this graph in logscale? How would it look like otherwise?
- The authors decided to show only a subset of the data. I wonder what the rest looks like
- There is no label/legend/... What is the meaning of this graph? If only I could access the generation script

As an Author

- I thought I used the same parameters but I'm getting different results!
- The new student wants to compare with the method I proposed last year
- My advisor asked me whether I took care of setting this or this but I can't remember
- The damned fourth reviewer asked for a major revision and wants me to change figure 3 :(
- Which code and which data set did I use to generate this figure?
- It worked yesterday!
- 6 months later: why did I do that?

My Feeling

Computer scientists have an incredibly poor training in probabilities, statistics, experimental management

Why should we? Computer are deterministic machines after all, right? ;)

Ten years ago, I've started realizing how lame the articles I reviewed (as well as those I wrote) were in term of experimental methodology.

- Yeah, I know, your method/algorithm is better than the others as demonstrated by the figures
- Not enough information to discriminate real effects from noise
- Little information about the workload
- Would the "conclusion" still hold with a slightly different workload?
- I'm tired of awful combination of tools (perl, gnuplot, sql, . . .) and bad methodology

Current practice in CS

Computer scientists tend to either:

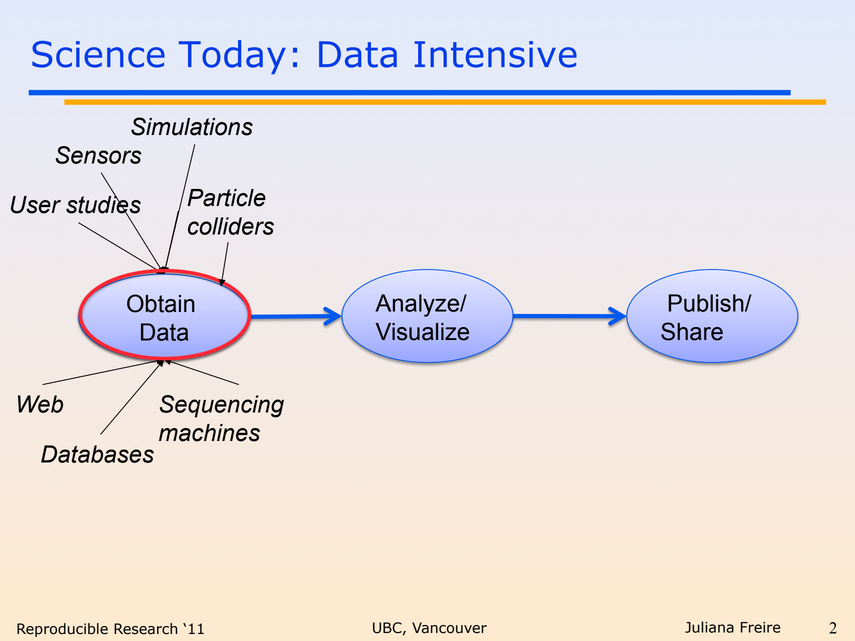
- vary one factor at a time, use a very fine sampling of the parameter range,
- run millions of experiments for a week varying a lot of parameters and then try to get something of it. Most of the time, they (1) don't know how to analyze the results (2) realize something went wrong...

Interestingly, most other scientists do the exact opposite.

These two flaws come from poor training and from the fact that C.S. experiments are almost free and very fast to conduct

- Most strategies of experimentation (DoE) have been designed to provide sound answers despite all the randomness and uncontrollable factors
- Maximize the amount of information provided by a given set of experiments
- Reduce as much as possible the number of experiments to perform to answer a given question under a given level of confidence

Takes a few lectures on Design of Experiments to improve but anyone can start by reading Jain's book on The Art of Computer Systems Performance Analysis



Science Today: Data Intensive

Simulations

Sensors

User studies

Particle colliders

Obtain Data

Analyze/ Visualize

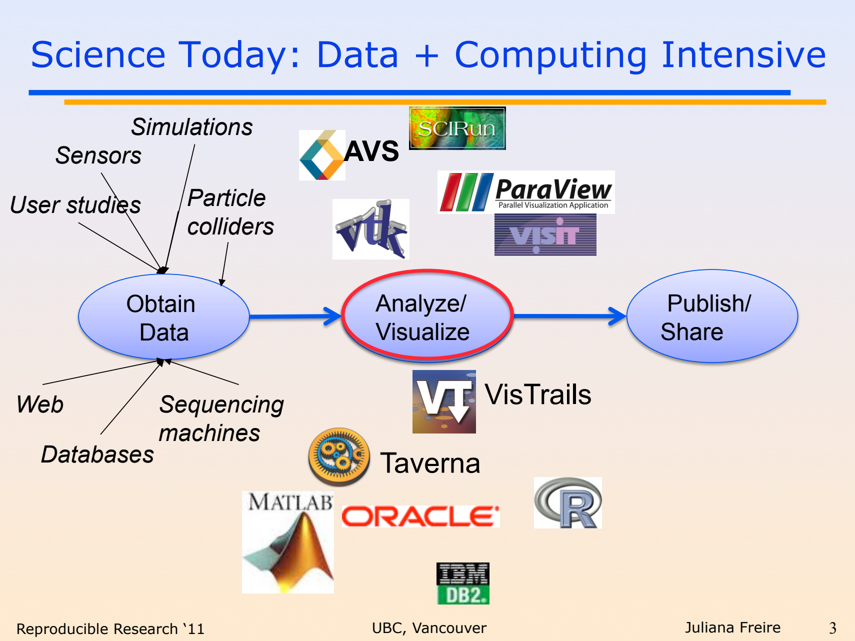
Publish/ Share

Web

Sequencing machines

Databases

Courtesy of Juliana Freire (AMP Workshop on Reproducible research)



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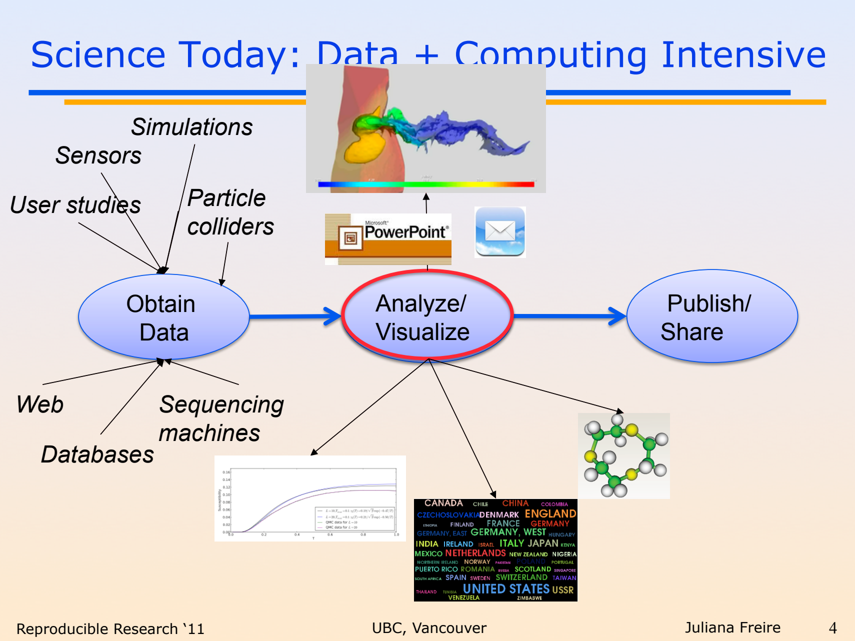

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MEXICO NETHERLANDS NEW ZEALAND NIGERIA
NORTHERN IRELAND NORWAY PAKISTAN POLAND PORTUGAL
PUERTO RICO ROMANIA RUSSIA SCOTLAND SINGAPORE
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THAILAND TUNISIA UNITED STATES USSR
VENEZUELA ZIMBABWE

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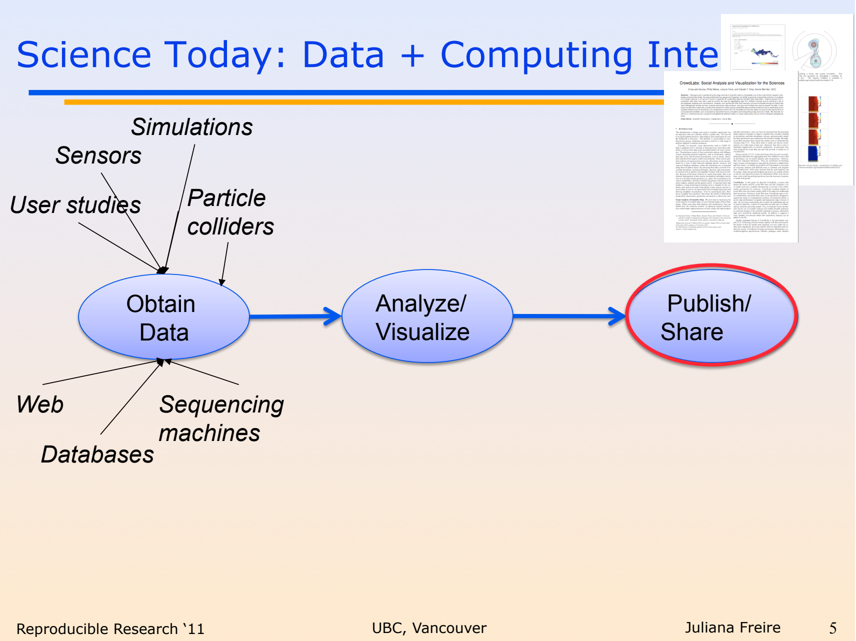

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CrowdLabs: Social Analysis and Visualization for the Sciences

Emanuele Santos, Phillip Mates, Juliana Freire, and Cláudio T. Silva, Senior Member, IEEE

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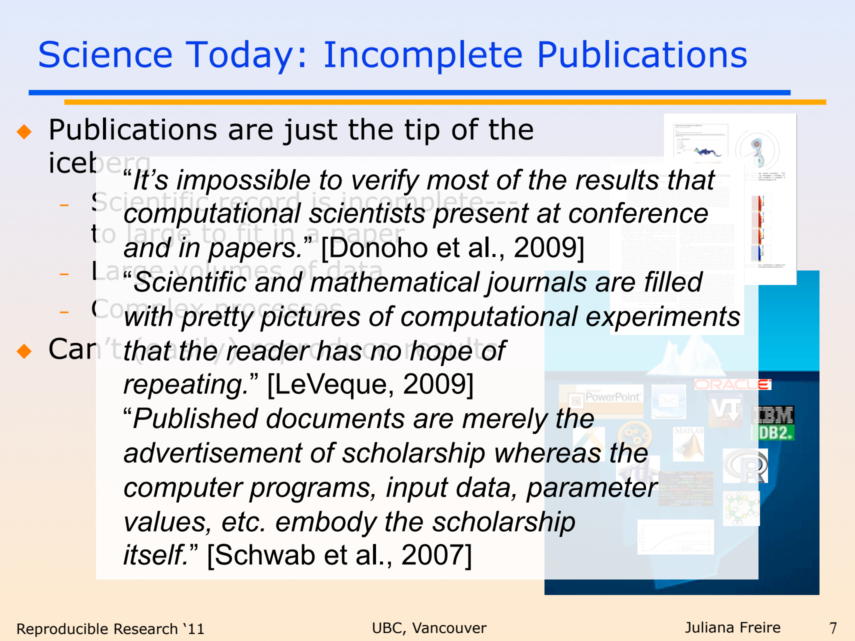
Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Science Today: Incomplete Publications

- Publications are just the tip of the iceberg
  - Scientific record is incomplete--- to large to fit in a paper
  - Large volumes of data
  - Complex processes
- Can't (easily) reproduce results

CrowdLabs: Social Analysis and Visualization for the Sciences
Microsoft PowerPoint
ORACLE
VT
IBM DB2
MATLAB
vtk
R

Courtesy of Juliana Freire (AMP Workshop on Reproducible research)



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"*It's impossible to verify most of the results that computational scientists present at conference and in papers.*" [Donoho et al., 2009]

"*Scientific and mathematical journals are filled with pretty pictures of computational experiments that the reader has no hope of repeating.*" [LeVeque, 2009]

"*Published documents are merely the advertisement of scholarship whereas the computer programs, input data, parameter values, etc. embody the scholarship itself.*" [Schwab et al., 2007]

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Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

A few Words on Scientific Fundation

- Falsifiability or refutability of a statement, hypothesis, or theory is an inherent possibility to prove it to be false (not "*commit fraud*" but "*prove to be false*").
- Karl Popper makes falsifiability the demarcation criterion to distinguish the scientific from the unscientific

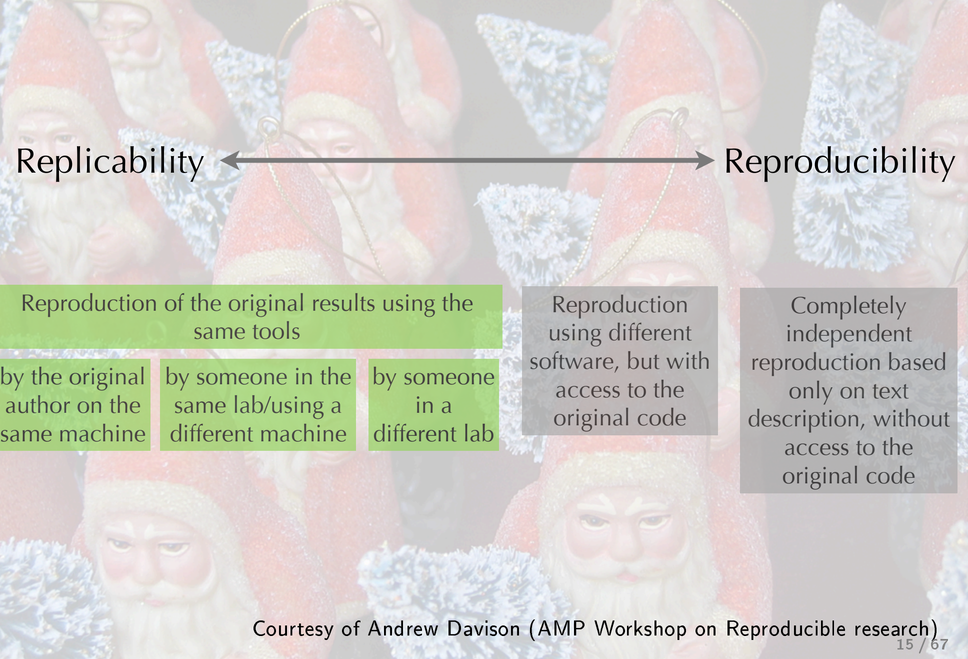
> *It is not only not right, it is not even wrong!*
> – *Wolfgang Pauli*

- Theories cannot be proved correct but they can be disproved. Only a few stand the test of batteries of critical experiments.
- It is not all black and white. There are many stories where scientists stick with their theories despite evidences and sometimes, they were even right to do so...

Testing and checking is thus one of the basis of science

Further readings: A Summary of Scientific Method*, Peter Kosso, Springer

Reproducibility: What Are We Talking About?



Replicability ⟷ Reproducibility

Reproduction of the original results using the same tools

- by the original author on the same machine
- by someone in the same lab/using a different machine
- by someone in a different lab

Reproduction using different software, but with access to the original code

Completely independent reproduction based only on text description, without access to the original code

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Why Are Scientific Studies so Difficult to Reproduce?

- Publication/Experimental bias
- Rewards for positive results
- Programming errors or data manipulation mistakes
- Poorly selected statistical tests
- Multiple testing, multiple looks at the data, multiple statistical analyses
- ~~Lack of easy-to-use tools~~

Courtesy of Adam J. Richards

Evidence for a Lack of Reproducibility

- Studies showing that scientific papers commonly leave out experimental details essential for reproduction and showing difficulties with replicating published experimental results:
  - J.P. Ioannidis. *Why Most Published Research Findings Are False* PLoS Med. 2005 August; 2(8)
- High number of failing clinical trials.
  - *Do We Really Know What Makes Us Healthy?*, New-York Times — September 16, 2007
  - *Lies, Damned Lies, and Medical Science*, The Atlantic. 2010, Nov.
- Increase in retracted papers:
  - Steen RG, *Retractions in the scientific literature: is the incidence of research fraud increasing?* J Med Ethics 37: 249–253.

Courtesy of Adam J. Richards

Why Bother Making Our Work Reproducible?

The Duke University scandal with scientific misconduct on lung cancer

- *Nature Medicine* - 12, 1294 - 1300 (2006) Genomic signatures to guide the use of chemotherapeutics, by Anil Potti and 16 other researchers from Duke University and University of South Florida
- Major commercial labs licensed it and were about to start using it before two statisticians discovered and publicized its faults

Dr. Baggerly and Dr. Coombes found errors almost immediately. Some seemed careless — moving a row or a column over by one in a giant spreadsheet — while others seemed inexplicable. The Duke team shrugged them off as "clerical errors."

The Duke researchers continued to publish papers on their genomic signatures in prestigious journals. Meanwhile, they started three trials using the work to decide which drugs to give patients.

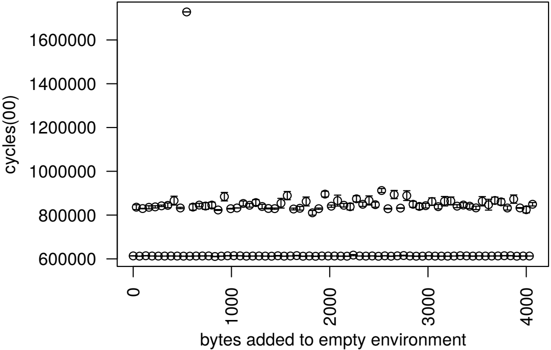
- Retracted: 07 January 2011. Ten papers that Potti coauthored in prestigious journals were retracted for varying reasons
- Some people die and may be getting worthless information that is based on bad science

Courtesy of Adam J. Richards

Is CS Concerned Really With This?

Yes, although designed and built by human beings, computers are so complex that mistakes are easy to do. . .

- T. Mytkowicz, A. Diwan, M. Hauswirth, and P. F. Sweeney. Producing wrong data without doing anything obviously wrong!. SIGPLAN Not. 44(3), March 2009



Key principles of experiment design

- Randomize to reduce bias
- Replicate to increase reliability

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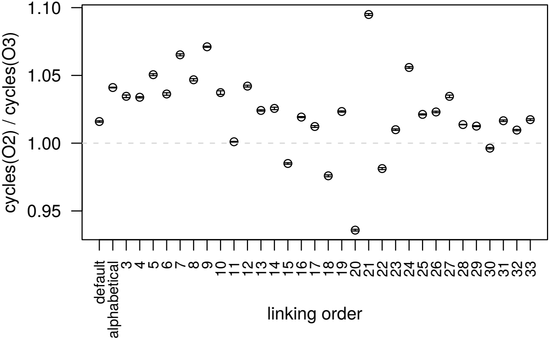

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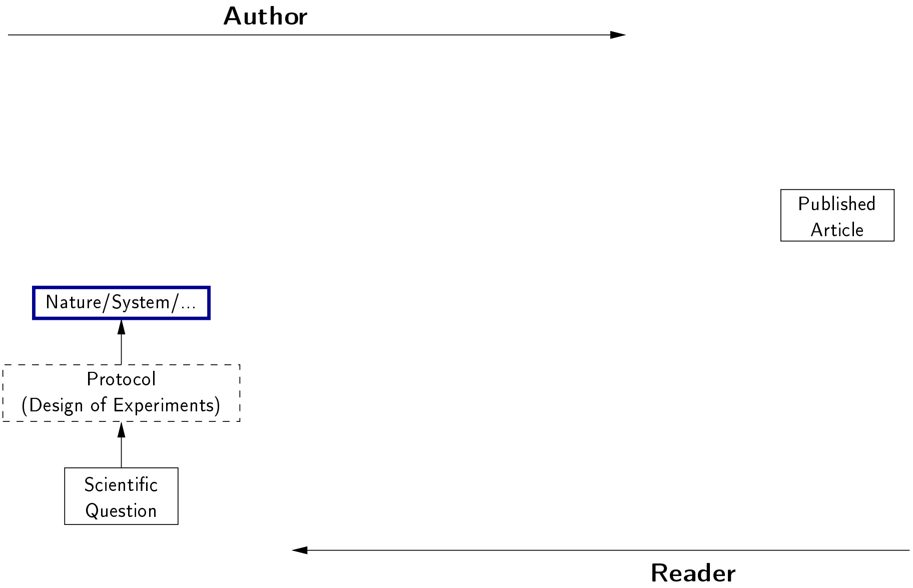
Reproducible Research: Trying to Bridge the Gap



Courtesy of Roger D. Peng (Coursera lecture on reproducible research, May 2014)

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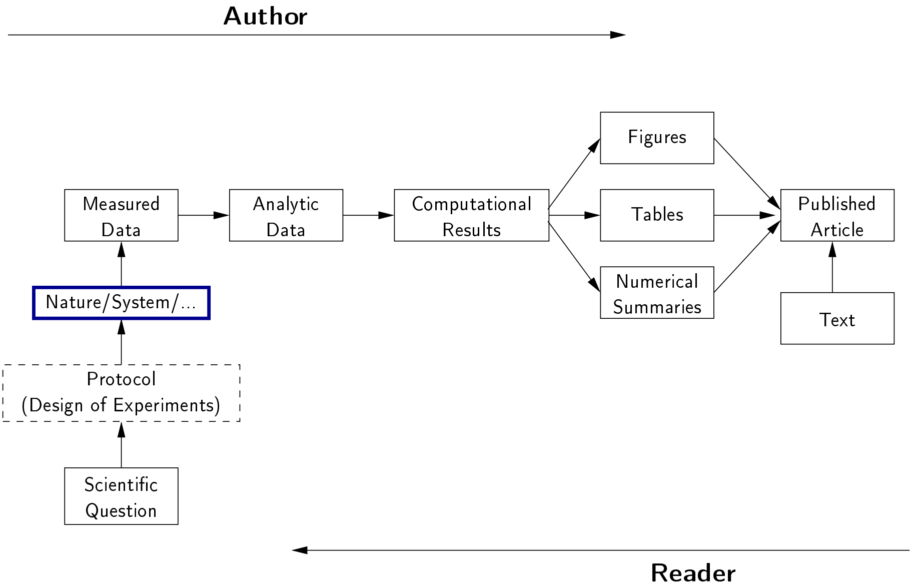

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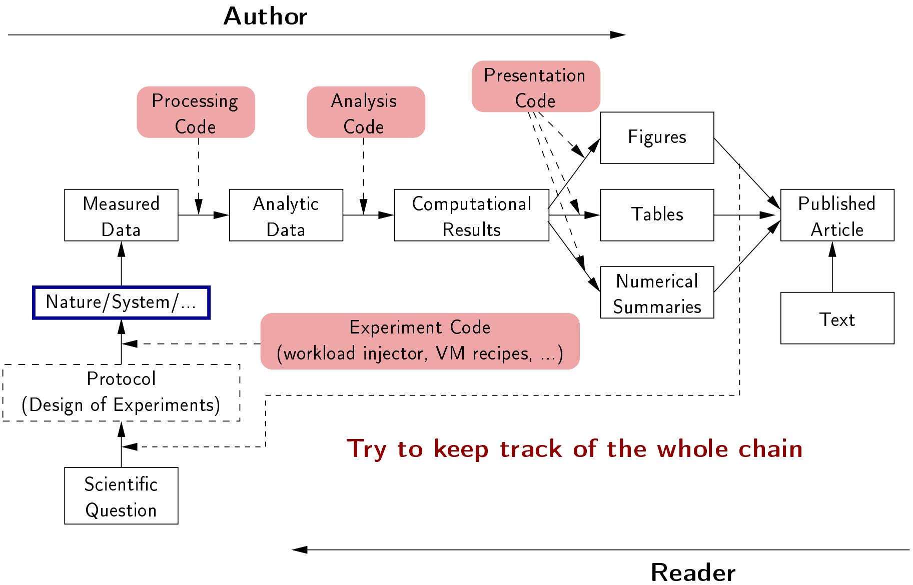

Try to keep track of the whole chain

Courtesy of Roger D. Peng (Coursera lecture on reproducible research, May 2014)

A Difficult Trade-off

Automatically keeping track of everything

- the code that was run (source code, libraries, compilation procedure)
- processor architecture, OS, machine, date, . . .

VM-based solutions and experiment engines

Ensuring others can redo/understand what you did

- Why did I run this?
- Does it still work when I change this piece of code for this one?

Laboratory notebook and recipes

Reproducible Research: the New Buzzword?

H2020-EINFRA-2014-2015

> *A key element will be capacity building to link literature and data in order to enable a more transparent evaluation of research and reproducibility of results.*

More and more workshops

- Workshop on Duplicating, Deconstructing and Debunking (WDDD) (2014 edition)
- Reproducible Research: Tools and Strategies for Scientific Computing (2011)
- Working towards Sustainable Software for Science: Practice and Experiences (2013)
- REPPAR'14: 1st International Workshop on Reproducibility in Parallel Computing
- Reproducibility@XSEDE: An XSEDE14 Workshop
- Reproduce/HPCA 2014
- TRUST 2014

Should be seen as opportunities to share experience.

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Many Alternative Tools Exist

- Naive way: sh + ssh + . . .

- Expo (2007-, G5K)
- XPflow (2012-, G5K)
- Execo (2013-, G5K)

$\left.\right\}$ although nothing specific to G5K

- Plush (2006-, PlanetLab)
- OMF (2009-, Wireless testbeds and Planetlab)
- Splay (2008, distributed algorithm comparison)
- . . .

They differ in the underlying paradigms and the platforms for which they have been designed

- A taxonomy of experiment management tools for distributed systems, T. Buchert, C. Ruiz , L. Nussbaum, O. Richard, FGCS, 2014

I'll present the few that I know and which are developed at Inria

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Expo

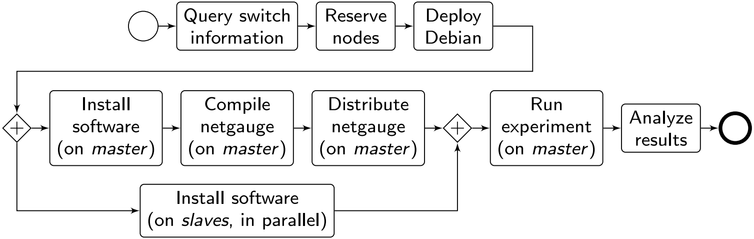
- Grenoble (B. Videau, C. Ruis, O. Richard) http://expo.gforge.inria.fr/
- DSL (Domain Specific Language) derived from Ruby and adapted to the management of experiment (based on taktuk, i.e., sh + ssh)
- At the moment Expo interacts with Planetlab and Grid5000 testbeds
- Resource and task abstractions, client-server organization, interactive or batch mode
- Native logging and archiving capabilities
  - every action performed on tasks, error flows, dates, . . .
  - lets you know what was run, when, where and how

```
reserv=ExpoEngine::new(@connection)
reserv.site=["bordeaux","lille","luxembourg","nancy","sophia"]
reserv.resources=["nodes=50","nodes=10","nodes=4","nodes=4","nodes=30"]
reserv.name = "Expo Scalability"
reserv.walltime=600

reserv.run!
ptask $all, "hostname"
reserv.stop!
```

XPflow

- Nancy (T. Buchert, L. Nussbaum) http://xpflow.gforge.inria.fr/
- DSL (Domain Specific Language) derived from Ruby and adapted to the management of experiment
- Resources, process, and activities
- Top-down rather than bottom-up: business process management
- Cope with failures through snapshotting and retry policy


Query switch information
Reserve nodes
Deploy Debian
Install software (on *master*)
Compile netgauge (on *master*)
Distribute netgauge (on *master*)
Install software (on *slaves*, in parallel)
Run experiment (on *master*)
Analyze results

Courtesy of T. Buchert

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```
process :exp do |site, switch|
    s = run g5k.switch, site, switch
    ns = run g5k.nodes, s
    r = run g5k.reserve_nodes,
        :nodes => ns, :time => '2h',
        :site => site, :type => :deploy
    master = (first_of ns)
    rest = (tail_of ns)
    run g5k.deploy,
        r, :env => 'squeeze-x64-nfs'
    checkpoint :deployed
    parallel :retry => true do
        forall rest do |slave|
            run :install_pkgs, slave
        end
        sequence do
            run :install_pkgs, master
            run :build_netgauge, master
            run :dist_netgauge,
                master, rest
        end
    end
    checkpoint :prepared
    output = run :netgauge, master, ns
    checkpoint :finished
    run :analysis, output, switch
end
```

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```

Activity :install_pkgs

```
activity :install_pkgs do|node|
    log 'Installing packages on ', node
    run 'g5k.bash', node do
        aptget :update
        aptget :upgrade
        aptget :purge, 'mx'
    end
end
```

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```

Activity :build_netgauge

```
activity :build_netgauge do |master|
    log "Building netgauge on #{master}"
    run 'g5k.copy', NETGAUGE, master, '~'
    run 'g5k.bash', master do
        build_tarball NETGAUGE, PATH
    end
    log "Build finished."
end
```

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```

Activity :dist_netgauge

```
activity :dist_netgauge do |m, s|
    master, slaves = m, s
    run 'g5k.dist_keys', master, slaves
    run 'g5k.bash', master do
        distribute BINARY,
            DEST, 'localhost', slaves
    end
end
```

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```

Activity :netgauge

```
activity :netgauge do |master, nodes|
    log "Running experiment..."
    out = run 'g5k.bash', master do
        cd PATH
        mpirun nodes, "./netgauge"
    end
    log "Experiment done."
end
```

Courtesy of T. Buchert

Execo

- Lyon (M. Imbert, L. Pouilloux) http://execo.gforge.inria.fr/
- Python-based API, script-oriented, fork+sh+ssh or taktuk
- Process: start/wait/kill, error/exit_code, stdout/stderr
- Heavy use of inheritence:
  - Process $\rightsquigarrow$ SshProcess
  - Engine $\rightsquigarrow$ g5k_cluster_engine/openstack_engine/vm5k

Kameleon

- Grenoble (C. Ruiz, S. Harrache, M. Mercier, O. Richard, . . .)
  http://kameleon.readthedocs.org/
- Generate customized appliances (kvm, LXC, Virtualbox, iso, . . .)
- Ruby-based, YAML description of recipes with steps and aliases, execution in contexts
- Automatically checkpoints to rebuild only what is required
- Relies on "under development" tools (e.g., qemu-nbd) but I managed to setup working VMs for today without much trouble

Providing not only VMs but also recipe is good!

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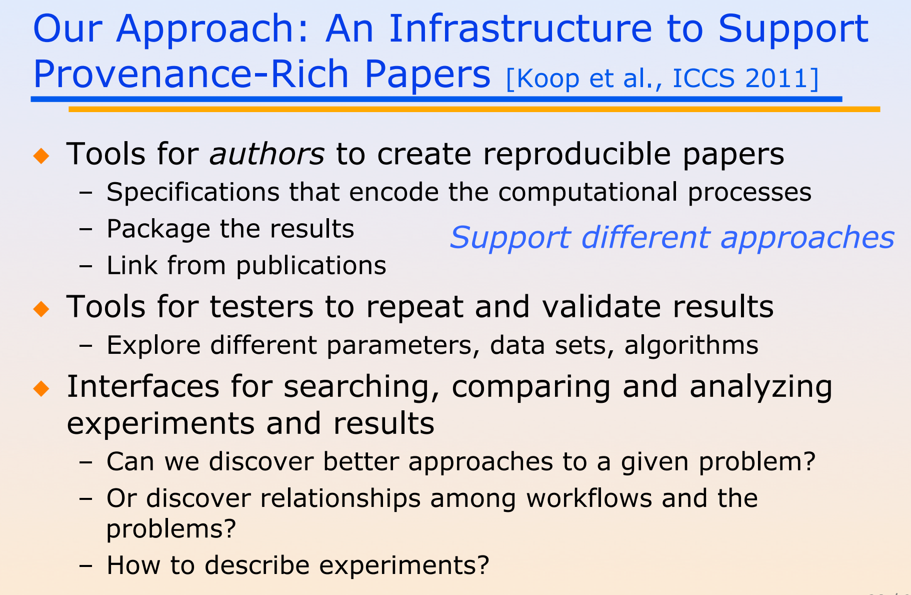
   - Emacs Demo of How to Keep Things Tidy

Vistrails: a Workflow Engine for Provenance Tracking



Our Approach: An Infrastructure to Support Provenance-Rich Papers [Koop et al., ICCS 2011]

- Tools for *authors* to create reproducible papers
  - Specifications that encode the computational processes
  - Package the results
  - Link from publications

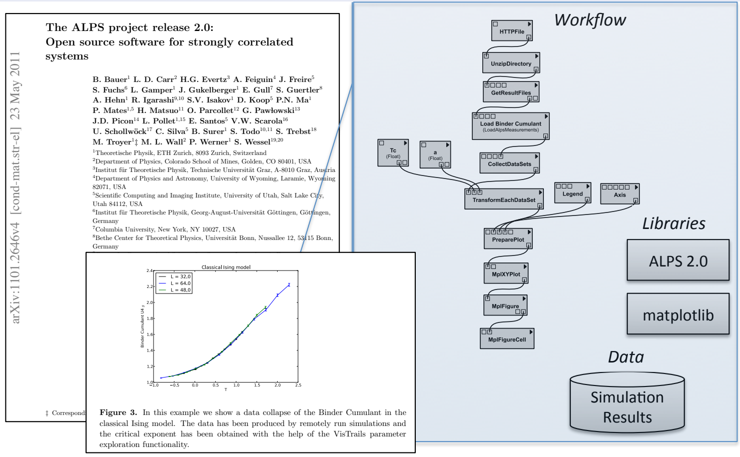
Support different approaches

- Tools for testers to repeat and validate results
  - Explore different parameters, data sets, algorithms
- Interfaces for searching, comparing and analyzing experiments and results
  - Can we discover better approaches to a given problem?
  - Or discover relationships among workflows and the problems?
  - How to describe experiments?

Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

Vistrails: a Workflow Engine for Provenance Tracking

An *Provenance-Rich* Paper: ALPS2.0



arXiv:1101.2646v4 [cond-mat.str-el] 23 May 2011

The ALPS project release 2.0:
Open source software for strongly correlated systems

B. Bauer[1] L. D. Carr[2] H.G. Evertz[3] A. Feiguin[4] J. Freire[5] S. Fuchs[6] L. Gamper[1] J. Gukelberger[1] E. Gull[7] S. Guertler[8] A. Hehn[1] R. Igarashi[9,10] S.V. Isakov[1] D. Koop[5] P.N. Ma[1] P. Mates[1,5] H. Matsuo[11] O. Parcollet[12] G. Pawłowski[13] J.D. Picon[14] L. Pollet[1,15] E. Santos[5] V.W. Scarola[16] U. Schollwöck[17] C. Silva[5] B. Surer[1] S. Todo[10,11] S. Trebst[18] M. Troyer[1]‡ M. L. Wall[2] P. Werner[1] S. Wessel[19,20]

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‡ Correspond

Figure 3. In this example we show a data collapse of the Binder Cumulant in the classical Ising model. The data has been produced by remotely run simulations and the critical exponent has been obtained with the help of the VisTrails parameter exploration functionality.

[Bauer et al., JSTAT 2011]

Courtesy of Juliana Freire (AMP Workshop on Reproducible research)

VCR: A Universal Identifier for Computational Results

Chronicing computations in real-time

VCR computation platform Plugin = Computation recorder

Regular program code

```
figure1 = plot(x)
save(figure1,'figure1.eps')
```

```
> file /home/figure1.eps saved
>
```

Courtesy of Matan Gavish and David Donoho (AMP Workshop on Reproducible research)

VCR: A Universal Identifier for Computational Results

Chronicing computations in real-time

VCR computation platform Plugin = Computation recorder

Program code with VCR plugin

```
repository vcr.nature.com
verifiable figure1 = plot(x)
```

```
> vcr.nature.com approved:
> access figure1 at https://vcr.nature.com/ffaaffb148d7
```

Courtesy of Matan Gavish and David Donoho (AMP Workshop on Reproducible research)

VCR: A Universal Identifier for Computational Results

Word-processor plugin App

LaTeX source

```
\includegraphics{figure1.eps}
```

LaTeX source with VCR package

```
\includeresult{vcr.thelancet.com/ffaaffb148d7}
```

Permanently bind printed graphics to underlying result content

Courtesy of Matan Gavish and David Donoho (AMP Workshop on Reproducible research)

VCR: A Universal Identifier for Computational Results

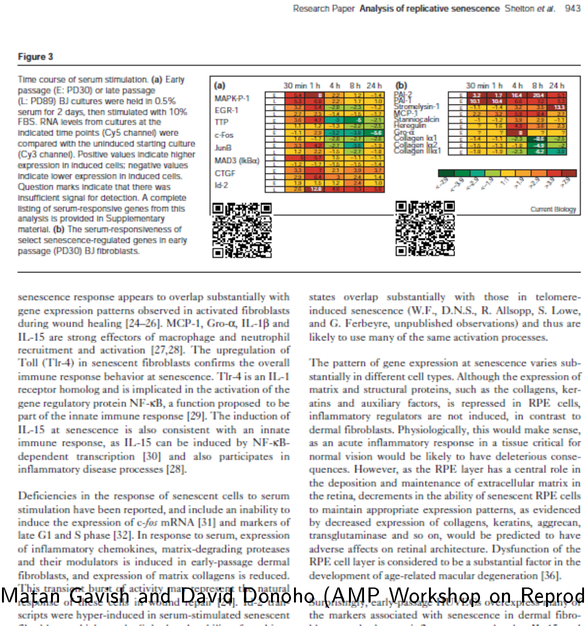


Figure 3

Time course of serum stimulation. **(a)** Early passage (E: PD30) or late passage (L: PD89) BJ cultures were held in 0.5% serum for 2 days, then stimulated with 10% FBS. RNA levels from cultures at the indicated time points (Cy5 channel) were compared with the uninduced starting culture (Cy3 channel). Positive values indicate higher expression in induced cells; negative values indicate lower expression in induced cells. Question marks indicate that there was insufficient signal for detection. A complete listing of serum-responsive genes from this analysis is provided in Supplementary material. **(b)** The serum-responsiveness of select senescence-regulated genes in early passage (PD30) BJ fibroblasts.

(a)

		30 min	1 h	4 h	8 h	24 h
MAPK-P-1	E	5.4	8	2.2	1.2	–1.4
	L	5.3	6.8	2.2	1.7	1.0
EGR-1	E	3.2	5.4	–2.8	–2.3	–1.2
	L	2.7	2.3	–1.4	–1.6	–1.7
TTP	E	3.6	4.7	–3	–5	–2.1
	L	1.1	1.2	–1.3	–2.2	–2.5
c-Fos	E	–1.1	2.9	–3.2	–3.8	–5.6
	L	1.6	–1.7	–2.8	–2.7	–2.6
JunB	E	3.3	4.2	–2.7	–3.6	–1.9
	L	1.2	2.2	–1.5	–2.7	–1.8
MAD3 (IkBα)	E	5	5.7	1.5	–1.1	–1.1
	L	–1.2	–1.7	–1.5	–1.5	–1.4
CTGF	E	3.3	7	2.1	3.9	3.7
	L	2.9	6.4	3	2.4	1.4
Id-2	E	1.9	1.5	1.2	2.4	1.0
	L	2.6	12.8	4.6	5.3	5.8

(b)

		30 min	1 h	4 h	8 h	24 h
PAI-2	E	3.2	1.7	16.4	20.4	5.1
PAI-1	E	10.1	10.4	6.6	7.2	5.3
Stromelysin-1	E	–1.1	–1.4	3.2	3.5	13.3
MCP-1	E	2.2	3.2	6.9	8.4	2.7
Stanniocalcin	E	–1	–1.2	3.9	2.9	–1.1
Heregulin	E	?	1.6	4.3	3.6	2.3
Gro-α	E	?	?	8	?	?
Collagen Iα1	E	–1.4	–1.1	–2.3	–8.6	–2.5
Collagen Iα2	E	–1.5	–1.3	–1.8	–4.9	–2
Collagen IIIα1	E	–1.8	–1.9	–2.3	–6.2	–3.8

senescence response appears to overlap substantially with gene expression patterns observed in activated fibroblasts during wound healing [24–26]. MCP-1, Gro-α, IL-1β and IL-15 are strong effectors of macrophage and neutrophil recruitment and activation [27,28]. The upregulation of Toll (Tlr-4) in senescent fibroblasts confirms the overall immune response behavior at senescence. Tlr-4 is an IL-1 receptor homolog and is implicated in the activation of the gene regulatory protein NF-κB, a function proposed to be part of the innate immune response [29]. The induction of IL-15 at senescence is also consistent with an innate immune response, as IL-15 can be induced by NF-κB-dependent transcription [30] and also participates in inflammatory disease processes [28].

Deficiencies in the response of senescent cells to serum stimulation have been reported, and include an inability to induce the expression of c-*fos* mRNA [31] and markers of late G1 and S phase [32]. In response to serum, expression of inflammatory chemokines, matrix-degrading proteases and their modulators is induced in early-passage dermal fibroblasts, and expression of matrix collagens is reduced. This transient burst of activity may represent the natural response of these cells in wound repair [24]. Id-2 transcripts were hyper-induced in serum-stimulated senescent

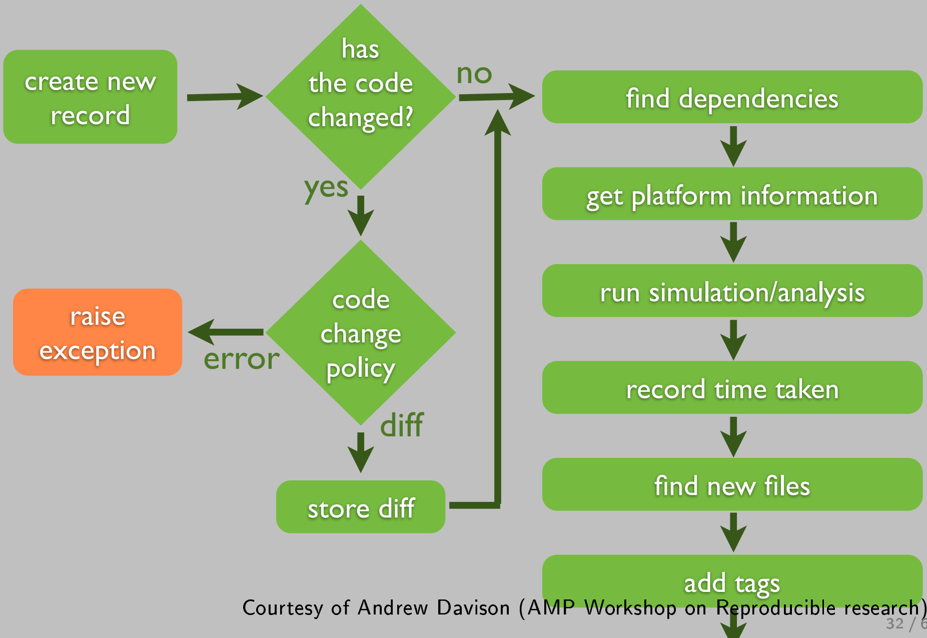
states overlap substantially with those in telomere-induced senescence (W.F., D.N.S., R. Allsopp, S. Lowe, and G. Ferbeyre, unpublished observations) and thus are likely to use many of the same activation processes.

The pattern of gene expression at senescence varies substantially in different cell types. Although the expression of matrix and structural proteins, such as the collagens, keratins and auxiliary factors, is repressed in RPE cells, inflammatory regulators are not induced, in contrast to dermal fibroblasts. Physiologically, this would make sense, as an acute inflammatory response in a tissue critical for normal vision would be likely to have deleterious consequences. However, as the RPE layer has a central role in the deposition and maintenance of extracellular matrix in the retina, decrements in the ability of senescent RPE cells to maintain appropriate expression patterns, as evidenced by decreased expression of collagens, keratins, aggrecan, transglutaminase and so on, would be predicted to have adverse affects on retinal architecture. Dysfunction of the RPE cell layer is considered to be a substantial factor in the development of age-related macular degeneration [36].

Surprisingly, early-passage HUVECs overexpress many of the markers associated with senescence in dermal fibro-

Courtesy of Matan Gavish and David Donoho (AMP Workshop on Reproducible research)

Sumatra: a lab notebook



Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: a lab notebook

```
$ smt comment 20110713-174949 "Eureka! Nobel prize
here we come."
```

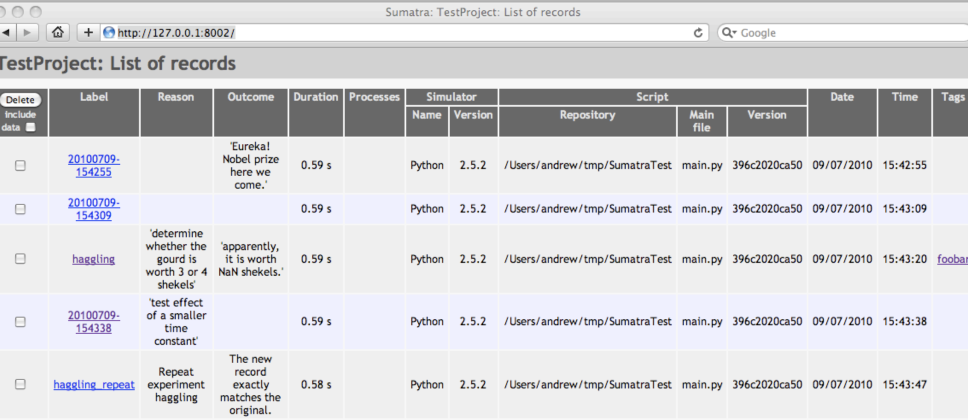
Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: a lab notebook

```
$ smt tag “Figure 6”
```

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

Sumatra: a lab notebook

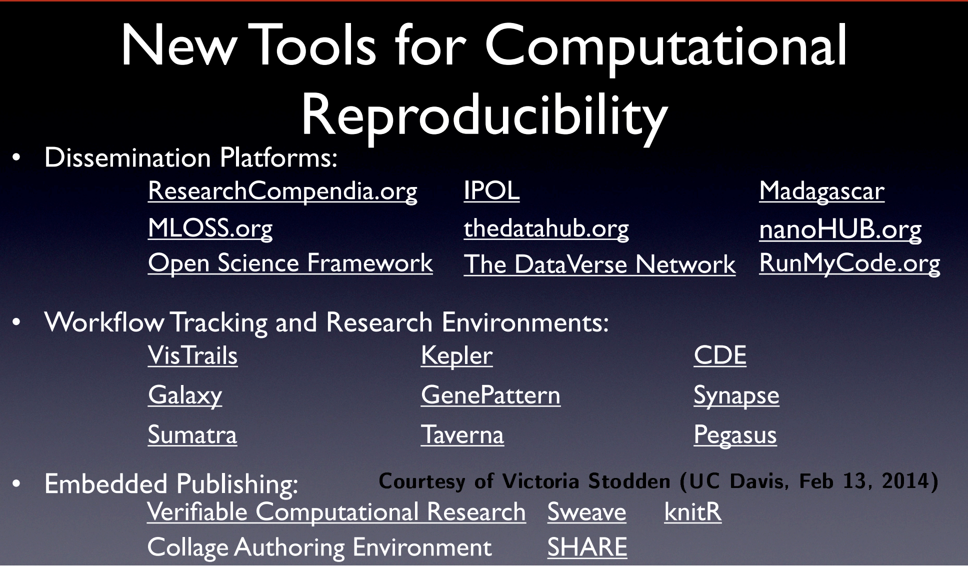


TestProject: List of records

Delete include data □	Label	Reason	Outcome	Duration	Processes	Simulator		Script			Date	Time	Tags
						Name	Version	Repository	Main file	Version			
□	20100709-154255		'Eureka! Nobel prize here we come.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:42:55	
□	20100709-154309			0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:09	
□	haggling	'determine whether the gourd is worth 3 or 4 shekels'	'apparently, it is worth NaN shekels.'	0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:20	foobar
□	20100709-154338	'test effect of a smaller time constant'		0.59 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:38	
□	haggling_repeat	Repeat experiment haggling	The new record exactly matches the original.	0.58 s		Python	2.5.2	/Users/andrew/tmp/SumatraTest	main.py	396c2020ca50	09/07/2010	15:43:47	

Courtesy of Andrew Davison (AMP Workshop on Reproducible research)

So many new tools



New Tools for Computational Reproducibility

- Dissemination Platforms:
  ResearchCompendia.org IPOL Madagascar
  MLOSS.org thedatahub.org nanoHUB.org
  Open Science Framework The DataVerse Network RunMyCode.org
- Workflow Tracking and Research Environments:
  VisTrails Kepler CDE
  Galaxy GenePattern Synapse
  Sumatra Taverna Pegasus
- Embedded Publishing:
  Verifiable Computational Research Sweave knitR
  Collage Authoring Environment SHARE

Courtesy of Victoria Stodden (UC Davis, Feb 13, 2014)

And also: **Figshare**, **ActivePapers**, **Elsevier executable paper**, ...

Sharing Data

What kinds of systems are available?

- "Good" - The cloud (Dropbox, Google Drive, Figshare)
- Better - Version control systems (SVN, Git and Mercurial)
- "Best" - Version control systems on the cloud (GitHub, Bitbucket)

It depends on the level of privacy you want but you should already know this tools.

Is this enough?

1. Use a workflow that documents both data and process
2. Use the machine readable CSV format
3. Provide raw data and meta data, not just statistical outputs
4. Never do data manipulation and statistical tests by hand
5. Use R, Python or another free software to read and process raw data (ideally to produce complete reports with code, results and prose)

Courtesy of Adam J. Richards

Litterate Programming

Donald Knuth: explanation of the program logic in a natural language interspersed with snippets of macros and traditional source code.

I'm way too 3133t to program this way but that's
exactly what we need for writing a reproducible article/analysis!

Org-mode (requires emacs)

My favorite tool.

- plain text, very smooth, works both for html, pdf, . . .
- allows to combine all my favorite languages even with sessions

Ipython notebook

If you are a python user, go for it! Web app, easy to use/setup. . .

KnitR (a.k.a. Sweave)

For non-emacs users and as a first step toward *reproducible papers*:

- Click and play with a modern IDE (e.g., Rstudio)

Outline

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   - Looks familiar?
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   - Many Different Alternatives for Reproducible Analysis
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   - Reproducible Documents: knitR
   - Introduction to R
   - Needful Packages by Hadley Wickam
3. Setting up a Laboratory Notebook
   - Emacs Demo of How to Keep Things Tidy

Why R?

R is a great language for data analysis and statistics

- Open-source and multi-platform
- Very expressive with high-level constructs
- Excellent graphics
- Widely used in academia and business
- Very active community
    - Documentation, FAQ on http://stackoverflow.com/questions/tagged/r
- Great integration with other tools

Why is R a pain for computer scientists?

- R is not really a programming language
- Documentation is for statisticians
- Default plots are ~~cumbersome~~ (meaningful)
- Summaries are ~~cryptic~~ (precise)
- Steep learning curve even for us, computer scientists whereas we generally switch seamlessly from a language to another! That's frustrating! ;)

Do's and dont's

~~R is high level, I'll do everything myself~~

- CTAN comprises 4,334 TEX, LATEX, and related packages and tools. Most of you do not use plain TEX.
- Currently, the CRAN package repository features 4,030 available packages.
- How do you know which one to use??? Many of them are highly exotic (not to say useless to you).

  I learnt with http://www.r-bloggers.com/
- Lots of introductions but not necessarily what you're looking for so I'll give you a short tour.

  You should quickly realize though that you need proper training in statistics and data analysis if you do not want tell nonsense.
- Again, you should read Jain's book on The Art of Computer Systems Performance Analysis
- You may want to follow online courses:
  - https://www.coursera.org/course/compdata
  - https://www.coursera.org/course/repdata

Install and run R on debian

```
apt-cache search r
```

Err, that'is not very useful :) It's the same when searching on google but once the filter bubble is set up, it gets better...

```
sudo apt-get install r-base
```

```
R
```

```
R version 3.0.2 (2013-09-25) -- "Frisbee Sailing"
Copyright (C) 2013 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.
>
```

Install a few cool packages

R has it's own package management mechanism so just run R and type the following commands:

- ddply, reshape and ggplot2 by Hadley Wickham (http://had.co.nz/)

```r
install.packages("plyr")
install.packages("reshape")
install.packages("ggplot2")
```

- knitR by (Yihui Xie) http://yihui.name/knitr/

```r
install.packages("knitr")
```

IDE

Using R interactively is nice but quickly becomes painful so at some point, you'll want an IDE.

Emacs is great but you'll need *Emacs Speaks Statistics*

```
sudo apt-get install ess
```

In this tutorial, I will briefly show you rstudio (https://www.rstudio.com/) and later how to use `org-mode`

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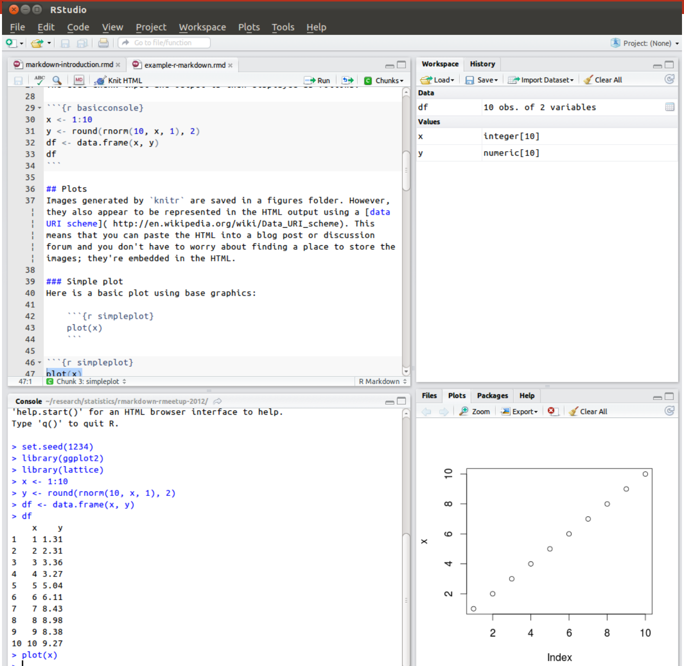
Rstudio screenshot



~~~
```{r basicconsole}
x <- 1:10
y <- round(rnorm(10, x, 1), 2)
df <- data.frame(x, y)
df
```

## Plots
Images generated by `knitr` are saved in a figures folder. However,
they also appear to be represented in the HTML output using a [data
URI scheme]( http://en.wikipedia.org/wiki/Data_URI_scheme). This
means that you can paste the HTML into a blog post or discussion
forum and you don't have to worry about finding a place to store the
images; they're embedded in the HTML.

### Simple plot
Here is a basic plot using base graphics:

    ```{r simpleplot}
    plot(x)
    ```

```{r simpleplot}
plot(x)
~~~

Data	
df	10 obs. of 2 variables
Values	
x	integer[10]
y	numeric[10]

```
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> set.seed(1234)
> library(ggplot2)
> library(lattice)
> x <- 1:10
> y <- round(rnorm(10, x, 1), 2)
> df <- data.frame(x, y)
> df
    x    y
1   1 1.31
2   2 2.31
3   3 3.36
4   4 3.27
5   5 5.04
6   6 6.11
7   7 8.43
8   8 8.98
9   9 8.38
10 10 9.27
> plot(x)
> 
```

Reproducible analysis in Markdown + R

- Create a new R Markdown document (Rmd) in rstudio
- R chunks are interspersed with “‘{r} and “‘
- Inline R code: ‘r sin(2+2)‘
- You can knit the document and share it via rpubs
- R chunks can be sent to the top-level with `Alt-Ctrl-c`
- I usually work mostly with the current environment and only knit in the end
- Other engines can be used (use rstudio completion)

```
‘‘‘{r engine=’sh’}
ls /tmp/
‘‘‘
```

- Makes reproducible analysis as simple as one click
- Great tool for quick analysis for self and colleagues, homeworks, . . .

Reproducible articles with LaTeX + R

- Create a new R Sweave document (Rnw) in rstudio
- R chunks are interspersed with <<>>= and @
- You can knit the document to produce a pdf
- You'll probably quickly want to change default behavior (activate the cache, hide code, ...). In the preembule:

```
<<echo=FALSE>>=
opts_chunk$set(cache=TRUE,dpi=300,echo=FALSE,fig.width=7,
                warning=FALSE,message=FALSE)
@
```

- Great for journal articles, theses, books, ...

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Data frames

A data frame is a data tables (with columns and rows). `mtcars` is a built-in data frame that we will use in the sequel

```
head(mtcars);
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear car
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

You can also load a data frame from a CSV file:

```
df <- read.csv("http://foo.org/mydata.csv", header=T,
       strip.white=TRUE);
```

You will get help by using ?:

```
?data.frame
?rbind
?cbind
```

Exploring Content (1)

```
names(mtcars);
```

```
 [1] "mpg"  "cyl"  "disp" "hp"   "drat" "wt"   "qsec" "vs"   "am"
[11] "carb"
```

```
str(mtcars);
```

```
'data.frame': 32 obs. of  11 variables:
 $ mpg : num  21 21 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 ...
 $ cyl : num  6 6 4 6 8 6 8 4 4 6 ...
 $ disp: num  160 160 108 258 360 ...
 $ hp  : num  110 110 93 110 175 105 245 62 95 123 ...
 $ drat: num  3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...
 $ wt  : num  2.62 2.88 2.32 3.21 3.44 ...
 $ qsec: num  16.5 17 18.6 19.4 17 ...
 $ vs  : num  0 0 1 1 0 1 0 1 1 1 ...
 $ am  : num  1 1 1 0 0 0 0 0 0 0 ...
 $ gear: num  4 4 4 3 3 3 3 4 4 4 ...
 $ carb: num  4 4 1 1 2 1 4 2 2 4 ...
```

Exploring Content (2)

```
dim(mtcars);
length(mtcars);
```

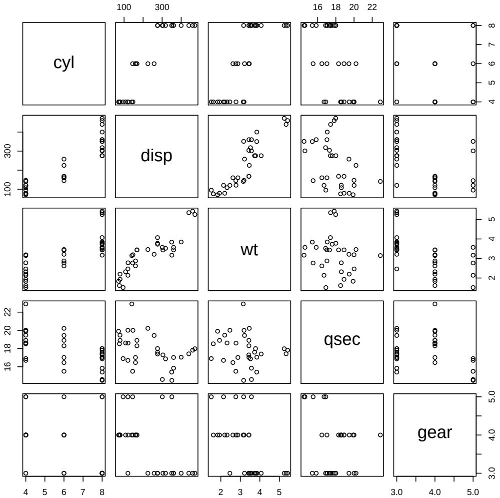
```
[1] 32 11
[1] 11
```

```
summary(mtcars);
```

```
     mpg             cyl             disp             hp       
Min.   :10.40   Min.   :4.000   Min.   : 71.1   Min.   : 52.0  
1st Qu.:15.43   1st Qu.:4.000   1st Qu.:120.8   1st Qu.: 96.5  
Median :19.20   Median :6.000   Median :196.3   Median :123.0  
Mean   :20.09   Mean   :6.188   Mean   :230.7   Mean   :146.7  
3rd Qu.:22.80   3rd Qu.:8.000   3rd Qu.:326.0   3rd Qu.:180.0  
Max.   :33.90   Max.   :8.000   Max.   :472.0   Max.   :335.0  
     drat             wt             qsec             vs        
Min.   :2.760   Min.   :1.513   Min.   :14.50   Min.   :0.0000  
1st Qu.:3.080   1st Qu.:2.581   1st Qu.:16.89   1st Qu.:0.0000  
Median :3.695   Median :3.325   Median :17.71   Median :0.0000  
Mean   :3.597   Mean   :3.217   Mean   :17.85   Mean   :0.4375  
3rd Qu.:3.920   3rd Qu.:3.610   3rd Qu.:18.90   3rd Qu.:1.0000  
```

Exploring Content (3)

```r
plot(mtcars[names(mtcars) %in% c("cyl","wt","disp","qsec","gear")])
```



Accessing Content

```
mtcars$mpg
```

```
 [1] 21.0 21.0 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 17.8 16.4 17
[16] 10.4 14.7 32.4 30.4 33.9 21.5 15.5 15.2 13.3 19.2 27.3 26.0 30
[31] 15.0 21.4
```

```
mtcars[2:5,]$mpg
```

```
[1] 21.0 22.8 21.4 18.7
```

```
mtcars[mtcars$mpg == 21.0,]
```

```
              mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4      21   6  160 110  3.9 2.620 16.46  0  1    4    4
Mazda RX4 Wag  21   6  160 110  3.9 2.875 17.02  0  1    4    4
```

```
mtcars[mtcars$mpg == 21.0 & mtcars$wt > 2.7,]
```

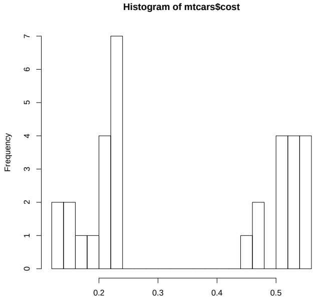
```
              mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4 Wag  21   6  160 110  3.9 2.875 17.02  0  1    4    4
```

Extending Content

```
mtcars$cost = log(mtcars$hp)*atan(mtcars$disp)/
 sqrt(mtcars$gear**5);
mean(mtcars$cost);
summary(mtcars$cost);
```

```
[1] 0.345994
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 0.1261  0.2038  0.2353  0.3460  0.5202  0.5534
```

```
hist(mtcars$cost,breaks=20);
```

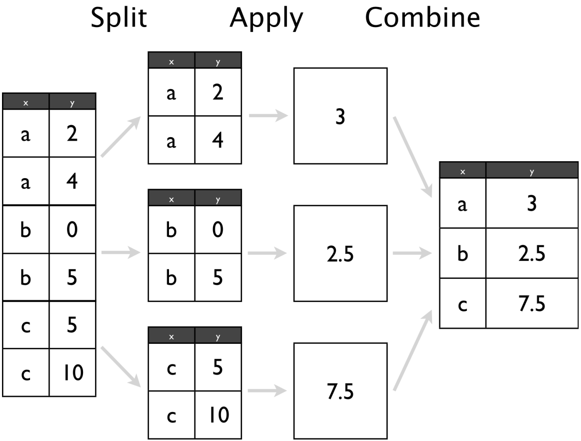


Outline

1. Reproducible Research
   - Looks familiar?
   - A few Tools for Experiment Setup and Management
   - Many Different Alternatives for Reproducible Analysis
2. R Crash Course
   - General Introduction
   - Reproducible Documents: knitR
   - Introduction to R
   - Needful Packages by Hadley Wickam
3. Setting up a Laboratory Notebook
   - Emacs Demo of How to Keep Things Tidy

plyr: the Split-Apply-Combine Strategy

Have a look at http://plyr.had.co.nz/09-user/ for a more detailed introduction.



Split Apply Combine

x	y
a	2
a	4
b	0
b	5
c	5
c	10

x	y
a	2
a	4

x	y
b	0
b	5

x	y
c	5
c	10

3

2.5

7.5

x	y
a	3
b	2.5
c	7.5

plyr: Powerfull One-liners

```r
library(plyr)
mtcars_summarized = ddply(mtcars,c("cyl","carb"), summarize,
      num = length(wt), wt_mean = mean(wt), wt_sd = sd(wt),
      qsec_mean = mean(qsec), qsec_sd = sd(qsec));
mtcars_summarized
```

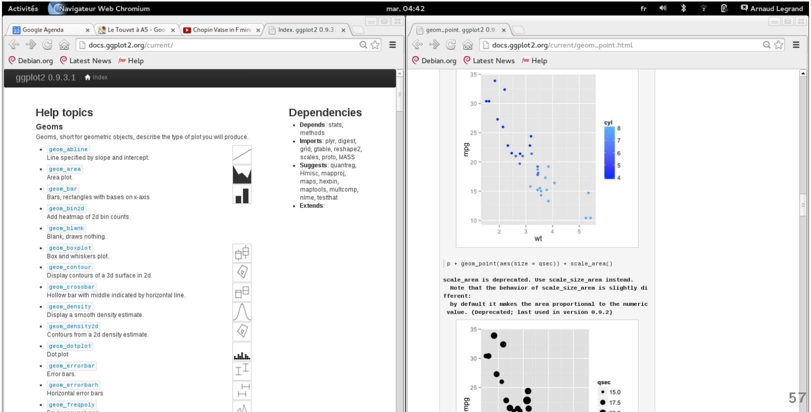
```
  cyl carb num  wt_mean     wt_sd qsec_mean   qsec_sd
1   4    1   5 2.151000 0.2627118  19.37800 0.6121029
2   4    2   6 2.398000 0.7485412  18.93667 2.2924368
3   6    1   2 3.337500 0.1732412  19.83000 0.5515433
4   6    4   4 3.093750 0.4131460  17.67000 1.1249296
5   6    6   1 2.770000        NA  15.50000        NA
6   8    2   4 3.560000 0.1939502  17.06000 0.1783255
7   8    3   3 3.860000 0.1835756  17.66667 0.3055050
8   8    4   6 4.433167 1.0171431  16.49500 1.4424112
9   8    8   1 3.570000        NA  14.60000        NA
```

If your data is not in the right form give a try to reshapeP/melt.

plyr next generation = dplyr

ggplot2: Modularity in Action

- ggplot2 builds on plyr and on a modular grammar of graphics
- ~~obnoxious function with dozens of arguments~~
- combine small functions using layers and transformations
- aesthetic mapping between observation characteristics (data frame column names) and graphical object variables
- an incredible documentation: http://docs.ggplot2.org/current/



Help topics

Geoms

Geoms, short for geometric objects, describe the type of plot you will produce.

- `geom_abline`
  Line specified by slope and intercept.
- `geom_area`
  Area plot.
- `geom_bar`
  Bars, rectangles with bases on x-axis
- `geom_bin2d`
  Add heatmap of 2d bin counts.
- `geom_blank`
  Blank, draws nothing.
- `geom_boxplot`
  Box and whiskers plot.
- `geom_contour`
  Display contours of a 3d surface in 2d.
- `geom_crossbar`
  Hollow bar with middle indicated by horizontal line.
- `geom_density`
  Display a smooth density estimate.
- `geom_density2d`
  Contours from a 2d density estimate.
- `geom_dotplot`
  Dot plot
- `geom_errorbar`
  Error bars.
- `geom_errorbarh`
  Horizontal error bars
- `geom_freqpoly`

Dependencies

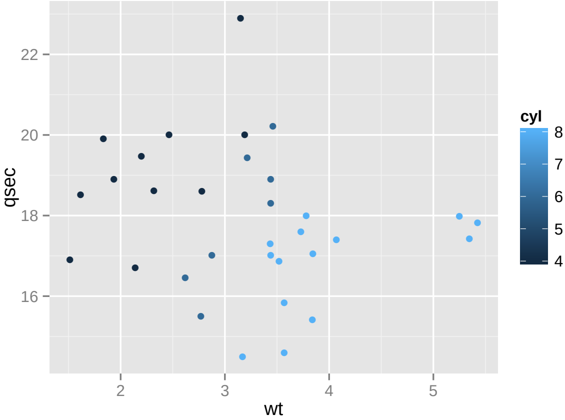
- **Depends**: stats, methods
- **Imports**: plyr, digest, grid, gtable, reshape2, scales, proto, MASS
- **Suggests**: quantreg, Hmisc, mapproj, maps, hexbin, maptools, multcomp, nlme, testthat
- **Extends**:

```
p + geom_point(aes(size = qsec)) + scale_area()
```

```
scale_area is deprecated. Use scale_size_area instead.
  Note that the behavior of scale_size_area is slightly di
fferent:
  by default it makes the area proportional to the numeric
 value. (Deprecated; last used in version 0.9.2)
```

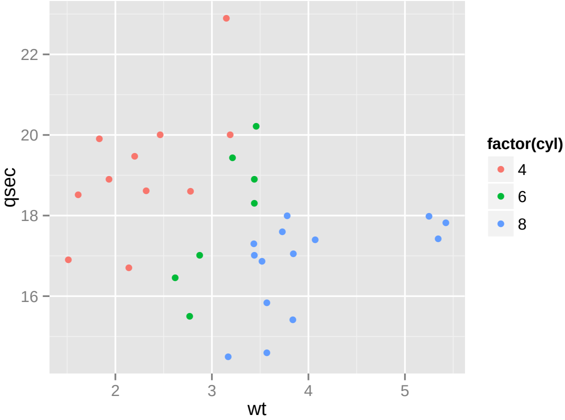
ggplot2: Illustration (1)

```
ggplot(data = mtcars, aes(x=wt, y=qsec, color=cyl)) +
        geom_point();
```



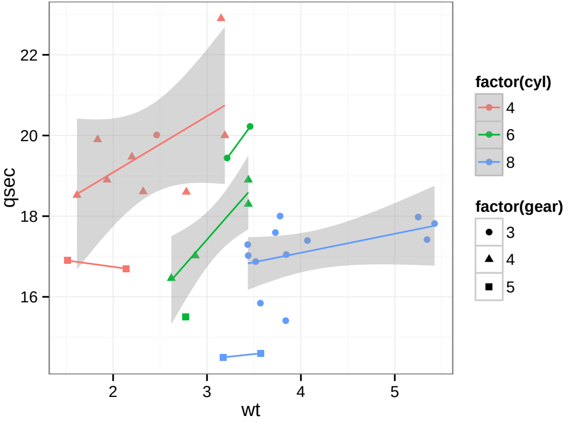
ggplot2: Illustration (2)

```
ggplot(data = mtcars, aes(x=wt, y=qsec, color=factor(cyl))) +
        geom_point();
```



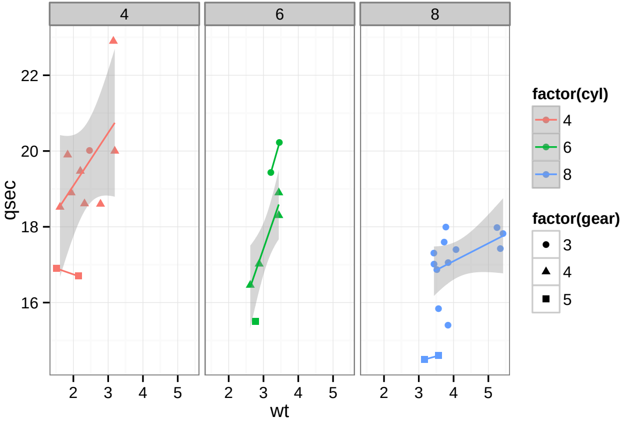
ggplot2: Illustration (3)

```
ggplot(data = mtcars, aes(x=wt, y=qsec, color=factor(cyl),
        shape = factor(gear))) +  geom_point() + theme_bw() +
        geom_smooth(method="lm");
```



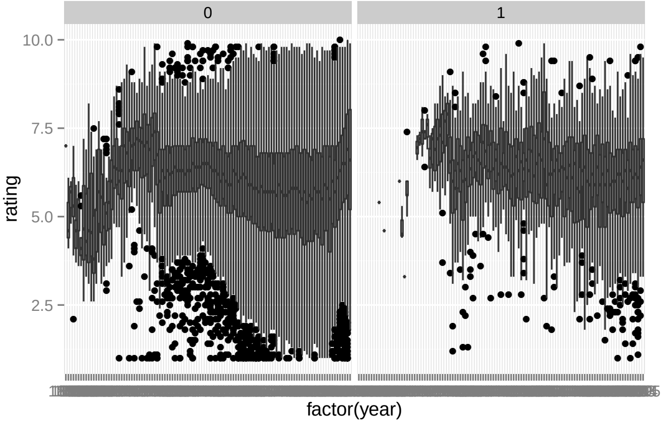
ggplot2: Illustration (4)

```
ggplot(data = mtcars, aes(x=wt, y=qsec, color=factor(cyl),
       shape = factor(gear))) + geom_point() + theme_bw() +
       geom_smooth(method="lm") + facet_wrap(~ cyl);
```



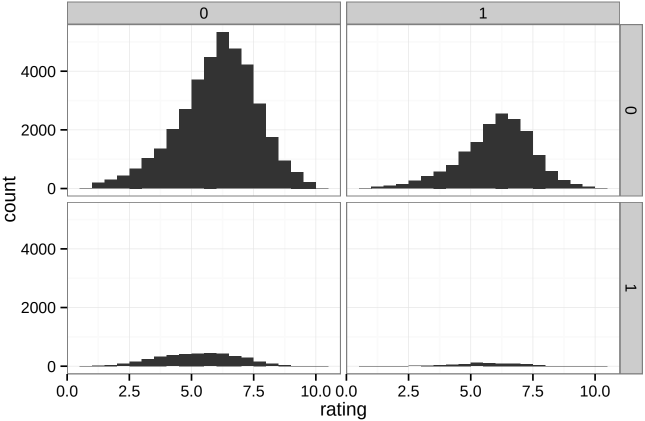
ggplot2: Illustration (5)

```
ggplot(data = movies, aes(x=factor(year),y=rating)) +
        geom_boxplot() + facet_wrap(~Romance)
```



ggplot2: Illustration (6)

```
ggplot(movies, aes(x = rating)) + geom_histogram(binwidth = 0.5)+
        facet_grid(Action ~ Comedy) + theme_bw();
```



Take away Message

- R is a great tool but is only a tool. There is no magic. You need to understand what you are doing and get a minimal training in statistics
- It is one of the building block of reproducible research (the *reproducible analysis* block) and will save you a lot of time
- Read at least Jain's book: The Art of Computer Systems Performance Analysis
- Jean-Marc Vincent and myself give a set of tutorials on performance evaluation to M2R (links provided at the end of these slides)
- There are introductory online courses on coursera (links provided at the end of these slides)

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Litterate Programming on a Daily Basis

Mastering Emacs

- `C-g`: get me out of here!
- `C-_`: undo
- Activate CUA keys in the Options menu

Mastering Org-mode

- `Tab` will fold/unfold stuff
- `C-c C-c`: do something (context-sensivite) where you are
- `<s` + `Tab`, `<b`, `<l`, `<r`, `<h`, ... for creating code blocks
- `C-c C-e`: export
- `C-c c`: capture content
- `C-c C-o=/=C-c l=/=C-c C-l`: open/store/insert links
- `C-c C-a`: attach a file
- `C-c C-d`: set deadline, `C-c C-t`: TODO/DONE

A few links to learn more

Emacs/Org-mode

- *Org for beginners* (worg)
- *My emacs configuration*
- *For Mac OS X users*
- *These slides and the VM images* I prepared with Kameleon

Performance Evaluation Lectures

- Jean-Marc Vincent and myself give a set of tutorials on performance evaluation to M2R
  - *2013 edition* (confidence intervals, linear regression, DoE)
  - *2011 edition* (visualization, measurement, checklists)
- There are interesting online courses on coursera (101s) By Roger D. Peng
  - *Computing For Data Analysis* (R)
  - *Reproducible Research* (actually reproducible data analysis)
  - *Exploratory Data Analysis* (ggplot2 + lattice)