

Reproducible Research: Concepts and Ideas

Reproducible Research

*Roger D. Peng, Associate Professor of Biostatistics
Johns Hopkins Bloomberg School of Public Health*

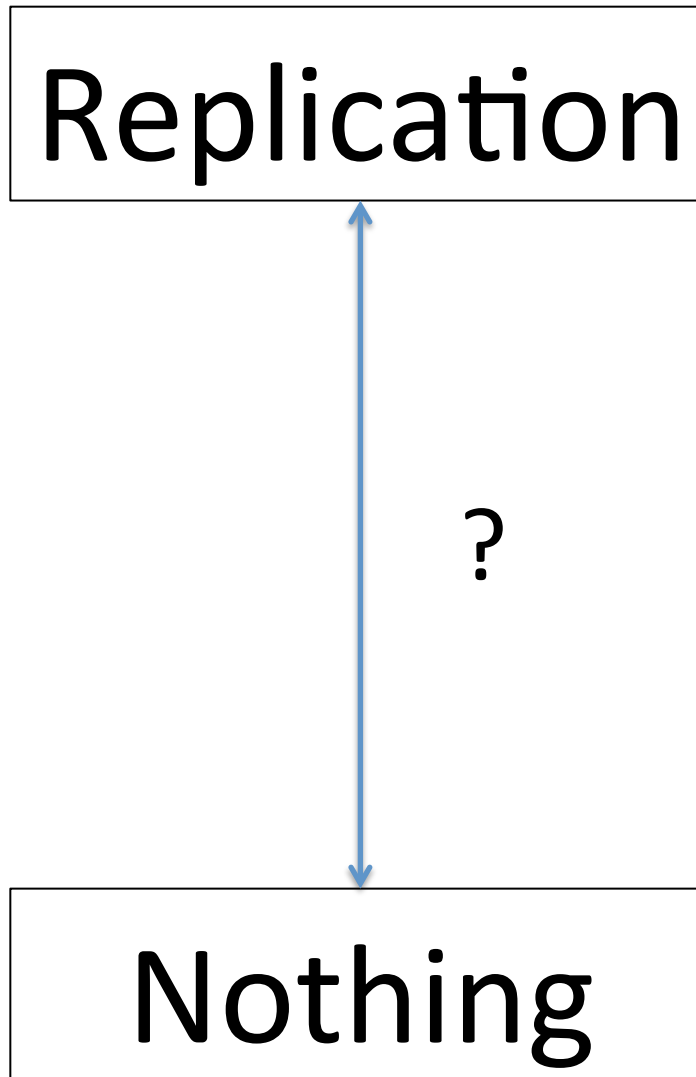
Replication

- The ultimate standard for strengthening scientific evidence is replication of findings and conducting studies with independent
 - Investigators
 - Data
 - Analytical methods
 - Laboratories
 - Instruments
- Replication is particularly important in studies that can impact broad policy or regulatory decisions

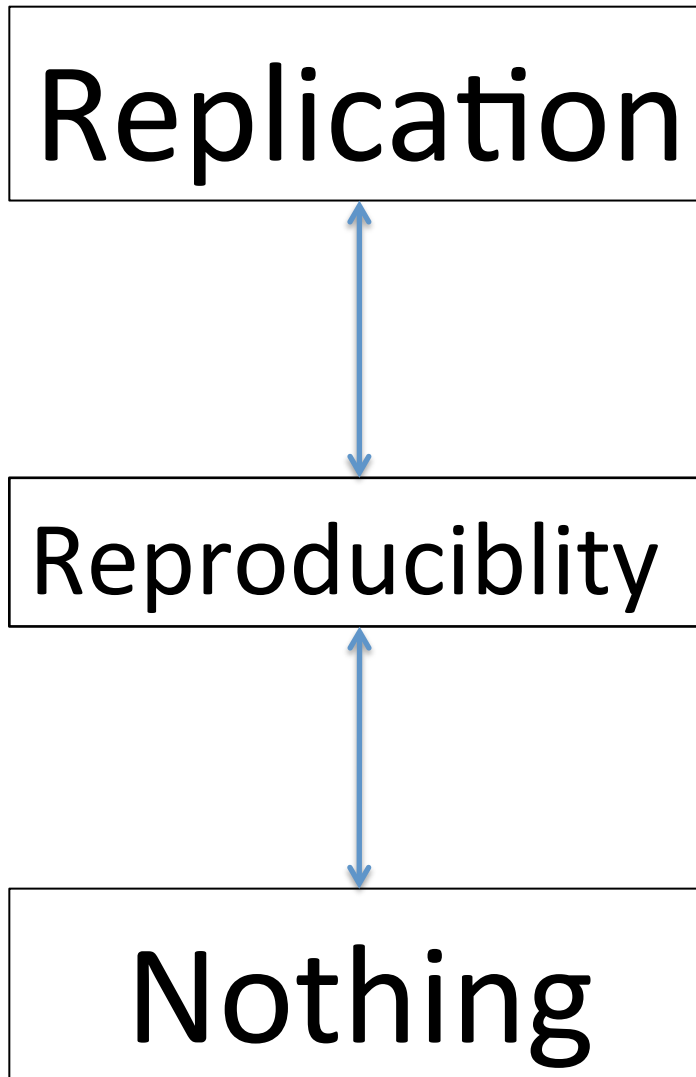
What's Wrong with Replication?

- Some studies cannot be replicated
 - No time, opportunistic
 - No money
 - Unique
- Reproducible Research: Make analytic data and code available so that others may reproduce findings

How Can We Bridge the Gap?



How Can We Bridge the Gap?



Why Do We Need Reproducible Research?

- New technologies increasing data collection throughput; data are more complex and extremely high dimensional
- Existing databases can be merged into new “megadatabases”
- Computing power is greatly increased, allowing more sophisticated analyses
- For every field “X” there is a field “Computational X”

Example: Reproducible Air Pollution and Health Research

- Estimating small (but important) health effects in the presence of much stronger signals
- Results inform substantial policy decisions, affect many stakeholders
 - EPA regulations can cost billions of dollars
- Complex statistical methods are needed and subjected to intense scrutiny

Internet-based Health and Air Pollution Surveillance System (iHAPSS)



ABOUT iHAPSS

iHAPSS is an internet system for monitoring the effects of air pollution on mortality and morbidity in the United States.

iHAPSS is funded by the [Health Effects Institute](#) (HEI). It provides published material, software and data to monitor the association between air pollution and mortality and morbidity.

iHAPSS is developed and maintained by the [Department of Biostatistics](#) at the Johns Hopkins Bloomberg School of Public Health.



PUBLICATIONS

Current and previous publications and reports.



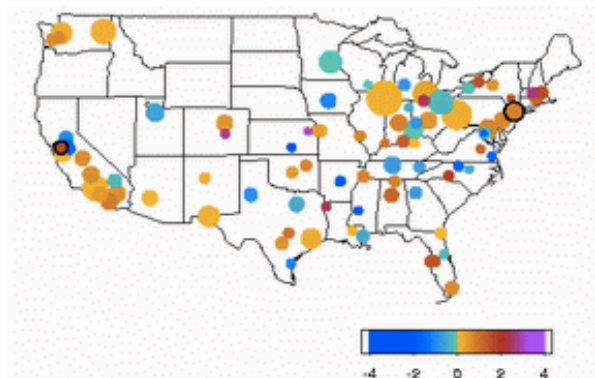
SOFTWARE

Tools for data analysis.



DATA

Air pollution and meteorological data for 108 U.S. cities 1987–2000.



<http://www.ihapss.jhsph.edu>

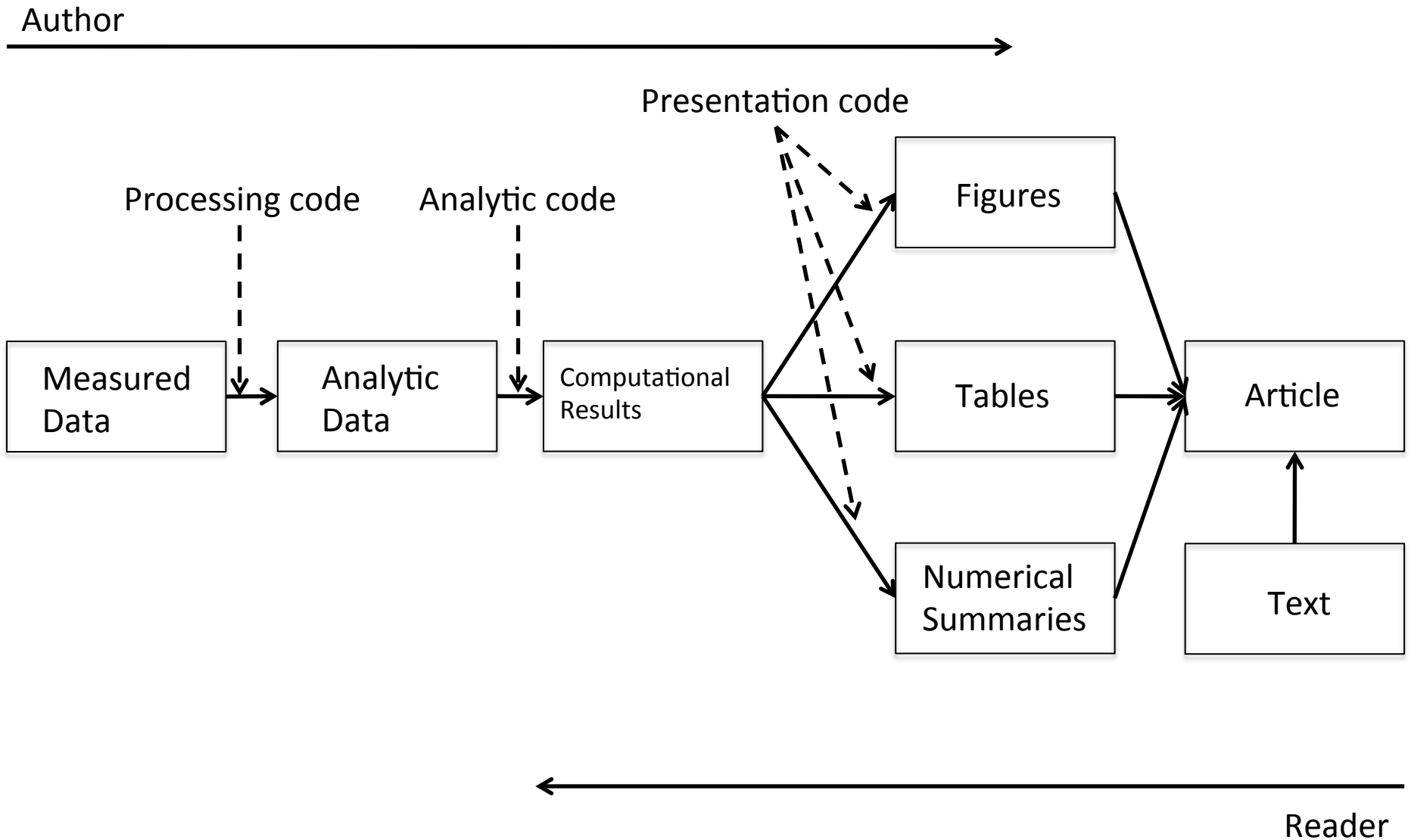
Research Pipeline



Article

Reader

Research Pipeline



Recent Developments in Reproducible Research



Data Replication & Reproducibility

PERSPECTIVE

Reproducible Research in Computational Science

Roger D. Peng

Computational science has led to exciting new developments, but the nature of the work has exposed limitations in our ability to evaluate published findings. Reproducibility has the potential to serve as a minimum standard for judging scientific claims when full independent replication of a study is not possible.

The Duke Saga



Recent Developments in Reproducible Research

REPORT BRIEF  MARCH 2012

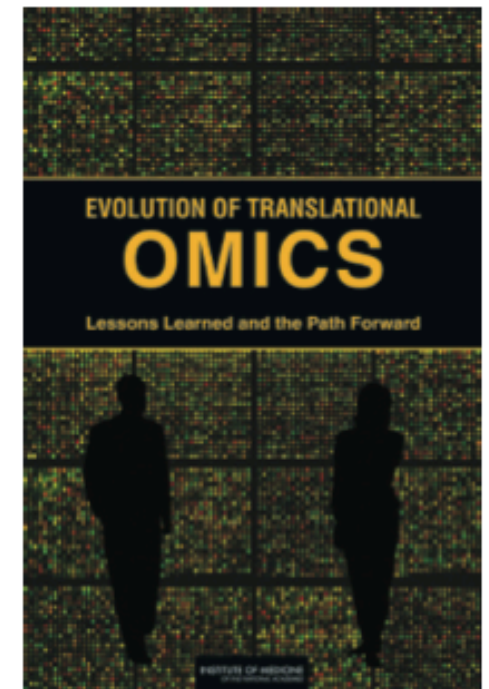
INSTITUTE OF MEDICINE
OF THE NATIONAL ACADEMIES

Advising the nation • Improving health

For more information visit www.iom.edu/translationalomics

Evolution of Translational Omics

Lessons Learned and the
Path Forward



The IOM Report

In the Discovery/Test Validation stage of omics-based tests:

- **Data/metadata** used to develop test should be made publicly available
- The **computer code** and fully specified computational procedures used for development of the candidate omics-based test should be made sustainably available
- “Ideally, the computer code that is released will **encompass all of the steps of computational analysis**, including all data preprocessing steps, that have been described in this chapter. All aspects of the analysis need to be transparently reported.”

What do We Need?

- Analytic data are available
- Analytic code are available
- Documentation of code and data
- Standard means of distribution

Who are the Players?

- Authors
 - Want to make their research reproducible
 - Want tools for RR to make their lives easier (or at least not much harder)
- Readers
 - Want to reproduce (and perhaps expand upon) interesting findings
 - Want tools for RR to make their lives easier

Challenges

- Authors must undertake considerable effort to put data/results on the web (may not have resources like a web server)
- Readers must download data/results individually and piece together which data go with which code sections, etc.
- Readers may not have the same resources as authors
- Few tools to help authors/readers (although toolbox is growing!)

In Reality...

- Authors
 - Just put stuff on the web
 - (Infamous) Journal supplementary materials
 - There are some central databases for various fields (e.g. biology, ICPSR)
- Readers
 - Just download the data and (try to) figure it out
 - Piece together the software and run it

Literate (Statistical) Programming

- An article is a stream of **text** and **code**
- Analysis code is divided into text and code “chunks”
- Each code chunk loads data and computes results
- Presentation code formats results (tables, figures, etc.)
- Article text explains what is going on
- Literate programs can be **weaved** to produce human-readable documents and **tangled** to produce machine-readable documents

Literate (Statistical) Programming

- Literate programming is a general concept that requires
 1. A documentation language (human readable)
 2. A programming language (machine readable)
- Sweave uses L^AT_EX and R as the documentation and programming languages
- Sweave was developed by Friedrich Leisch (member of the R Core) and is maintained by R core
- **Main web site:** <http://www.statistik.lmu.de/~leisch/Sweave>

Sweave Limitations

- Sweave has many limitations
- Focused primarily on LaTeX, a difficult to learn markup language used only by weirdos
- Lacks features like caching, multiple plots per chunk, mixing programming languages and many other technical items
- Not frequently updated or very actively developed

Literate (Statistical) Programming

- knitr is an alternative (more recent) package
- Brings together many features added on to Sweave to address limitations
- knitr uses R as the programming language (although others are allowed) and variety of documentation languages
 - LaTeX, Markdown, HTML
- knitr was developed by Yihui Xie (while a graduate student in statistics at Iowa State)
- See <http://yihui.name/knitr/>

Summary

- Reproducible research is important as a **minimum standard**, particularly for studies that are difficult to replicate
- Infrastructure is needed for **creating** and **distributing** reproducible documents, beyond what is currently available
- There is a growing number of tools for creating reproducible documents



Structure of a Data Analysis

Part 1

Roger D. Peng, Associate Professor of Biostatistics
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Steps in a data analysis

- Define the question
- Define the ideal data set
- Determine what data you can access
- Obtain the data
- Clean the data
- Exploratory data analysis
- Statistical prediction/modeling
- Interpret results
- Challenge results
- Synthesize/write up results
- Create reproducible code

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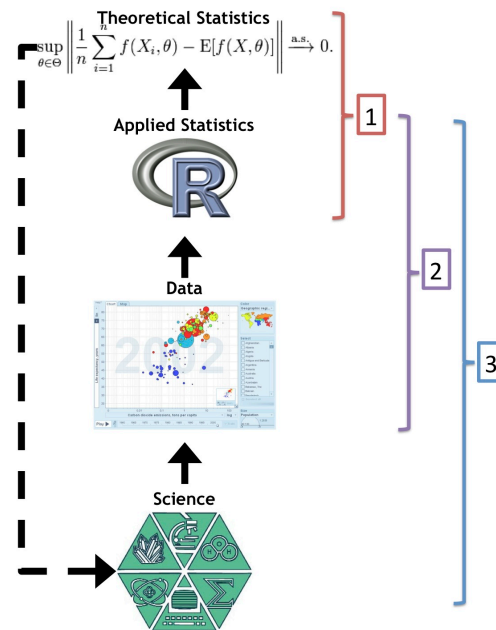
The key challenge in data analysis

"Ask yourselves, what problem have you solved, ever, that was worth solving, where you knew all of the given information in advance? Where you didn't have a surplus of information and have to filter it out, or you had insufficient information and have to go find some?"



[Dan Myer, Mathematics Educator](#)

Defining a question



1. Statistical methods development
2. Danger zone!!!
3. Proper data analysis

An example

Start with a general question

Can I automatically detect emails that are SPAM that are not?

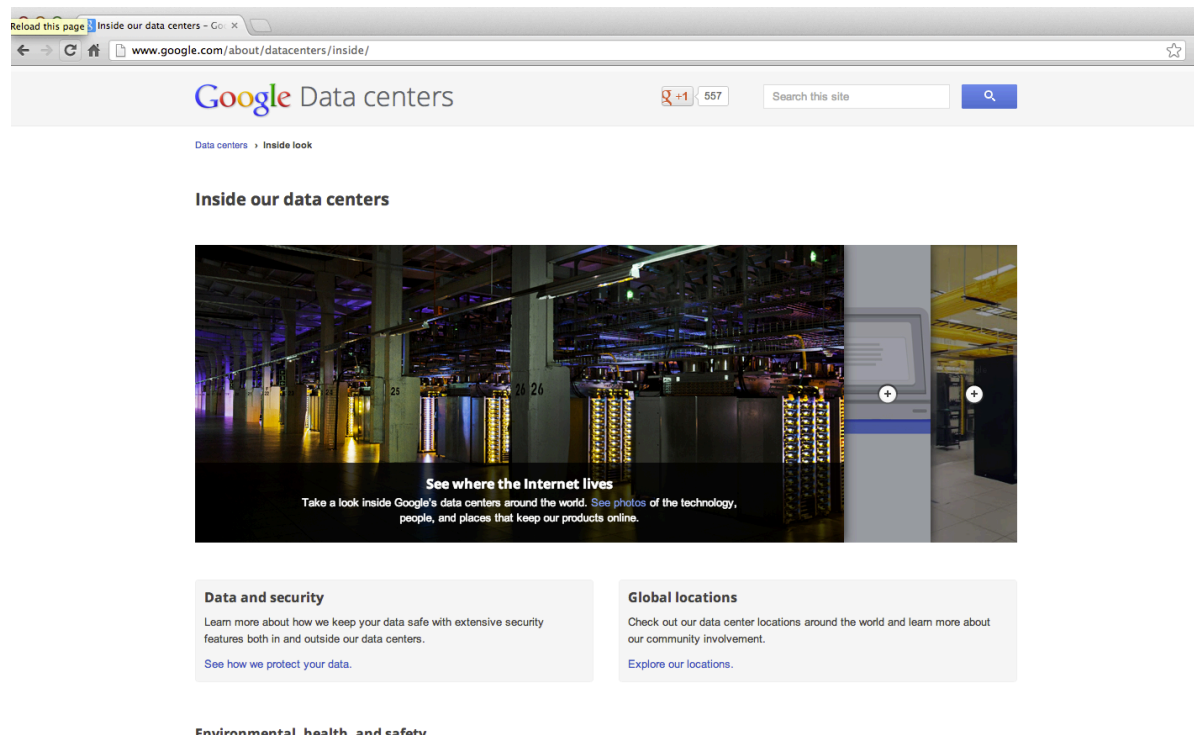
Make it concrete

Can I use quantitative characteristics of the emails to classify them as SPAM/HAM?

Define the ideal data set

- The data set may depend on your goal
 - Descriptive - a whole population
 - Exploratory - a random sample with many variables measured
 - Inferential - the right population, randomly sampled
 - Predictive - a training and test data set from the same population
 - Causal - data from a randomized study
 - Mechanistic - data about all components of the system

Our example

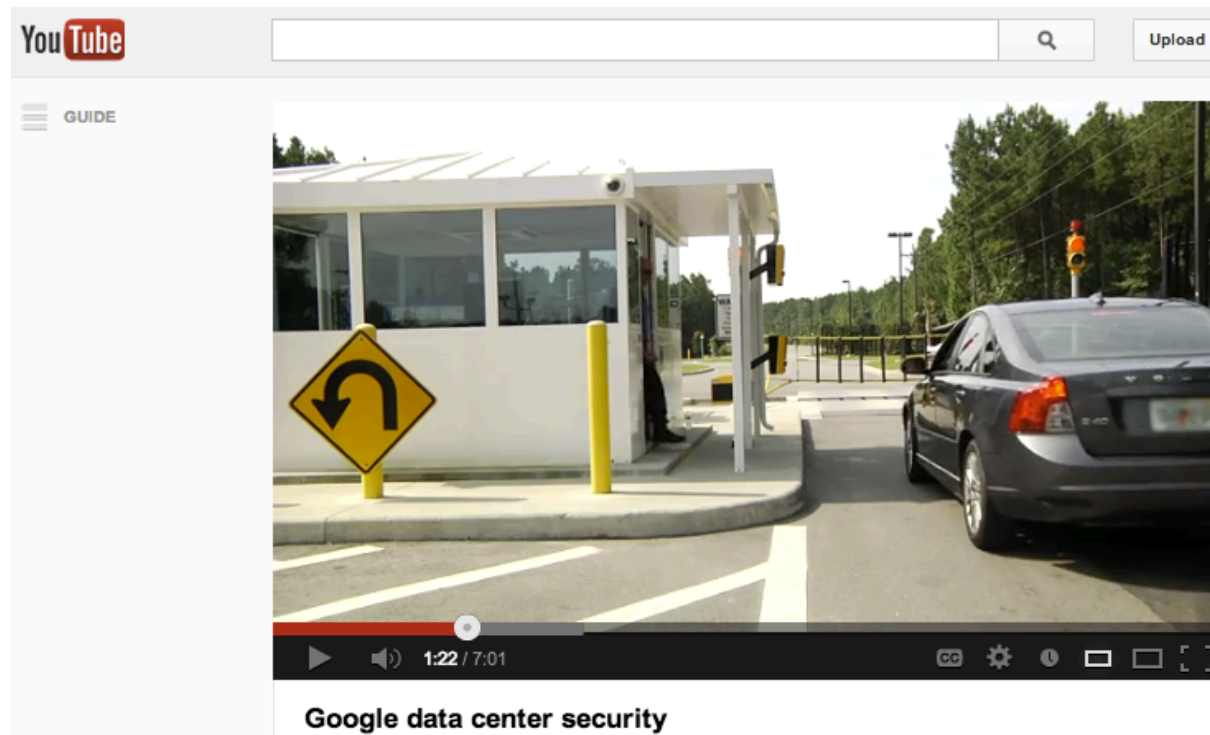


<http://www.google.com/about/datacenters/inside/>

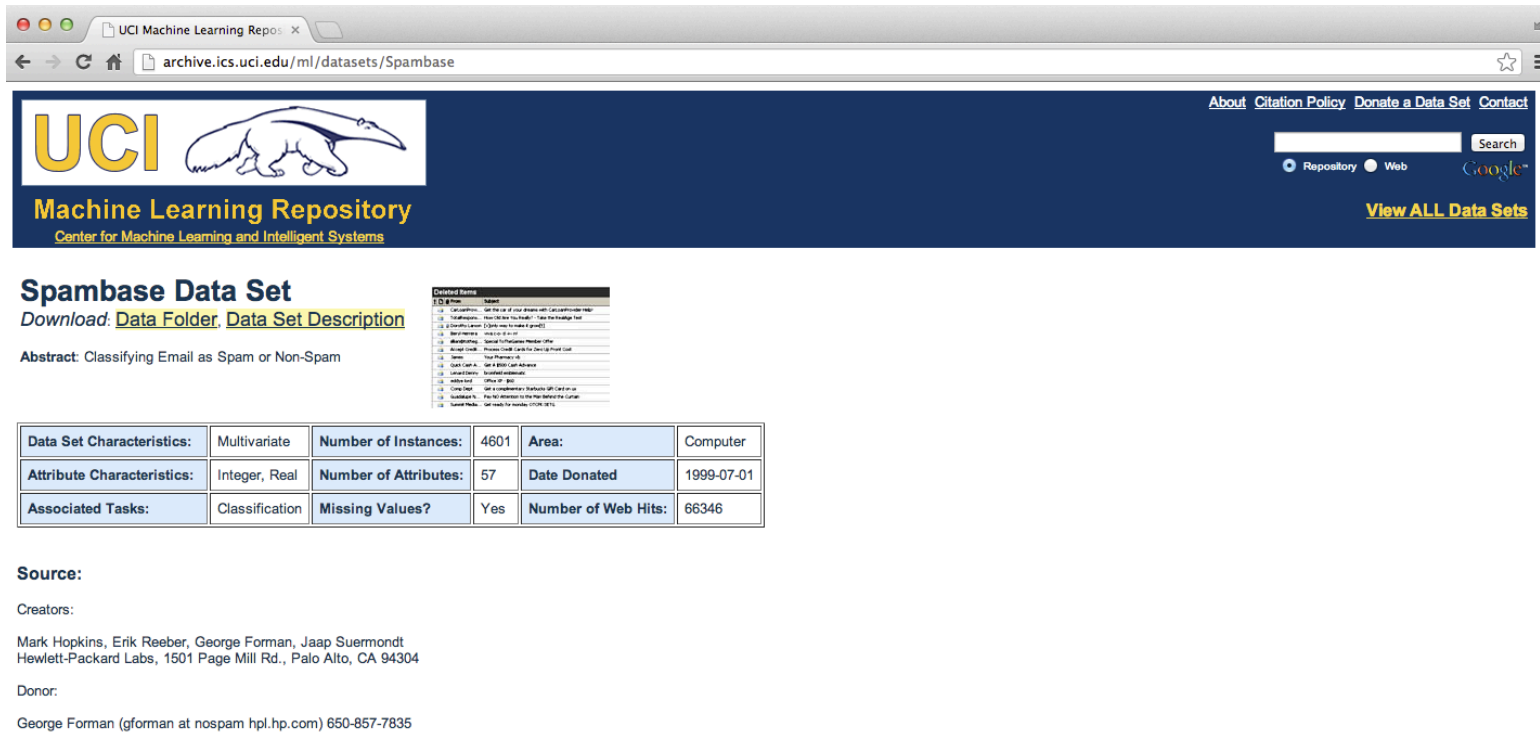
Determine what data you can access

- Sometimes you can find data free on the web
- Other times you may need to buy the data
- Be sure to respect the terms of use
- If the data don't exist, you may need to generate it yourself

Back to our example



A possible solution



The screenshot shows a web browser window with the address bar displaying "archive.ics.uci.edu/ml/datasets/Spambase". The page features the UCI Machine Learning Repository logo and navigation links. The main content area is titled "Spambase Data Set" and includes a download link, an abstract, a table of data set characteristics, a source section, and a list of creators.

Spambase Data Set
Download: [Data Folder](#), [Data Set Description](#)

Abstract: Classifying Email as Spam or Non-Spam

Data Set Characteristics:	Multivariate	Number of Instances:	4601	Area:	Computer
Attribute Characteristics:	Integer, Real	Number of Attributes:	57	Date Donated	1999-07-01
Associated Tasks:	Classification	Missing Values?	Yes	Number of Web Hits:	66346

Source:

Creators:

Mark Hopkins, Erik Reeber, George Forman, Jaap Suermondt
Hewlett-Packard Labs, 1501 Page Mill Rd., Palo Alto, CA 94304

Donor:

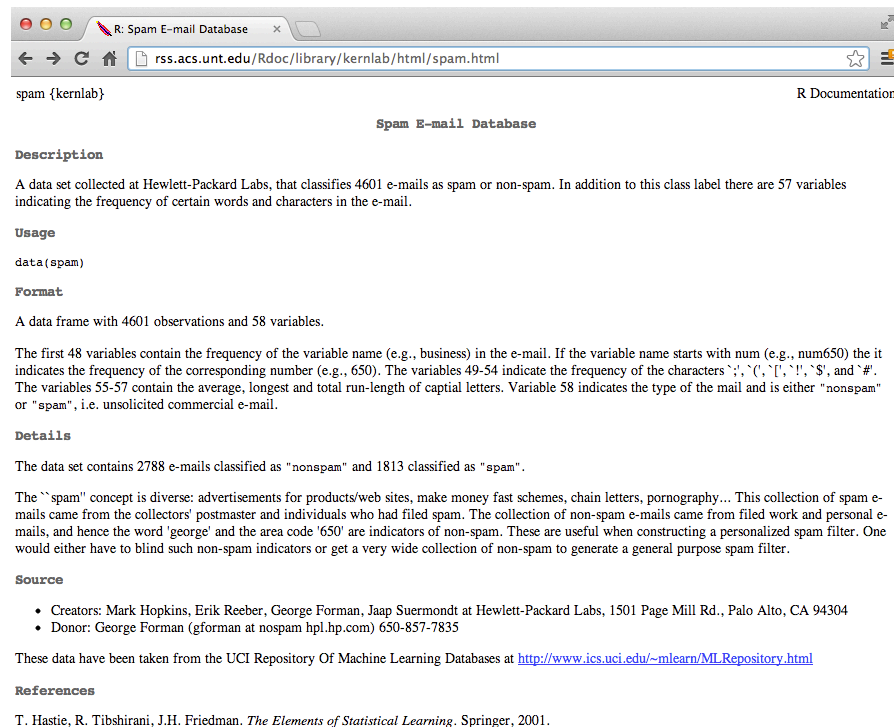
George Forman (gforman at nospam hpl.hp.com) 650-857-7835

<http://archive.ics.uci.edu/ml/datasets/Spambase>

Obtain the data

- Try to obtain the raw data
- Be sure to reference the source
- Polite emails go a long way
- If you will load the data from an internet source, record the url and time accessed

Our data set



The screenshot shows a web browser window with the title "R: Spam E-mail Database". The address bar displays the URL "rss.acs.unt.edu/Rdoc/library/kernlab/html/spam.html". The page content includes the following sections:

- spam {kernlab}** (top left)
- R Documentation** (top right)
- Spam E-mail Database** (center)
- Description**

A data set collected at Hewlett-Packard Labs, that classifies 4601 e-mails as spam or non-spam. In addition to this class label there are 57 variables indicating the frequency of certain words and characters in the e-mail.
- Usage**

`data(spam)`
- Format**

A data frame with 4601 observations and 58 variables.

The first 48 variables contain the frequency of the variable name (e.g., business) in the e-mail. If the variable name starts with num (e.g., num650) the it indicates the frequency of the corresponding number (e.g., 650). The variables 49-54 indicate the frequency of the characters ';', '^', '(', '[', '!', '\$', and '#'. The variables 55-57 contain the average, longest and total run-length of capital letters. Variable 58 indicates the type of the mail and is either "nospam" or "spam", i.e. unsolicited commercial e-mail.
- Details**

The data set contains 2788 e-mails classified as "nospam" and 1813 classified as "spam".

The "spam" concept is diverse: advertisements for products/web sites, make money fast schemes, chain letters, pornography... This collection of spam e-mails came from the collectors' postmaster and individuals who had filed spam. The collection of non-spam e-mails came from filed work and personal e-mails, and hence the word 'george' and the area code '650' are indicators of non-spam. These are useful when constructing a personalized spam filter. One would either have to blind such non-spam indicators or get a very wide collection of non-spam to generate a general purpose spam filter.
- Source**
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 - Donor: George Forman (gforman at nospam hpl.hp.com) 650-857-7835
- These data have been taken from the UCI Repository Of Machine Learning Databases at <http://www.ics.uci.edu/~mllearn/MLRepository.html>
- References**

T. Hastie, R. Tibshirani, J.H. Friedman. *The Elements of Statistical Learning*. Springer, 2001.

<http://search.r-project.org/library/kernlab/html/spam.html>

Clean the data

- Raw data often needs to be processed
- If it is pre-processed, make sure you understand how
- Understand the source of the data (census, sample, convenience sample, etc.)
- May need reformatting, subsampling - record these steps
- **Determine if the data are good enough** - if not, quit or change data

Our cleaned data set

```
# If it isn't installed, install the kernlab package with install.packages()
library(kernlab)
data(spam)
str(spam[, 1:5])
```

```
'data.frame':  4601 obs. of  5 variables:
 $ make      : num  0 0.21 0.06 0 0 0 0 0 0 0.15 0.06 ...
 $ address: num  0.64 0.28 0 0 0 0 0 0 0 0.12 ...
 $ all       : num  0.64 0.5 0.71 0 0 0 0 0 0.46 0.77 ...
 $ num3d     : num  0 0 0 0 0 0 0 0 0 0 ...
 $ our       : num  0.32 0.14 1.23 0.63 0.63 1.85 1.92 1.88 0.61 0.19 ...
```

<http://search.r-project.org/library/kernlab/html/spam.html>



Structure of a Data Analysis

Part 2

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Steps in a data analysis

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An example

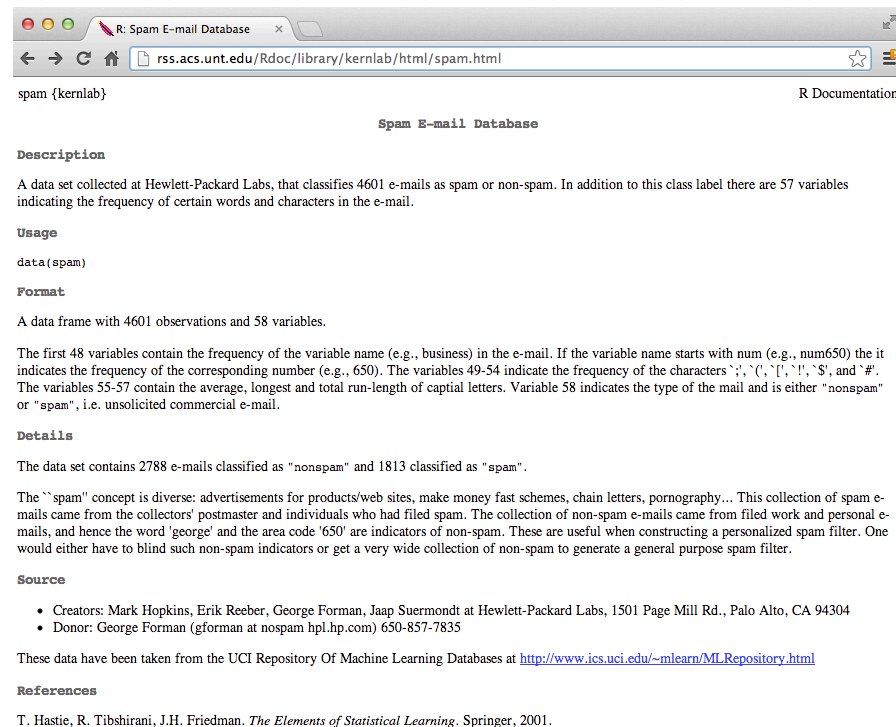
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Can I automatically detect emails that are SPAM or not?

Make it concrete

Can I use quantitative characteristics of the emails to classify them as SPAM/HAM?

Our data set



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<http://search.r-project.org/library/kernlab/html/spam.html>

Subsampling our data set

We need to generate a test and training set (prediction)

```
# If it isn't installed, install the kernlab package
library(kernlab)
data(spam)
# Perform the subsampling
set.seed(3435)
trainIndicator = rbinom(4601, size = 1, prob = 0.5)
table(trainIndicator)
```

```
## trainIndicator
##      0      1
## 2314 2287
```

```
trainSpam = spam[trainIndicator == 1, ]
testSpam = spam[trainIndicator == 0, ]
```

Exploratory data analysis

- Look at summaries of the data
- Check for missing data
- Create exploratory plots
- Perform exploratory analyses (e.g. clustering)

Names

```
names(trainSpam)
```

```
## [1] "make"          "address"       "all"
## [4] "num3d"         "our"           "over"
## [7] "remove"        "internet"      "order"
## [10] "mail"          "receive"       "will"
## [13] "people"        "report"        "addresses"
## [16] "free"          "business"      "email"
## [19] "you"           "credit"        "your"
## [22] "font"          "num000"        "money"
## [25] "hp"            "hpl"           "george"
## [28] "num650"        "lab"           "labs"
## [31] "telnet"        "num857"        "data"
## [34] "num415"        "num85"         "technology"
## [37] "num1999"       "parts"         "pm"
## [40] "direct"        "cs"            "meeting"
## [43] "original"      "project"       "re"
## [46] "edu"           "table"         "conference"
## [49] "charSemicolon" "charRoundbracket" "charSquarebracket"
## [52] "charExclamation" "charDollar"      "charHash"
## [55] "capitalAve"    "capitalLong"    "capitalTotal"
## [58] "type"
```

Head

```
head(trainSpam)
```

```
##      make address  all num3d  our over remove internet order mail receive
## 1  0.00      0.64 0.64      0 0.32 0.00   0.00      0  0.00 0.00   0.00
## 7  0.00      0.00 0.00      0 1.92 0.00   0.00      0  0.00 0.64   0.96
## 9  0.15      0.00 0.46      0 0.61 0.00   0.30      0  0.92 0.76   0.76
## 12 0.00      0.00 0.25      0 0.38 0.25   0.25      0  0.00 0.00   0.12
## 14 0.00      0.00 0.00      0 0.90 0.00   0.90      0  0.00 0.90   0.90
## 16 0.00      0.42 0.42      0 1.27 0.00   0.42      0  0.00 1.27   0.00
##      will people report addresses free business email  you credit your font
## 1  0.64      0.00      0      0 0.32      0  1.29 1.93   0.00 0.96   0
## 7  1.28      0.00      0      0 0.96      0  0.32 3.85   0.00 0.64   0
## 9  0.92      0.00      0      0 0.00      0  0.15 1.23   3.53 2.00   0
## 12 0.12      0.12      0      0 0.00      0  0.00 1.16   0.00 0.77   0
## 14 0.00      0.90      0      0 0.00      0  0.00 2.72   0.00 0.90   0
## 16 0.00      0.00      0      0 1.27      0  0.00 1.70   0.42 1.27   0
##      num000 money hp hpl george num650 lab labs telnet num857 data num415
## 1      0  0.00 0  0      0      0  0  0      0      0 0.00      0
## 7      0  0.00 0  0      0      0  0  0      0      0 0.00      0
## 9      0  0.15 0  0      0      0  0  0      0      0 0.15      0
## 12     0  0.00 0  0      0      0  0  0      0      0 0.00      0
## 14     0  0.00 0  0      0      0  0  0      0      0 0.00      0
```

Summaries

```
table(trainSpam$type)
```

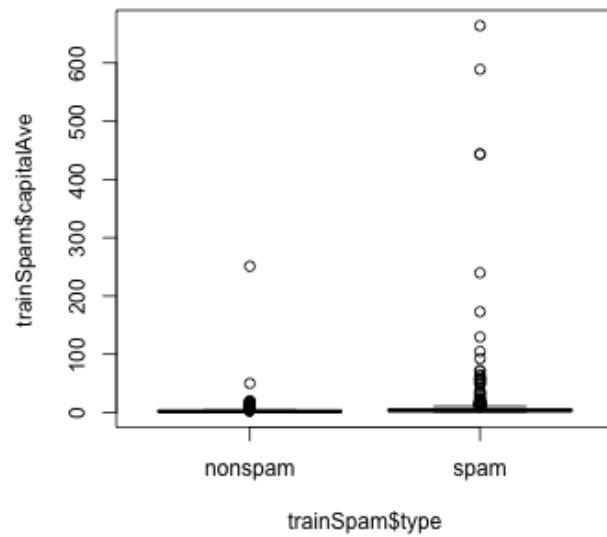
```
##
```

```
## nonspam    spam
```

```
##      1381     906
```

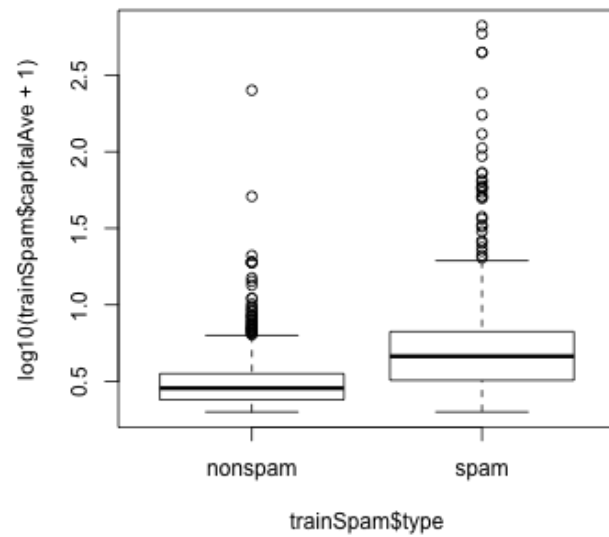

Plots

```
plot(trainSpam$capitalAve ~ trainSpam$type)
```



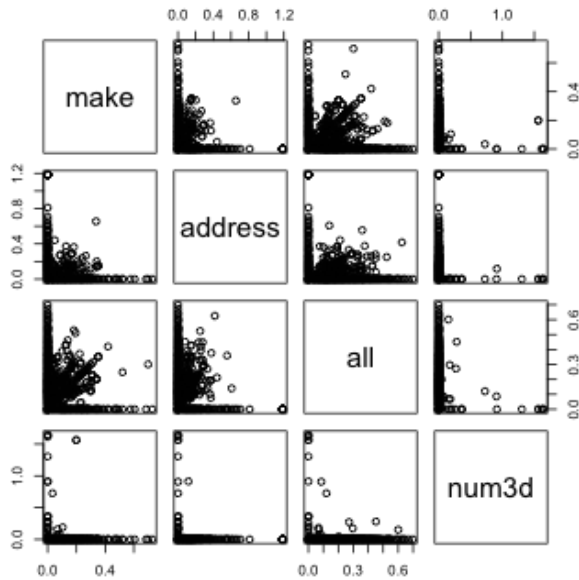
Plots

```
plot(log10(trainSpam$capitalAve + 1) ~ trainSpam$type)
```



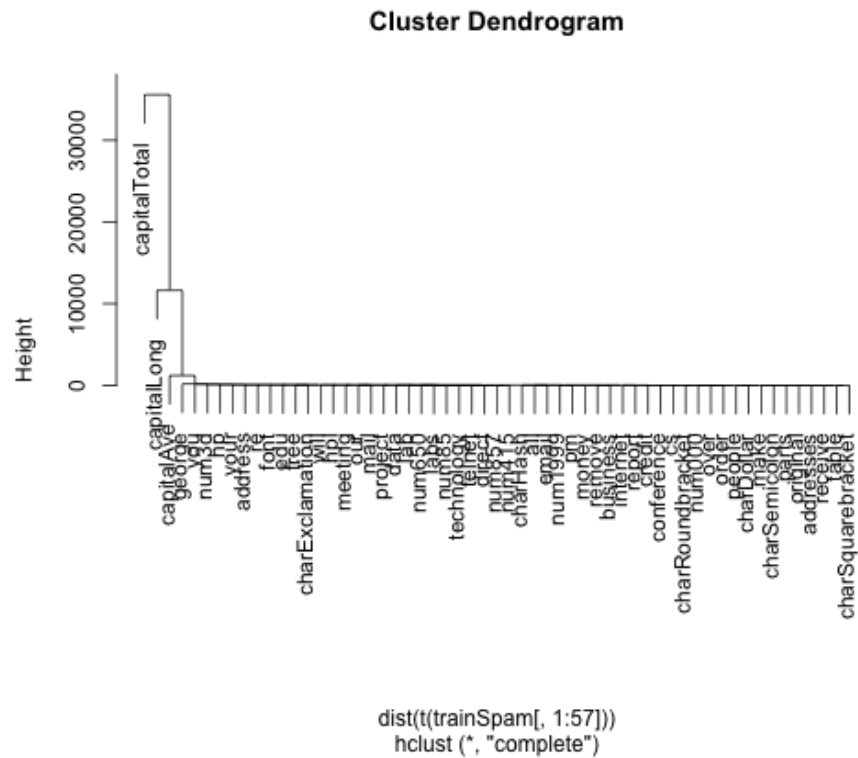
Relationships between predictors

```
plot(log10(trainSpam[, 1:4] + 1))
```



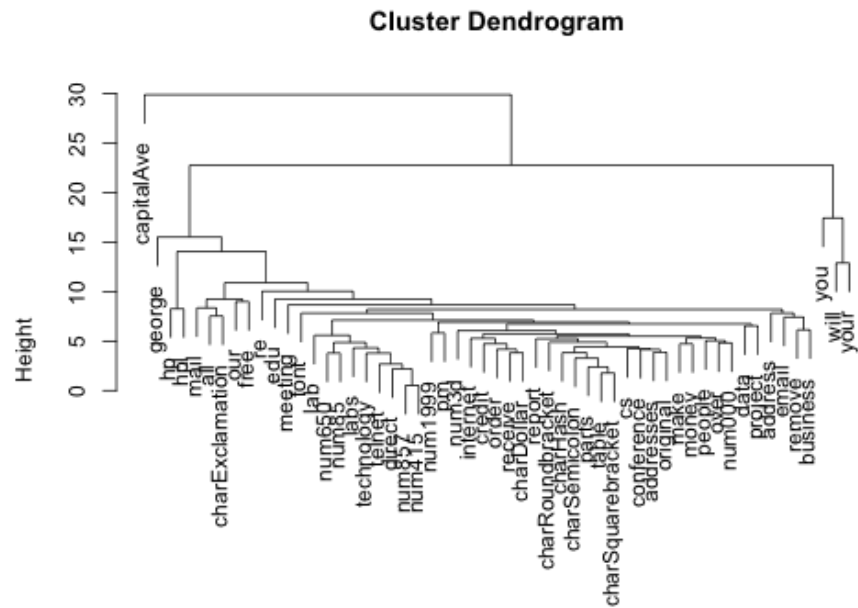
Clustering

```
hCluster = hclust(dist(t(trainSpam[, 1:57])))  
plot(hCluster)
```



New clustering

```
hClusterUpdated = hclust(dist(t(log10(trainSpam[, 1:55] + 1))))  
plot(hClusterUpdated)
```



```
dist(t(log10(trainSpam[, 1:55] + 1)))  
hclust (*, "complete")
```

Statistical prediction/modeling

- Should be informed by the results of your exploratory analysis
- Exact methods depend on the question of interest
- Transformations/processing should be accounted for when necessary
- Measures of uncertainty should be reported

Statistical prediction/modeling

```
trainSpam$numType = as.numeric(trainSpam$type) - 1
costFunction = function(x, y) sum(x != (y > 0.5))
cvError = rep(NA, 55)
library(boot)
for (i in 1:55) {
  lmFormula = reformulate(names(trainSpam)[i], response = "numType")
  glmFit = glm(lmFormula, family = "binomial", data = trainSpam)
  cvError[i] = cv.glm(trainSpam, glmFit, costFunction, 2)$delta[2]
}
```

```
## Which predictor has minimum cross-validated error?
names(trainSpam)[which.min(cvError)]
```

```
## [1] "charDollar"
```

Get a measure of uncertainty

```
## Use the best model from the group
predictionModel = glm(numType ~ charDollar, family = "binomial", data = trainSpam)

## Get predictions on the test set
predictionTest = predict(predictionModel, testSpam)
predictedSpam = rep("nonspam", dim(testSpam)[1])

## Classify as `spam' for those with prob > 0.5
predictedSpam[predictionModel$fitted > 0.5] = "spam"
```


Get a measure of uncertainty

```
## Classification table  
table(predictedSpam, testSpam$type)
```

```
##  
## predictedSpam nonspam spam  
##      nonspam      1346    458  
##      spam         61    449
```

```
## Error rate  
(61 + 458)/(1346 + 458 + 61 + 449)
```

```
## [1] 0.2243
```

Interpret results

- Use the appropriate language
 - describes
 - correlates with/associated with
 - leads to/causes
 - predicts
- Give an explanation
- Interpret coefficients
- Interpret measures of uncertainty

Our example

- The fraction of characters that are dollar signs can be used to predict if an email is Spam
- Anything with more than 6.6% dollar signs is classified as Spam
- More dollar signs always means more Spam under our prediction
- Our test set error rate was 22.4%

Challenge results

- Challenge all steps:
 - Question
 - Data source
 - Processing
 - Analysis
 - Conclusions
- Challenge measures of uncertainty
- Challenge choices of terms to include in models
- Think of potential alternative analyses

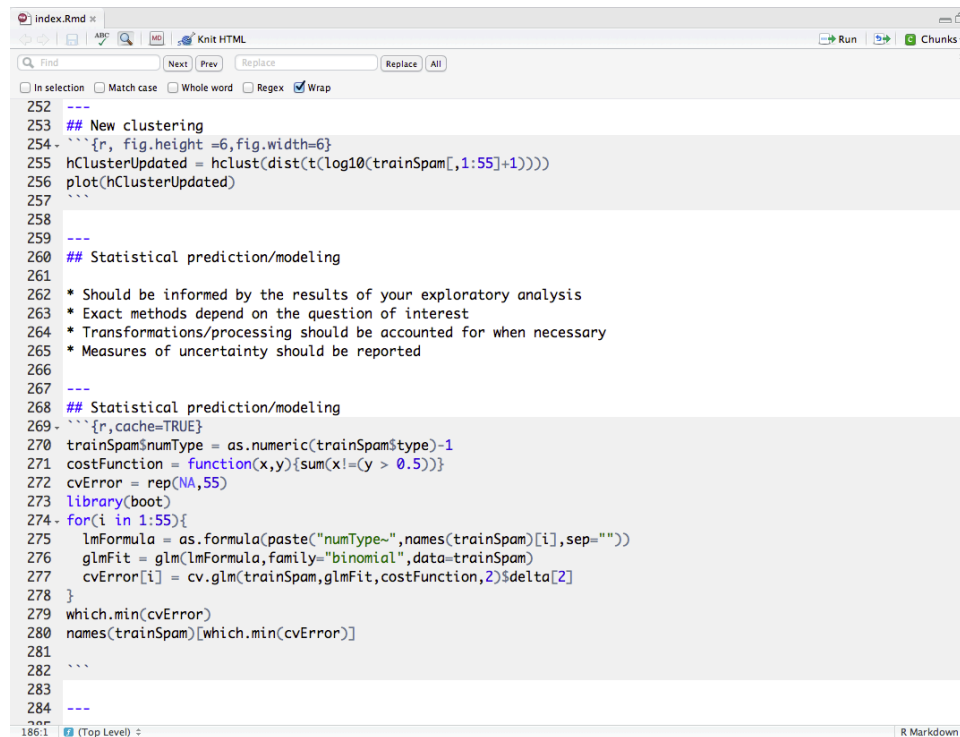
Synthesize/write-up results

- Lead with the question
- Summarize the analyses into the story
- Don't include every analysis, include it
 - If it is needed for the story
 - If it is needed to address a challenge
- Order analyses according to the story, rather than chronologically
- Include "pretty" figures that contribute to the story

In our example

- Lead with the question
 - Can I use quantitative characteristics of the emails to classify them as SPAM/HAM?
- Describe the approach
 - Collected data from UCI -> created training/test sets
 - Explored relationships
 - Choose logistic model on training set by cross validation
 - Applied to test, 78% test set accuracy
- Interpret results
 - Number of dollar signs seems reasonable, e.g. "Make money with Viagra \$ \$ \$ \$!"
- Challenge results
 - 78% isn't that great
 - I could use more variables
 - Why logistic regression?

Create reproducible code



```
252 ---
253 ## New clustering
254 ```{r, fig.height = 6, fig.width = 6}
255 hClusterUpdated = hclust(dist(t(log10(trainSpam[,1:55]+1))))
256 plot(hClusterUpdated)
257 ```
258 ---
259 ---
260 ## Statistical prediction/modeling
261
262 * Should be informed by the results of your exploratory analysis
263 * Exact methods depend on the question of interest
264 * Transformations/processing should be accounted for when necessary
265 * Measures of uncertainty should be reported
266
267 ---
268 ## Statistical prediction/modeling
269 ```{r, cache=TRUE}
270 trainSpam$numType = as.numeric(trainSpam$type)-1
271 costFunction = function(x,y){sum(x!=(y > 0.5))}
272 cvError = rep(NA,55)
273 library(boot)
274 for(i in 1:55){
275   lmFormula = as.formula(paste("numType~",names(trainSpam)[i],sep=""))
276   glmFit = glm(lmFormula,family="binomial",data=trainSpam)
277   cvError[i] = cv.glm(trainSpam,glmFit,costFunction,2)$delta[2]
278 }
279 which.min(cvError)
280 names(trainSpam)[which.min(cvError)]
281 ```
282 ---
283 ---
284 ---
```



Organizing a Data Analysis

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Johns Hopkins Bloomberg School of Public Health

Data analysis files

- Data
 - Raw data
 - Processed data
- Figures
 - Exploratory figures
 - Final figures
- R code
 - Raw / unused scripts
 - Final scripts
 - R Markdown files
- Text
 - README files
 - Text of analysis / report

Raw Data

ALLERGIES	MEDICATION HISTORY
Last Updated: 01 Dec 2011 @ 0851	Last Updated: 11 Apr 2011 @ 1737
<p>llergy Name: TRIMETHOPRIM</p> <p>ocation: DAYT29</p> <p>ate Entered: 09 Mar 2011</p> <p>eaction:</p> <p>llergy Type: DRUG</p> <p>A Drug Class: ANTI-INFECTIVES,OTHER</p> <p>bserved/Historical: HISTORICAL</p> <p>omments: The reaction to this allergy was MILD (NO SQUELAE)</p>	<p>Medication: AMLODIPINE BESYLATE 10MG TAB</p> <p>Instructions: TAKE ONE TABLET BY MOUTH TAKE ONE-HALF TABLET FOR : GRAPEFRUIT JUICE--</p> <p>Status: Active</p> <p>Refills Remaining: 3</p> <p>Last Filled On: 20 Aug 2010</p> <p>Initially Ordered On: 13 Aug 2010</p> <p>Quantity: 45</p> <p>Days Supply: 90</p> <p>Pharmacy: DAYTON</p> <p>Prescription Number: 2718953</p>
<p>llergy Name: TRAMADOL</p> <p>ocation: DAYT29</p> <p>ate Entered: 09 Mar 2011</p> <p>eaction: URINARY RETENTION</p> <p>llergy Type: DRUG</p> <p>A Drug Class: NON-OPIOID ANALGESICS</p> <p>bserved/Historical: HISTORICAL</p> <p>omments: gradually worsening difficulty emptying bladder</p>	<p>Medication: IBUPROFEN 600MG TAB</p> <p>Instructions: TAKE ONE TABLET BY MOUTH FOUR TIMES A DAY WITH FOOD</p> <p>Status: Active</p> <p>Refills Remaining: 3</p> <p>Last Filled On: 20 Aug 2010</p> <p>Initially Ordered On: 01 Jul 2010</p> <p>Quantity: 300</p>

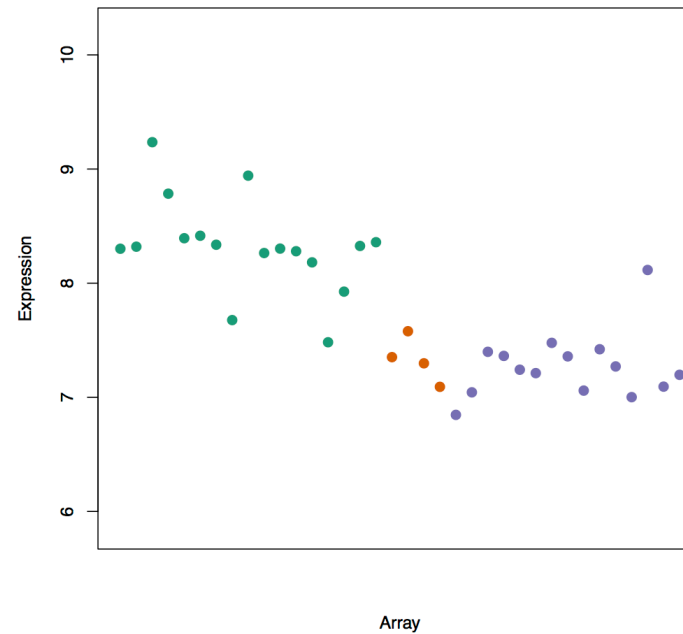
- Should be stored in your analysis folder
- If accessed from the web, include url, description, and date accessed in README

Processed data

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
	id	problem_id	subject_id	start	stop	time_left	answer									
2	1	498	17	1307119989	1307120016	2369	A									
3	2	150	15	1307119991	1307120009	2376	D									
4	3	313	16	1307119994	1307120009	2376	E									
5	4	12	13	1307119995	1307120019	2366	B									
6	5	273	14	1307119996	1307120028	2357	A									
7	6	101	19	1307119996	1307120021	2364	B									
8	7	105	18	1307119998	1307120048	2337	B									
9	8	162	12	1307120004	1307120042	2343	C									
10	9	70	15	1307120011	1307120038	2347	C									
11	10	300	16	1307120012	1307120092	2293	B									
12	11	494	17	1307120017	1307120075	2310	D									
13	12	357	13	1307120021	1307120118	2267	A									
14	13	522	19	1307120025	1307120152	2233	D									
15	14	232	14	1307120030	1307120158	2227	C									
16	15	344	15	1307120041	1307120117	2268	B									
17	16	160	17	1307120079	1307120249	2136	D									
18	17	516	16	1307120094	1307120159	2226	B									
19	18	472	12	1307120119	1307120170	2215	A									
20	19	43	15	1307120122	1307120140	2245	C									
21	20	353	13	1307120144	1307120199	2186	C									
22	21	218	15	1307120152	1307120272	2113	E									
23	22	69	16	1307120163	1307120188	2197	D									
24	23	562	16	1307120190	1307120301	2084	D									
25	24	121	19	1307120253	1307120294	2091	E									
26	25	297	15	1307120277	1307120342	2043	B									
27	26	495	13	1307120281	1307120353	2032	E									
28	27	94	14	1307120288	1307120343	2042	E									
29	28	22	18	1307120310	1307120365	2020	C									
30	29	64	19	1307120310	1307120385	2000	B									
31	30	502	16	1307120323	1307120336	2049	B									
32	31	44	16	1307120339	1307120352	2033	A									
33	32	315	14	1307120348	1307120362	2023	B									
34	33	385	15	1307120352	1307120553	1832	E									
35	34	550	13	1307120356	1307120444	1941	B									
36	35	92	14	1307120368	1307120397	1988	B									
37	36	395	16	1307120377	1307120426	1959	D									
38	37	267	17	1307120382	1307120515	1870	E									
39	38	257	14	1307120401	1307120427	1958	C									
40	39	312	19	1307120407	1307120548	1837	D									
41	40	321	18	1307120431	1307120449	1936	A									
42	41	220	16	1307120437	1307120510	1875	A									

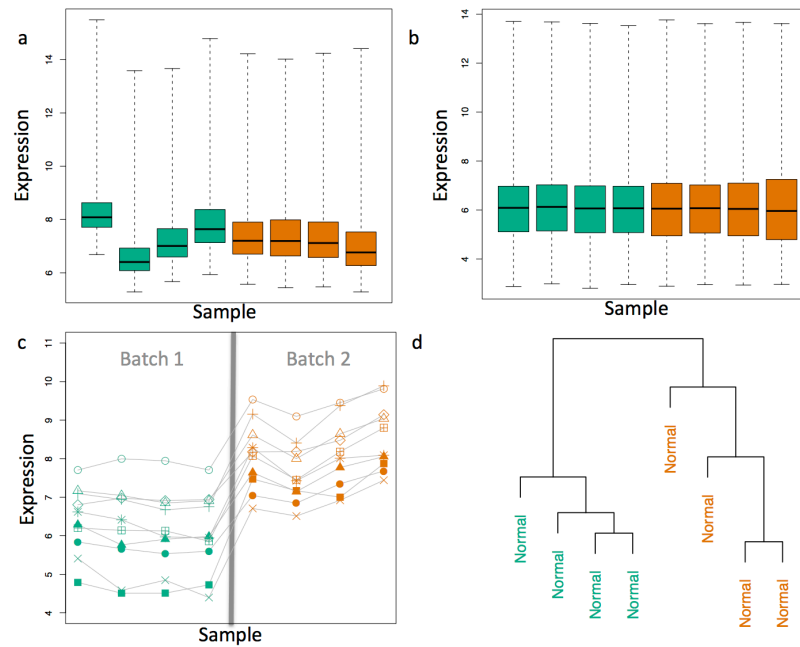
- Processed data should be named so it is easy to see which script generated the data.
- The processing script - processed data mapping should occur in the README
- Processed data should be [tidy](#)

Exploratory figures



- Figures made during the course of your analysis, not necessarily part of your final report.
- They do not need to be "pretty"

Final Figures



- Usually a small subset of the original figures
- Axes/colors set to make the figure clear
- Possibly multiple panels

Raw scripts

```
1 source("regmodel.R")
2
3 dp <- ddm[, c("group", "pm25_0", "pm25_1", "symfree0", "symfree1")]
4 dp$p_id <- row.names(dp)
5
6 fitx0 <- lm(pm25_1 ~ pm25_0 + age + no2_0 + pm10_0, data = subset(ddm, group == 0))
7 fitx1 <- lm(pm25_1 ~ ns(pm25_0, 2) + age + no2_0 + pm10_0, data = subset(ddm, group == 1))
8
9 fity0 <- glm(cbind(symfree1, 14-symfree1) ~ symfree0 + age + factor(gender), data = subset(ddm, group == 0))
10 fity1 <- glm(cbind(symfree1, 14-symfree1) ~ symfree0 + age + factor(gender), data = subset(ddm, group == 1))
11
12 y10 <- predict(fity0, subset(ddm, group == 1), type = "response") * 14
13 y01 <- predict(fity1, subset(ddm, group == 0), type = "response") * 14
14 p10 <- predict(fitx0, subset(ddm, group == 1))
15 p01 <- predict(fitx1, subset(ddm, group == 0))
16
17 yy <- data.frame(p_id = as.integer(c(names(y10), names(y01))),
18                 symfree00 = c(y10, y01))
19 pp <- data.frame(p_id = as.integer(c(names(p10), names(p01))),
20                 pm25_00 = c(p10, p01))
21
22 m <- merge(dp, yy, by = "p_id")
23 mm <- merge(m, pp, by = "p_id")
```

- May be less commented (but comments help you!)
- May be multiple versions
- May include analyses that are later discarded

Final scripts

```
49 #####
50 ## Main 'pgibbs()' function
51
52
53 pgibbs <- function(gibbsState,
54                   maxit = 80000,
55                   verbose = TRUE,
56                   dbfile = "statepgibbs",
57                   deleteCache = FALSE,
58                   singleAgeCat = TRUE,
59                   sigmaE = NULL,
60                   delta = NULL) {
61   library(MASS)
62
63   ## Setup database of results
64   if(file.exists(dbfile)) {
65     if(deleteCache) {
66       message("removing existing cache file")
67       file.remove(dbfile)
68     }
69     else
70       stop(sprintf("cache file '%s' already exists", dbfile))
71   }
```

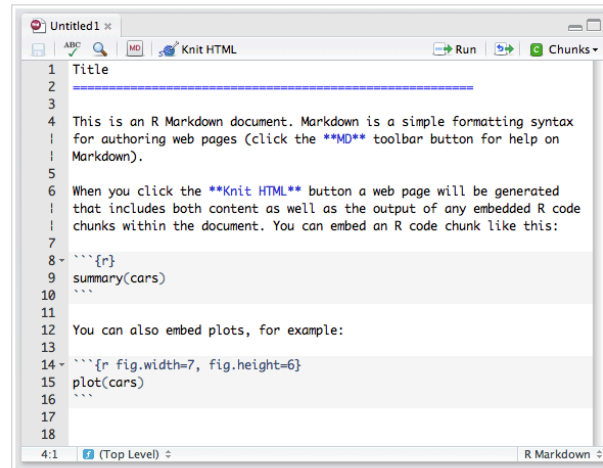
- Clearly commented
 - Small comments liberally - what, when, why, how
 - Bigger commented blocks for whole sections
- Include processing details
- Only analyses that appear in the final write-up

R markdown files

R Markdown Documents

To work with R Markdown (.Rmd) files in RStudio you first need to ensure that the [knitr](#) package (version 0.5 or later) is installed.

To create a new R Markdown file, go to **File | New** and select **R Markdown**. A new file is created with a default template to get you oriented:

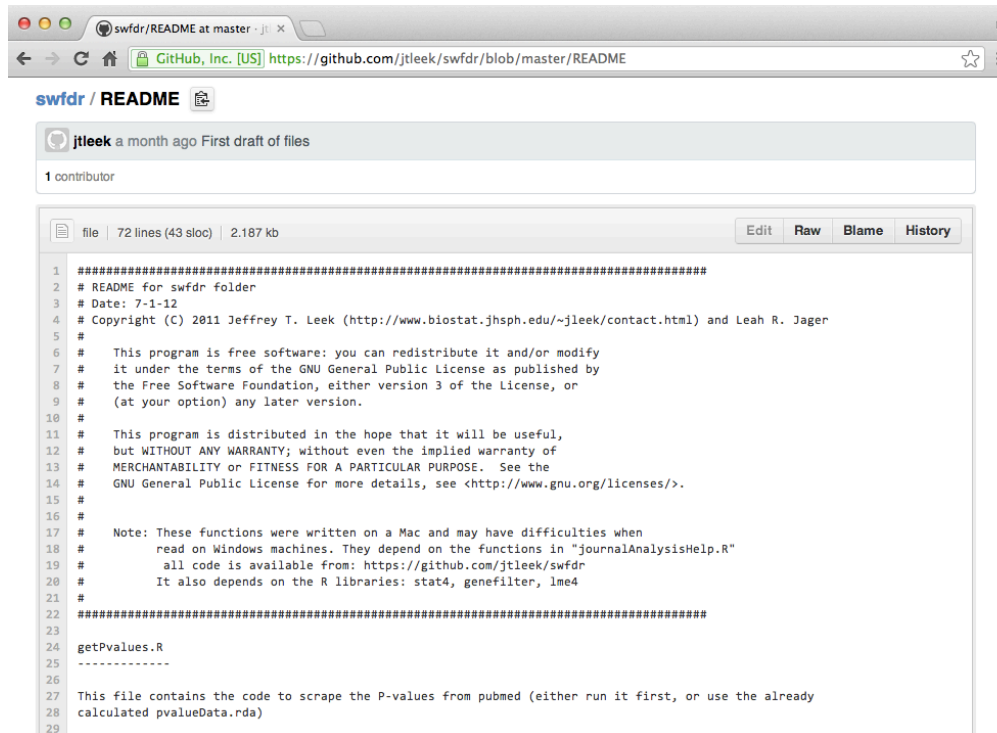


Note that the toolbar provides some useful tools for working with R Markdown:

- **Quick Reference** — Click the **MD** toolbar button to open a quick reference guide for Markdown.
- **Knit HTML** — Click to knit the current document to HTML, see the **Knitting to HTML** section below for more details.
- **Run** — Run the current line or selection of lines in the console. This allows running R code inside a code chunk similar to a normal R source file.
- **Chunks** — The chunks menu provides assistance with inserting, running, and chunk navigation. See the **Chunk Menu and Options** section below for more details.

- [R markdown](#) files can be used to generate reproducible reports
- Text and R code are integrated
- Very easy to create in [Rstudio](#)

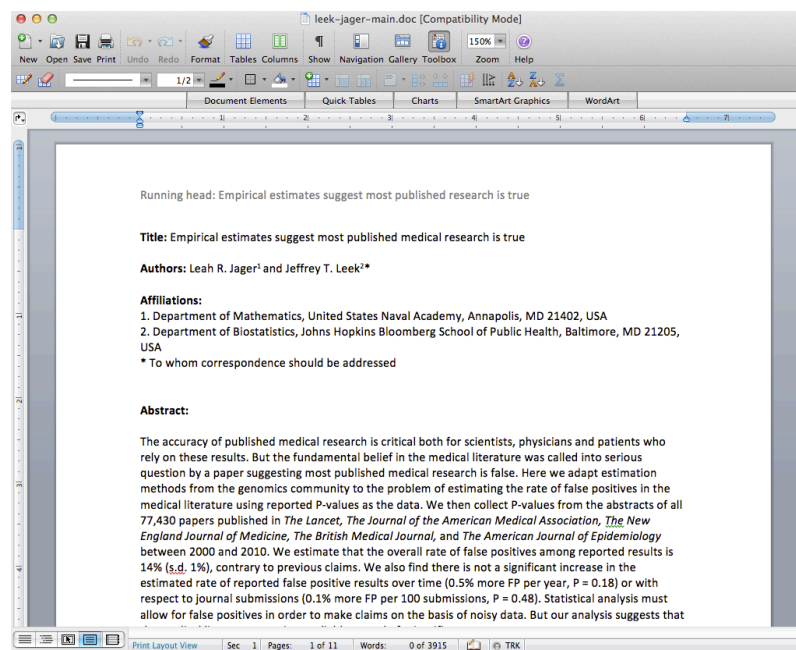
Readme files

A screenshot of a web browser displaying a GitHub repository page. The browser's address bar shows the URL 'https://github.com/jtleek/swfdr/blob/master/README'. The page title is 'swfdr / README'. Below the title, it says 'jtleek a month ago First draft of files' and '1 contributor'. The main content is a README file with 72 lines (43 sloc) and 2.187 kb. The file content is as follows:

```
1 #####
2 # README for swfdr folder
3 # Date: 7-1-12
4 # Copyright (C) 2011 Jeffrey T. Leek (http://www.biostat.jhsph.edu/~jtleek/contact.html) and Leah R. Jager
5 #
6 # This program is free software: you can redistribute it and/or modify
7 # it under the terms of the GNU General Public License as published by
8 # the Free Software Foundation, either version 3 of the License, or
9 # (at your option) any later version.
10 #
11 # This program is distributed in the hope that it will be useful,
12 # but WITHOUT ANY WARRANTY; without even the implied warranty of
13 # MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
14 # GNU General Public License for more details, see <http://www.gnu.org/licenses/>.
15 #
16 #
17 # Note: These functions were written on a Mac and may have difficulties when
18 # read on Windows machines. They depend on the functions in "journalAnalysisHelp.R"
19 # all code is available from: https://github.com/jtleek/swfdr
20 # It also depends on the R libraries: stat4, genefilter, lme4
21 #
22 #####
23
24 getPValues.R
25 -----
26
27 This file contains the code to scrape the P-values from pubmed (either run it first, or use the already
28 calculated pvalueData.rda)
29
```

- Not necessary if you use R markdown
- Should contain step-by-step instructions for analysis
- Here is an example <https://github.com/jtleek/swfdr/blob/master/README>

Text of the document



- It should include a title, introduction (motivation), methods (statistics you used), results (including measures of uncertainty), and conclusions (including potential problems)
- It should tell a story
- *It should not include every analysis you performed*
- References should be included for statistical methods

Further resources

- Information about a non-reproducible study that led to cancer patients being mistreated: [The Duke Saga Starter Set](#)
- [Reproducible research and Biostatistics](#)
- [Managing a statistical analysis project guidelines and best practices](#)
- [Project template](#) - a pre-organized set of files for data analysis