Interfacing R with the Web for Accessible, Portable, and Reproducible Data Science

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Contents

1	Problem statement 3				
2	Ove	Overview 4			
	2.1	The in	mportance of interface design	4	
	2.2	Interfa	aces for working with web content	4	
	2.3	Interfa	aces to data on the web	5	
		2.3.1	Data packages	6	
		2.3.2	Packaging access to data	6	
	2.4	Interfa	aces to web services	6	
	2.5	Interfa	aces for dynamic interactive statistical web graphics	6	
		2.5.1	Why interactive?	6	
		2.5.2	Indirect versus direct manipulation	7	
		2.5.3	GUI Toolkits	8	
		2.5.4	Web Technologies	8	
		2.5.5	Direct manipulation	8	
		2.5.6	Web-based technology	8	
		2.5.7	The paradigm of linked views	8	
		2.5.8	A grammar for linked views	9	
3	Sco	pe		9	
4	Tan	ning P	ITCHf/x Data with XML2R and pitchRx	10	
5	Curating open data in R			10	
6	LDAvis: A method for visualizing and interpreting topics 1			10	
7	Two new keywords for interactive, animated plot design: clickSelects and showSelected 10				
8	Web-based interactive statistical graphics				
9	Test	Testing interactive web-based graphics software from R.			

	11
References	11

1 Problem statement

"[The web] has helped broaden the focus of statistics from the modeling stage to all stages of data science: finding relevant data, accessing data, reading and transforming data, visualizing the data in rich ways, modeling, and presenting the results and conclusions with compelling, interactive displays." - (Nolan and Lang 2014)

The web, as a platform, has the potential to provide solutions to problems that have impeded broad distribution of statistical computing research products for decades. It requires interfaces to leverage web services in a way that is practically useful for people doing data analysis and statistics, and also develop new methodology in the process. Web technologies have evolved at a rapid pace, and as new web services have appeared new custom interfaces have been developed, which has taken substantial community effort. The CRAN task view on web technologies and services (Chamberlain et al. 2015), documents many customized interfaces for the R project, currently the world's leading open source data science software (R Core Team 2015).

R has a long history of serving as an interface to computational facilities for the use by people doing data analysis and statistics research. In fact, the motivation behind the birth of R's predecessor, S, was to provide a direct, consistent, and interactive interface to the best computational facilities already available in languages such as FORTRAN and C (Becker and Chambers 1978). This empowers users to focus on the primary goal statistical modeling and exploratory data analysis, rather than the computational implementation details. By providing more and better interfaces to web services, we can continue to empower R users in a similar way, by making it easier to acquire or share data, create interactive web graphics, perform cloud computing, practice reproducible research, collaborate remotely, and share their work with a larger audience.

Portability has prevented the broad dissemination of interactive statistical graphics. Interactive graphics software traditionally builds on toolkits like GTK+ or openGL that provide widgets for making interface elements, and also event loops for catching user input. These toolkits need to be installed locally on a user's computer, across various platforms, which adds to installation complexity, impeding portability. Modern web browsers with HTML5 support are now ubiquitous, and provide a cross-platform solution for sharing interactive statistical graphics. However, interfacing web-based visualizations with statistical analysis software remains difficult, and still requires juggling many languages and technologies. By providing better interfaces for creating web-based interactive statistical graphics, we can make them more accessible, and therefore make it easier to share statistical research to a wider audience. This research addresses this gap.

2 Overview

This section describes the background and an overview of my research on making web-based interactive graphics and data on the web more accessible. I currently maintain a number of software projects (including 7 different R packages) that address this common theme. It also points to my plans for completing my thesis research.

2.1 The importance of interface design

Unwin and Hofmann (2009) discuss the strengths, weaknesses, and differences between using graphical and command-line interfaces for data analysis. Graphical user interfaces (GUIs) can be much more intuitive to use, but at the cost of being less flexible, precise, and repeatable. Unwin and Hofmann argue statistical software should strive to achieve a synergy of two that leverages both of their strengths. That is, a command-line interface when we can precisely describe what we want and a graphical interface for "searching for information and interesting structures without fully specified questions."

Unwin and Hofmann further discuss the different audiences these interfaces attract. Command-line interfaces typically attract "power users" such as applied statisticians and statistical researchers in a university, whereas more casual users of statistical software typically prefer a GUI. In later sections, we discuss GUIs in greater detail within the context of interactive statistical graphics. For now, we briefly discuss some best practices for designing a command-line interface for statistical computing in R.

Before authoring an interface, one should establish the target audience, the class of problems it should address, and loosely define how the interface should actually work. During this process, it may also be helpful to identify your audience as being primarily composed of *software developers* or *data analysts*. Developers are typically more interested in using the interface to develop novel software or incorporating the functionality into a larger scientific computing environment (Jereon Ooms 2014). In this case, interactive exploration and troubleshooting is not always a luxury, so robust functionality is of utmost importance. On the other hand, analysts interfaces should work well in an interactive environment since this caters to rapid prototyping of ideas and troubleshooting of errors.

Good developer interfaces often make it easier to implement good analyst interfaces. A great recent example of a good developer interface is the R package **Rcpp**, which provides a seamless interface between R with C++ (Eddelbuettel 2013). To date, more than 500 R packages use **Rcpp** to make interfaces that are both expressive and efficient, including the highly influential analyst interfaces such as **tidyr** and **dplyr** (Wickham 2014); (Wickham and Francois 2015). These interfaces help analysts focus on the primary task of wrangling data into a form suitable for visualization and statistical modeling, rather than focusing on the implementation details behind how the transformations are performed. (Donoho 2015) argues that these interfaces "May have more impact on today's practice of data analysis than many highly-regarded theoretical statistics papers".

Evaluating statistical computing interfaces is certainly a subjective matter since we all have different tastes, different backgrounds, and have different needs. It seems reasonable to evaluate an interface based on its effectiveness and efficiency in aiding a user complete their task, but as (Unwin and Hofmann 2009) points out, "There is a tendency to judge software by the most powerful tools they provide (whether with a good interface or not)". As a result, all too often, analysts must spend time gaining the skills of a software developer. Good analyst interfaces often abstract functionality from developer interfaces in a way that allow analysts to focus on their primary task of acquiring/analyzing/modeling/visualizing data, rather than the implementation details. The next section focuses such work in the realm of acquiring data from the web and interactive statistical web graphics.

2.2 Interfaces for working with web content

R has a rich history of interfacing with web technologies for accomplishing a variety of tasks such as requesting, manipulating, and creating web content. As an important first step, extending ideas from (Chambers 1999),

Brian Ripley implemented the connections interface for file-oriented input/output in R (Ripley 2001). This interface supports a variety of common transfer protocols (HTTP, HTTPS, FTP), providing access to most files on the web that can be identified with a Uniform Resource Locator (URL). Connection objects are actually external pointers, meaning that, instead of immediately reading the file, they just point to the file, and make no assumptions about the actual contents of the file.

Many functions in the base R distribution for reading data (e.g., scan, read.table, read.csv, etc.) are built on top of connections, and provide additional functionality for parsing well-structured plain-text into basic R data structures (vector, list, data frame, etc.). However, the base R distribution does not provide functionality for parsing common file formats found on the web (e.g., HTML, XML, JSON). In addition, the standard R connection interface provides no support for communicating with web servers beyond a simple HTTP GET request (Lang 2006).

The RCurl, XML, and RJSONIO packages were major contributions that drastically improved our ability to request, manipulate, and create web content from R (Nolan and Lang 2014). The RCurl package provides a suite of high and low level bindings to the C library libcurl, making it possible to transfer files over more network protocols, communicate with web servers (e.g., submit forms, upload files, etc.), process their responses, and handle other details such as redirects and authentication (Lang 2014a). The XML package provides low-level bindings to the C library libxml2, making it possible to download, parse, manipulate, and create XML (and HTML) (Lang and CRAN Team 2015). To make this possible, XML also provides some data structures for representing XML in R. The RJSONIO package provides a mapping between R objects and JavaScript Object Notation (JSON) (Lang 2014b). These packages were heavily used for years, but several newer interfaces have made these tasks easier and more efficient.

The curl, httr, and jsonlite packages are more modern R interfaces for requesting content on the web and interacting with web servers. The curl package provides a much simpler interface to libcurl that also supports streaming data (useful for transferring large data), and generally has better performance than RCurl (Ooms 2015). The httr package builds on curl and organizes it's functionality around HTTP verbs (GET, POST, etc.) (Wickham 2015a). Since most web application programming interfaces (APIs) organize their functionality around these same verbs, it is often very easy to write R bindings to web services with httr. The httr package also builds on jsonlite since it provides consistent mappings between R/JSON and most modern web APIs accept and send messages in JSON format (Jeroen Ooms 2014). These packages have already had a profound impact on the investment required to interface R with web services.

The **rvest** package builds on **httr** and makes it easy to manipulate content in HTML/XML files (Wickham 2015b). Using **rvest** in combination with SelectorGadget, it is often possible to extract structured information (e.g., tables, lists, links, etc) from HTML with almost no knowledge/familiarity with web technologies. The **XML2R** package has a similar goal of providing an interface to acquire and manipulate XML content into tabular R data structures without any working knowledge of XML/XSLT/XPath (Sievert 2014a). As a result, these interfaces reduce the startup costs required for analysts to acquire data from the web.

Packages such as **XML**, **XML2R**, and **rvest** can download and parse the source of web pages, which is *static*, but if we wish to extract *dynamic* web content from R, we need additional tools. The R package **rdom** fills this void and makes it easy to render and access the Document Object Model (DOM) using the headless browsing engine phantomjs (Sievert 2015). The R package **RSelenium** can also render dynamic web pages and simulate user actions, but its broad scope and heavy software requirements make it harder to use and less reliable compared to **rdom** (Harrison 2014).

Any combination of these interfaces may be useful in developing high-level interfaces to specific web services or acquiring content for analysis.

2.3 Interfaces to data on the web

These high-level interfaces provide a nice resource for both teaching and practicing applied statistics, and serve as a model for providing access to clean versions of messy datasets on the web (Unwin 2010).

2.3.1 Data packages

If the data source is fairly small, somewhat static, and freely available with an open license, then we can directly provide data via R packaging mechanism.

It is recommended that the package author include scripts used to acquire and transform

2.3.2 Packaging access to data

R packages that provide an interface to data can be more desirable than repackaging the data for several reasons. In some cases, it helps avoid legal issues with rehosting copyrighted data. Furthermore, the source code of R packages can always be inspected, so users can verify the cleaning and transformations performed on the data to ensure its integrity. They are also versioned, which makes the data acquisition, and thus any downstream analysis, more reproducible and transparent. It is also possible handle dynamic data with such interfaces, meaning that new data can be acquired without any change to source code.

Perhaps the largest centralized effort in this direction is lead by rOpenSci, a community of R developers that, at the time of writing, maintains more than 50 packages providing access to scientific data ranging from bird sightings, species occurrence, and even text/metadata from academic publications. This provides a tremendous service to researchers who want to spend their time building models and deriving insights from data, rather than learning the programming skills necessary to acquire and clean it.

It's becoming increasingly clear that "meta" packages that standardize the interface to data acquisition/curation in a particular domain would be tremendously useful. However, it is not clear how such interfaces should be designed. The etl package (a joint work with Ben Baumer) is one step in this direction and actually aims to provide a standardized interface for any data access package that fits into an Extract-Transform-Load paradigm (Baumer and Sievert). The package provides generic extract-transform-load functions, but requires developers to write custom extract-transform methods for the specific data source. In theory, the default load method works for any application; as well as other database management operations such as update and clean.

The Open Data CRAN Task View does a great job of summarizing data access packages in R, and even breaks them down by their domain application (e.g., Government, Finance, Earth Science, etc). It also details more general tools for requesting, parsing, and working with popular file formats on the web from R that many of the data access packages use to implement their functionality. Two other packages I maintain: **XML2R** and **rdom** fit into this broader category.

2.4 Interfaces to web services

The scope of functionality readily available through R packages is constantly expanding thanks to these general purpose interfaces. For example, it is now easy to install R packages hosted on the web (devtools), perform cloud computing (analogsea), archive/share computational outputs (dvn, rfigshare, RAmazonS3, googlesheets, rdrop2, etc.), create/share web graphics (plotly), and acquire all sorts of data (too many to list).

2.5 Interfaces for dynamic interactive statistical web graphics

2.5.1 Why interactive?

Our ability to find interesting structures in high-dimensional data is fundamentally limited by the 2D display of a computer screen (or paper). We can visualize a handful of dimensions by encoding data values in the visual attributes of marks on a static plot, but this approach often limited by perceptual issues when viewers try to decode values. There are also certain layouts, such as a scatterplot-matrix, and non-orthogonal coordinate systems (e.g., parallel coordinate plots), which allow us to see view high-dimensional relationships,

but don't scale well to many variables and/or many observations. There are also many ways to perform dimension reduction (e.g., multidimensional scaling), but this can lead to over-generalizations that miss interesting details in the data. In short, any visualization of high dimensional data has to be compressed in some way, but interactivity allows us to obtain details-on-demain and reveal high-dimensional structures that may otherwise go unnoticed.

The ASA Section on Statistical Computing and Graphics maintains a video library which captures many useful dynamic interactive statistical graphics techniques. Several videos show how xgobi (predecessor to ggobi), a dynamic interactive statistical graphics system, can be used to reveal high-dimensional relationships and structures that cannot be easily identified using numerical methods alone (Swayne, Cook, and Buja 1998). Another notable video shows how the interactive graphics system mondrian can be used to quickly find interesting patterns in high-dimensional data using exploratory data analysis (EDA) techniques (Theus and Urbanek 2008). The most recent video is the first web-based visualization and shows how interactive techniques can be used to help interpret a topic model (a statistical mixture model applied to text data) using **LDAvis** (Sievert and Shirley 2014).

2.5.2 Indirect versus direct manipulation

Even within the statistical graphics community, the term *interactive* graphics can mean wildly different things to different people (Swayne and Klinke 1999). Some early statistical literature on the topic uses interactive in the sense that an interactive command-line prompt allows users to create graphics on-the-fly (R. A. Becker 1984). That is, users enter commands into the command-line prompt, the prompts evaluates the command, and prints the result (known as the read–eval–print loop (REPL)). Modifying a command to generate another variation of a particular result (e.g., to restyle a static plot) can be thought of as a type of interaction that some might call *indirect manipulation*.

Indirect manipulation can be achieved both from the command-line or from a graphical user interface (GUI). Indirect manipulation from the command-line is more flexible since we have complete control over the commands, but it is also more cumbersome since we must translate our thoughts into code. Indirect manipulation via a GUI is more restrictive, but it helps reduces the the gulf of execution for end-users (i.e., easier to generate desired output) (Hutchins, Hollan, and Norman 1985). In this sense, a GUI can be useful, even for experienced statistical programmers, when the command-line interface impedes our primary task of deriving insight from data.

In many cases, the gulf of execution can be further reduced through direct manipulation. Roughly speaking, within the context of interactive graphics, direct manipulation occurs whenever we interact with a plot and reveal new information tied to the event. (Cook and Swayne 2007) use the terms dynamic graphics and direct manipulation to characterize "plots that respond in real time to an analyst's queries and change dynamically to re-focus, link to information from other sources, and re-organize information." Perhaps the most powerful direct manipulation technique is the paradigm of linked views (Wilhelm 2005), which will be discussed in more detail in a later section.

A simple example to help demonstrate the differences between these interactive techniques would be in an analysis of variance (ANOVA) via multiple boxplots. By default, most plotting libraries sort categories alphabetically, but this is usually not optimal for visual comparison of groups. With a static plotting library such as **ggplot2**, we could indirectly manipulate the default by going back to the command-line, reordering the factor levels of the categorical variables, and regenerate the plot (Wickham 2009). This is flexible and precise since we may order the levels by any measure we wish (e.g., Median, Mean, IQR, etc.), but it would be much quicker and easier if we had a GUI with a drop-down menu for most of the reasonable sorting options. In a general purpose interactive graphics system such as mondrian, we can use direct manipulation to directly click and drag on the categories to reorder them, making it quick and easy to compare any two groups of interest (Theus and Urbanek 2008).

¹For example, http://stat-graphics.org/movies/xgobi.html and http://stat-graphics.org/movies/grand-tour.html

²http://stat-graphics.org/movies/tour-de-france.html

³http://stat-graphics.org/movies/ldavis.html

2.5.3 GUI Toolkits

A wide array of GUI toolkits have been available in R for years, and many of them interface to GUI construction libraries written in lower-level languages. A couple fairly recent and popular examples include the RGtk2 package which provides R bindings to the GTK+ 2.0 library written C and the rJava package which provides R bindings to Java (Lawrence and Temple Lang 2010); (Urbanek 2015). More recently, GUI development has moved to the web browser. Probably the most attractive consequence of writing a GUI for the web browser is that users do not have to install any software in order to use the interface.

The R package **shiny** makes it incredibly easy to create web-based GUIs with support for indirect manipulation (Chang et al. 2015). Since **shiny** is based on a client-server model, it is sometimes referred to as a web application (app) framework. In a client-server model, end-users interact with the client, and when necessary, the client can requests resources from the server, or even request that the some code, that can't evaluated in a web browser (e.g., R code), be evaluated and its output returned to the client. There are a number of other R packages that allow one to write web apps which leverage R functionality (e.g., **FastRWeb**, **httpuv**, **opencpu**) (Urbanek and Horner 2015), but **shiny** is probably the most popular since apps can be written entirely in R using a very powerful yet approachable reactive programming framework for handling user events. There are many convenient shortcuts for creating **shiny** input widgets, making it incredibly easy to go from R script to an interactive web app.

Although it is very easy to write a **shiny** app with indirect manipulation, it is often much harder to construct a web app with direct manipulation. A myriad of JavaScript charting libraries have appeared in recent years which make it easy to perform simple direct manipulation (e.g., mousing over points to reveal information), and these are often easy to plug into a shiny app,

2.5.4 Web Technologies

d3js

2.5.5 Direct manipulation

Refer to http://stat-graphics.org/movies/focussing-linking.html

- plotly has tools for focusing
- animint has tools for linking

2.5.6 Web-based technology

The **htmlwidgets** package provides a framework for creating HTML widgets that render in various contexts including the R console, 'R Markdown' documents, and 'Shiny' web applications (Vaidyanathan et al. 2015). (TODO: use this a transition point for moving to GUI/shiny applications?)

Functional programming paradigm works well for computational problems with well defined input/output. With interactive web graphics you want to the output to be dynamic, meaning that users can modify the "inputs" even after the output has been determined.

2.5.7 The paradigm of linked views

(Wilhelm 2003); (Wilhelm 2005); (Wilhelm 2008)

2.5.8 A grammar for linked views

The clickSelects/showSelected paradigm makes it easy to select/query points belonging to arbitrary group(s) and visualize those points in another data space. This differs from the classing linked brushing approach where points must belong to contiguous regions within a subset of the data space.

- Talk about rggobi and controlling a standalone application from the command-line?
- R bindings that talk to JSON specifications are most similar to this approach

3 Scope

This section describes work to be achieved before completion of the thesis. Most of the work involves writing and revising papers. I have a very early start on two papers that will summarize modern interfaces in R for interactive web graphics as well as curating data on the web.

Toby Dylan Hocking, Susan VanderPlas, and I have a paper in progress which outlines the design of **animint** and it's interesting features https://github.com/tdhock/animint-paper. We've submitted this paper to IEEE Transactions on Visualization and Computer Graphics, and were told to revise and resubmit. We intend on revising and submitting to the Journal of Computational and Graphical Statistics by January 2016. The revision includes a restructuring of the content/ideas and new features implemented during Google Summer of Code 2015. The paper will be included as one of the chapters in my thesis.

We have a long TODO list with known bugs and features we'd like to implement in **animint** after we submit to JCGS. As of writing, I'm working on numerous bug fixes in **plotly**, introduced by a massive reworking of **ggplot2** internals in version 1.1. I intended on making similar fixes for **animint** so users can rely on the CRAN version of **ggplot2**, rather than our fork on GitHub. This work simply ensures packages are *usable*, but I'm also interested in expanding the scope of **animint**, which may lead to paper(s) after the thesis is submitted:

- 1. The current design of **animint** requires pre-computation of every state the visualization can possibly take on. One benefit of this approach is that we don't need any special software besides a web browser for viewing, and bodes well for cognostic-like applications, but when the number of states is very large, pre-computation can take a long time, and the amount of data that the browser tries to upload can be very large. Instead of pre-computing these states, we could dynamically compute states, only when user requests them, using a HTTP requests. The **plumbr** and **opencpu** packages assist in creating a REST API providing the ability to execute arbitrary R functions over HTTP, allowing us to define endpoints at compile time, create/destroy them during the rendering/viewing stage, and all of this could be done on a viewer's machine if R is installed. This addition to **animint** would be helpful for visualizations with many states, but in order to retain responsiveness, each state would need to be relatively cheap to compute.
- 2. Integrate crossfilter.js into **animint**. This should help relax current restrictions that summary statistics impose on showing/selecting values.

In February 2015, I was invited to write a chapter on MLB Pitching Expertise and Evaluation for the Handbook of Statistical Methods for Design and Analysis in Sports, a volume that is planned to be one of the Chapman & Hall/CRC Handbooks of Modern Statistical Methods. I've since brought on Brian Mills as a co-author, and we submitted a draft in early November. This chapter uses data collection and visualization functionality in the **pitchRx** package, but it more focused on modeling this data with Generalized Additive Models. The book likely won't be published until after this thesis is completed, and the chapter probably won't be included in the thesis, but I do intend on working on revisions of this chapter in the meantime.

4 Taming PITCHf/x Data with XML2R and pitchRx

Pitch f/x refers a massive, publicly available baseball dataset hosted on the web in XML and JSON format. Since this data is large, increases on a daily basis, and only licensed for individual use, the **pitchRx** package provides a simple interface to download, parse, clean, and transform the data from its source (instead of directly distributing the data). If acquiring large amounts of data, to avoid memory limitations, users may divert incoming data in chunks to a database using any valid R database connection (Databases 2014). It also provides a convenient function to update an existing database with the most recently available data.

The **openWAR** package also provides high-level access to Pitch f/x data, but it is currently more limited in the data it can acquire (Baumer, Jensen, and Matthews 2015). It also currently depends on the difficult to install **Sxslt** package, impeding portability (Lang). **openWAR** depends on **Sxslt** to help transform XML files to R data frames via XSL Transformations (XSLT). Without advanced knowledge of XSLT, one must define transformations by hard coding assumptions about the XML format, such as the names of fields of interest. New variables have been added into Pitch f/x several times, and **pitchRx** automatically picks them up, thanks to functionality provided by **XML2R**.

XML2R makes it easy to wrangle relational data stored as a collection of XML files into a list of data frames. Its interface satisfies principles from pure functional programming: the output of each function can be completely determined from the input. The interface is also predictable: each function inputs and outputs a list of observations (an observation is a matrix with one row). This interface makes it much easier to implement and maintain higher-level interfaces to specific XML data sources, such as **pitchRx** and **bbscrapeR** (Sievert 2014b).

To see the fully published article "Taming PITCHf/x Data with XML2R and pitchRx", see http://rjournal.github.io/archive/2014-1/sievert.pdf

5 Curating open data in R

Work in progress. See https://github.com/cpsievert/thesis/blob/master/curate.Rmd

6 LDAvis: A method for visualizing and interpreting topics

http://nlp.stanford.edu/events/illvi2014/papers/sievert-illvi2014.pdf

7 Two new keywords for interactive, animated plot design: click-Selects and showSelected

Currently in revision. See https://github.com/tdhock/animint-paper/blob/master/HOCKING-animint.pdf

8 Web-based interactive statistical graphics

Work in progress. See https://github.com/cpsievert/thesis/blob/master/web-graphics.Rmd

9 Testing interactive web-based graphics software from R

The current trend in web-based interactive statistical graphics is provide various language bindings to JavaScript charting libraries. To test whether the entire software stack is working as intended, it's common

to verify properties of the data sent to the binding, but this does not guarantee that the end result is what we expect. A proper testing framework for this type of software should be able to construct and manipulate the Document Object Model (DOM) using technologies available to modern web browsers. To our knowledge, **animint** is the first R package to implement this testing approach, and some of the lessons learned could be used to construct a more reliable and easier to use testing suite.

10 Timeline

- January: Submit animint paper.
- March: Submit curating data paper.
- April: Submit Web Graphics paper
- May:

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