Having your cake and eating it too: Scripted workflows for image manipulation

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ABSTRACT
The reproducibility issue in science has come under increased scrutiny. One consistent suggestion lies in the use of scripted methods or workflows for data analysis. Image analysis is one area in science in which little can be done in scripted methods. The SWIIM Project (Scripted Workflows to Improve Image Manipulation) is designed to generate workflows from popular image manipulation tools. In the project, 2 approaches are being taken to construct workflows in the image analysis area. First, the open-source tool GIMP is being enhanced to produce an active log (which can be run on a stand-alone basis to perform the same manipulation). Second, the R system Shiny tool is being used to construct a graphical user interface (GUI) which works with EBImage code to modify images, and to produce an active log which can perform the same operations. This process has been successful to date, but is not complete. The basic method for each component is discussed, and example code is shown.

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1. INTRODUCTION

1.1 Workflows in science

A scientific workflow is a tool to structure and regularize a process ([12] [21] [15]). A good description is as follows:

“Scientific workflows attempt to automate repetitive computation and analysis by chaining together related processes. Automating repetitive time-consuming tasks allows scientists to keep pace with ever-growing volumes of data. Furthermore, workflows can aid in the reproducibility of scientific computations by providing a formal declaration of an analysis. Reproducibility is central to the scientific method, and detailed workflow provenance in formation ensures an analysis can be reproduced and extended.” [21]

Workflows have been the subject of much investigation. They take many different forms. Some workflows are defined by an interactive process, while others are defined by scripts. In using a scripted workflow, the process which the workflow performs becomes public, transparent, and reproducible.

1.2 Reproducibility

Reproducible research methods are increasingly important in science([11][18][19][23][32][31][39][42]). “Reproducibility of research” is defined by the different issues which result in problems obtaining the same results from a study. Are the results the same from a second processing of the same data?

“Getting the same result” can mean different things. The most specific is seemingly the simplest: When reanalysing a given dataset using the same methods, can identical outcome values (test statistics, p values, summary statistics) be obtained? This may be termed “data reproducibility”. A somewhat different form of reproducibility may involve running the study again with different subjects to examine the “scientific reproducibility” of the study. Each type of reproducibility examines the different aspects to the degree to which the results of a study are repeatable. Science involves determining a process which can be repeated and produce the same results, and thus reproducibility is the essence of science.

Obtaining the same result from a given set of data sounds obvious and trivial, but there are a number of reasons why this can be problematic. First, certain types of analyses are not closed-form but rather are iterative and approximating (with a loss function and convergence criteria). Unless the same convergence criteria, start values, and step sizes are used, it is entirely possible to get different outcomes. This
is particularly true in cases in which the outcome surface is relatively flat. Second, analyses may be done in an interactive manner, and thus the tracking of the exact processes involved can sometimes be difficult. When interactive methods are used, it is possible that steps are forgotten, or that steps are done in different orders, or that the specific details in a step are not correctly noted. Third, the version of software used for analysis may change from one use to the next. Newer versions can include different convergence criteria or even different methods for estimation. Fourth, the persons using the software can be different, and use the software in different ways. In the well-known Potti et al case, the original data were analyzed by a physician who was not well trained in proper data analysis, proper data storage, or proper use of training and validation samples ([1] [33]). Later analysis by better-trained bioinformatics scientists found many errors, including changes in the version of the main data analysis tool ([1]).

In producing scientific articles, the data must be structured for the analysis first. This is the “data management” process, and is often a key step in the process. Values are corrected. Occasionally data are removed. The statistical analysis which examines the data is next performed. Again, this must be carefully documented to produce valid outcomes ([31] [5] [38] [43]). Scripted methods (i.e., analysis performed using programs of computer code) are necessary for reproducible results ([32] [5] [38] [30]). The code can be inspected, transferred to others, used on more than one project, and modified easily. It also functions as the memory of the project([41]).

The use of analysis code also is “transparent” or able to be inspected by others. Transparent, scripted code ensures that the author of a scientific document can produce the same results later, and can demonstrate to others (e.g., journal editors, colleagues) exactly how the published information was created from source materials. In science, repeating an analysis must produce the same result.

1.3 Image manipulation

Scientific image manipulation is a key part of many areas, particularly basic biology and chemistry ([25] [4] [8] [24] [34] [36] [35]). It is the process of preparing images for publication. Scientific journals have clear and well-defined requirements for proper preparation of images ([25] [8] [36]). Such scientific image manipulation follows general guidelines:

1. specific features may not be changed or modified;
2. adjustments to the full image (brightness, contrast color values) are usually acceptable;
3. if separate images are grouped together, this must be explicit; and
4. the original image must be retained and be available for examination. [25]

There is a clear and well defined difference between preparation of scientific images and preparation of aesthetic images ([7] [6] [3]). Methods acceptable for aesthetic image preparation include many techniques which would not be allowed in scientific images.

Image processing is primarily done using interactive tools such as Adobe Photoshop([16]) ImageJ([9]) and GIMP([40]). These programs can read in images, modify them in many ways, and save the results. It is sometimes difficult to reproduce the interactive process of producing an image for a publication from a source image. This is due in part to the use of the computer mouse, and partly due to the difficulty of remembering operations.

When images are prepared for scientific presentation, reproducibility problems are common. The difficulties in reproducibility, due to the interactive nature of the process, partly arise due to the “semi-continuous” nature of the process. When cropping (selecting a small part of the picture for presentation), a selection is made using the mouse. Although this is done using positions which are numbers, the scale is large and the position is difficult to remember exactly. When increasing brightness-contrast, the increases are done using a scale which emphasizes relative amounts; the exact value is a number, but the number is likely not remembered exactly. While a person could remember such values, the exact numbers are quite difficult to remember, and the process is not conducive to simple recollection.

Image fraud is a serious and pressing issue in science([4] [24] [35] [27]). Image fraud includes a number of processes (e.g., image reuse, improper preparation, improper combination of images). The “Retraction Watch” blog provides a contemporaneous record of research fraud.[22] In examining this blog, it is clear that a large proportion of retractions involve image fraud. As of 2017/03/31, 512 of the entries in the blog are related to image fraud. Improper image preparation occurs commonly; some reports suggest that 25% of all submissions to journals have improper image preparation.[35] 20 years of discussing the problem have not reduced the incidence of the problem. Different approaches are needed.

1.4 Journaling

Writing code for analysis is a difficult skill. Interactive methods for data analysis are preferred by some as being simpler and more intuitive. When an analysis is performed by a graphical user interface (GUI; a window with buttons and controls), this is termed an “interactive approach”. The reproducibility of interactive approaches is questioned by many.[38] That is because interactive methods often involve important but small decisions, which are often hard to remember and write down. Details are difficult to remember correctly. If the interactive process is at all involved or complicated, the many decisions which are made “on the fly” are difficult to remember later, and may be hard to communicate in a scientifically complete manner.

There is a middle ground. In many high-level programs (e.g., SAS/JMP([17])), the analyst can perform the analysis interactively, while the program simultaneously creates code which performs the same analysis. This process of program-created code is termed “journaling”. The journaling process creates a log or record, which can then be used to perform the analysis
The SWIIM project is designed to generate workflows from the following operations:

A “journaling” approach to image processing is needed. In the SWIIM project, several approaches to journaling are being implemented. The project is creating such an image-manipulation journaling tool by working with open-source tools, to produce an executable log (the journal) of the analysis performed using the tool. The GIMP program will be enhanced to perform a journaling function, by adding code to the program. With the R system, a set of tools will be added to the existing methods to perform programmatic image analysis. In both cases, the modifications will allow the user

1. to examine what specifically was done with the image;
2. to perform the same modifications when “replayed” on the original image; and
3. to step through the modifications to examine them in detail.

Fraudulent and inappropriate image manipulation is a serious problem in science. The use of interactive methods makes it very difficult to provide a clear tracking of all processes performed on an image. A methodology which performs image manipulation using scripting can provide transparency in processing, but this is difficult to learn and use. The best approach to improve reproducibility of image manipulation is a journaling approach where valid operations performed interactively would produce code. The code could be run to produce the same result, and the code could be examined to see what had been done.

2 METHODS

The SWIIM project is designed to generate workflows from popular image manipulation tools. Two basic approaches are used in this effort:

1. GIMP: modify an existing open-source image manipulation tool to journal, or produce an active log which can manipulate images.
2. R: use open-source tools in the R system to manipulate images in a GUI.

Contemporary image manipulation toolkits include a large number of functions, many of which are strictly aesthetic, and inappropriate for the preparation of scientific images. The SWIIM project will concentrate on the journaling process for the following operations:

1. Import files with formats of jpg, tiff, png, bmp
2. Rotate image 90, 180, 270
3. Flip image through 3rd dimension (vertical, horizontal)
4. Crop image
5. Brightness-contrast adjustment on image
6. Color balance adjustment on image
7. Threshold adjustment and histogram balance
8. Meld images (insert one image into another) with borders
9. Hue (red, blue, green) adjustment
10. Export file with formats of jpg, tiff, png, bmp

2.1 Application: GIMP

GIMP is a full-featured image manipulation and modification program which can perform many types of image manipulations, including all scientific image manipulations.[40] GIMP processing involves using a GUI which allows images to be imported, manipulated, modified, and altered, and then saved in a variety of output formats. The functions for image manipulation can be invoked by clicking buttons, selecting items from pull-down lists, or typing keys. In addition, a full-featured scripting language (script-fu) can be used to construct scripted programs for image manipulation.

GIMP is written in C.[40] A journaling function will be added by modifying GIMP source code ([2] [29] [28]) or by creating a “plug-in”. In GIMP, the “parasite” system is being used to retain the sequence of actions which have been applied to a given image on the way from input to export. The parasite system allows the user to associate an arbitrary string to an image or processing session. At a specific point in the processing, the information in the “parasite” system can be recovered and used to create the journal for the process, and this journal can be saved to an output file. The process involves determining the exact actions which occurred, as well as determining the values of indexes or locations used in the process. This requires determining where key strokes and button selections (which had led to a specific modification point) are processed. Additionally, the values of selections (i.e., sliders, verniers) must recovered. Creating this kind of code-generating add-on or addition to GIMP is an objective of the GIMP community, and has support from developers and maintainers.

A code system is needed to provide the journaling function for the interactive manipulations. There are two which are being set up in GIMP. These are basically 2 code systems which will be used for the GIMP component. First, the ImageMagick system, a function-base graphics toolset[20] will be used. ImageMagick has well-defined functions which perform each of the actions defined above. For a more faithful and complete emulation of code to the interactive process, the script-fu system will be employed. This is a stand-alone GIMP language which is used to write scripts[13][14]. ImageMagick is somewhat less complicated and difficult than is script-fu, which is a fully-featured programming language. By using ImageMagick code, simple and equivalent modifications can be made to images. The advantage of this approach is that ImageMagick can be used to do a proof of concept, which will be followed up by script-fu over time. While ImageMagick can perform functions which are equivalent to those in GIMP, script-fu will perform functions which are exactly the same. Using script-fu functions will produce an exact match of images. Using ImageMagick will produce a visually equivalent image, but the image will not match on the pixel level.

2.2 Application: R/Shiny

The R system is a general-purpose system of statistical, data management, and data display techniques. It is open-source, and is produced by a number of different contributors ([10]).
The R system has the Shiny GUI building application ([37]). Using Shiny, a GUI can be built with buttons, controls, and menus to control processes. The processes controlled here are image analysis and image manipulation processes. The tool which is being constructed is called ShinyImage. For image manipulation, the ShinyImage tool uses the EBImage toolkit([26]) for image processing. Performing operations involves using the GUI to select an operation, executing that operation on the image, and reflecting the change in the image in the Shiny GUI. The journaling process involves writing the commands to a journaling log file. The log file can be examined for a record of the processing, and executed to perform the operations again.

3 STATUS OF PROJECT
The SWIIM project is coming to the end of the first year. Progress been made, but the modifications are not complete.

3.1 Developments to date: GIMP
(1) Full compile has been achieved. This requires that all supporting programs and files be obtained.
(2) The location of “open file” operation has been identified. File name has been written to an ImageMagick file. The separate file can be processed to modify the image.
(3) The location of the “crop” operation has been identified and this has been translated into ImageMagick code, and written to a file.
(4) The location of the “brightness-contrast” operation has been identified and this has been translated into ImageMagick code, and written to a file. The different systems use different values for the brightness and contrast modifications, but this has been correctly aligned.
(5) The location of the “hue” modification operation has been identified and this has been translated into ImageMagick code, and written to a file. The different systems use different values for the brightness and contrast modifications, but this has been correctly aligned.
(6) The location of “export file” operation has been identified. File name has been written to an ImageMagick file.
(7) The files produced are equivalent.

The code to perform simple operations is shown in Figure 3.

Figure 1: GIMP Window Setup

Figure 3: ImageMagick code
3.2 Developments to date: R

The ShinyImage tool has been initiated and the basic GUI set up. The following steps have been taken:

1. ShinyImage, a prototype image manipulation interface, has been developed. Figure 2 shows the ShinyImage GUI.
2. The basic representation approach has been determined (use of EBImage).
3. The crop, contrast adjustment, and undo/redo operations have been implemented. All changed versions of the image are recorded.
4. The user interface is incomplete, and we will be adding pull-down menus, online help, more flexible display (e.g., several versions of the image displayed side-by-side) and so on.
5. Additional image processing operations will be added. To accommodate larger images, some capability of parallel processing will be added.
6. EBImage code is used as the scripting language. The EBImage code can either perform the manipulation on the image, or work through the GUI. The code is saved in a file during the operation of ShinyImage.

An example of EBImage scripting code is shown in Figure 4.

3.3 Plans for the future

The SWIIM project has made good progress to date. The GIMP track has set up ImageMagick code to perform the same tasks. The next step is to devise script-fu code to perform the same processes. Script-fu is more complex than is ImageMagick.

For the R track, the process needs to be finished to perform the basic tasks on the task list.

3.4 Support status

The SWIIM project has been supported by grants from ORI (ORI2016000141 and ORI2017000232). Support is in place until 2018, with a contingent extension to 2019.

4 CONCLUSIONS

Image manipulation is performed interactively in most cases for scientific images. This is not an optimal situation. The prevalence of image fraud is high. Image fraud may occur due to ignorance, but it also seems to occur because images do not agree with the conclusions that they “wish” to draw. As image manipulation is done in a non-transparent, interactive
manner, fraud is common, since some scientists clearly appear to believe that they can “get away with it”.

The SWIIM project intends to improve the manipulation of images, and to reduce the incidence of image fraud. The project is modifying existing image manipulation tools (i.e., GIMP) to produce a “journal”, a log of the modification process which is also executable. A journal (an executable log) which performs the same functions as can be done interactively introduces transparency into the process. Transparent processes promote honest behavior. In addition, the journal is executable. Reviewers can, if they wish, run the journal, and see that the image intended for publication comes from the source image. This should have the effect of encouraging more appropriate behavior. In addition, editors of scientific journals can ask the author of submitted manuscripts to produce these executable journaled logs.

The R approach is a different, but equally valuable, approach to the same problem. Many scientists work with R, but do not have a convenient method to employ scripted image tools. By providing a method to use the scripted tools in a GUI, but producing a journal log for later re-use or examination, the R user can extend the ability of the R system to handle image manipulation.

Scientists can use scripted methods to perform image manipulation with ImageMagick, EBImage, script-fu, or other scripted tools. This is not common, however. ImageMagick is not difficult to learn, but there is a learning curve. Image manipulation is not intuitively done using scripted commands. Cropping a region (selecting a sub-region in the image) can be done with a scripted command, but this is not obvious, because the image is difficult to visualize in terms of pixels. Interactive methods are much easier to work with.

The journal is a workflow. Thus, the modified image manipulation GIMP tool is a workflow generator. ShinyImage, a newly constructed image manipulation tool, performs the image manipulation process with the same workflow as is saved. Reproducible AND transparent image manipulation is possible only with scripts/workflows. By producing the script/workflow (the journal log) as a consequence of the editing operation, the best of both worlds is retained. You can have your cake and eat it too.
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