A Method to Automate Processing Provenance in AFNI

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AIM

A lightweight approach to document and replicate all processing steps on a dataset

Motivation

- Considerable heterogeneity in data analysis pipelines
  - ◊ Carp (2012) showed almost every study uses a unique combination of analysis parameters/procedures
  - ◊ Due in part to improving tools and changes in “best practices”
- Much processing in neuroimaging is done through scripts (e.g. AFNI or FSL)
  - ◊ Asymmetric relationship between scripts and the files they create: Can determine from a script what files it creates, not vice versa
- File provenance (place or source of origin) is highly desirable for reproducible research

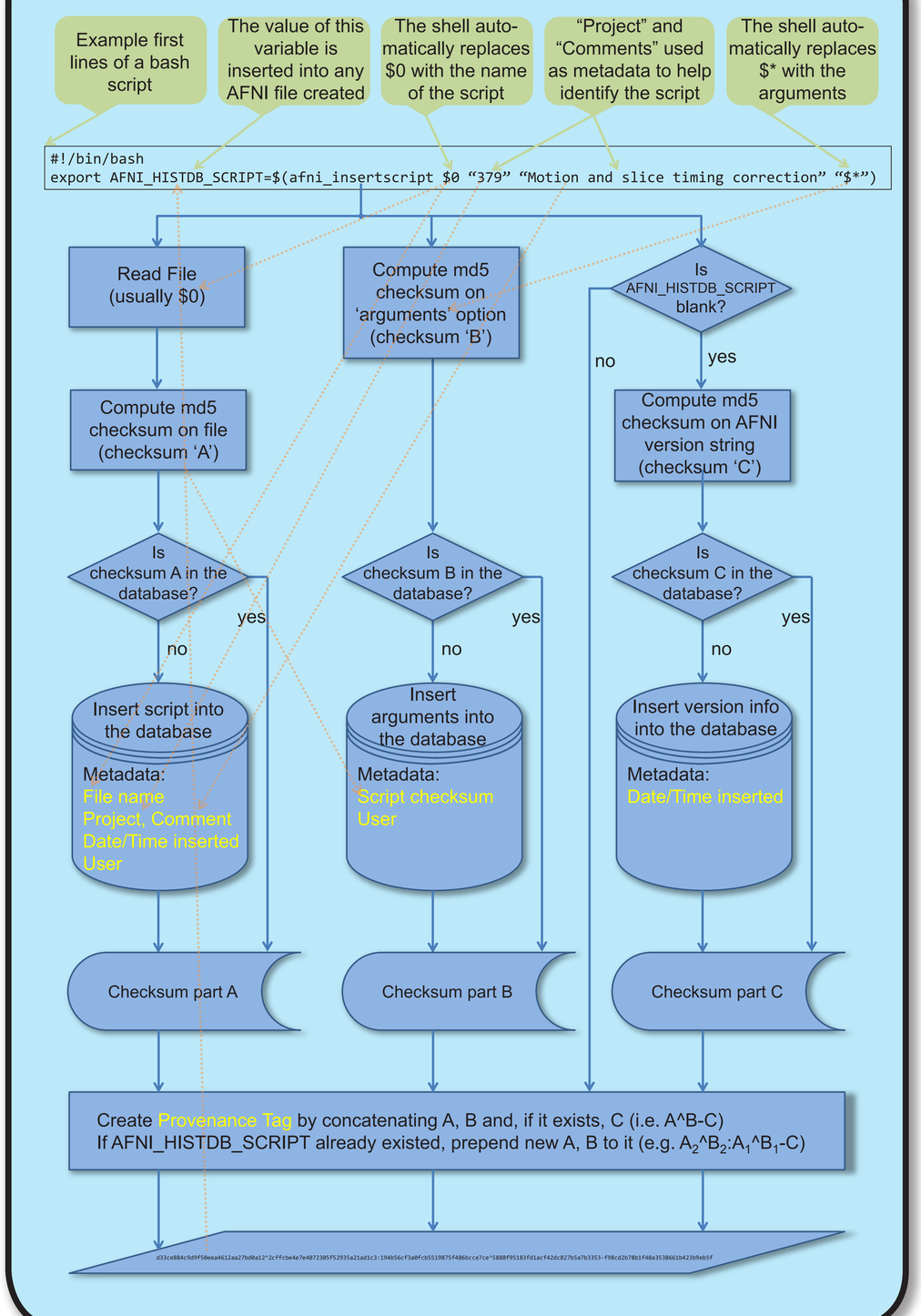
Prior Work

- The first provenance challenge (Moreau (2008)) specifically addressed the problem of an fMRI pipeline
  - ◊ 16 teams responded to the challenge, but it seems that none of the proffered solutions are in routine use in the neuroimaging community
    - » Many require using a specific ‘workflow’ that performs the appropriate documentation
      - * Often more difficult to create workflows than it is simple scripts
    - » Some require operating in a special environment that tracks all system calls
      - * Lacks simple annotation capabilities
      - * Querying the system quite challenging
- Arguably, the most popular neuroimaging provenance system is within the LONI pipeline (MacKenzie-Graham (2008))
  - ◊ Workflow based system with all of those advantages/disadvantages
- AFNI already has a history system that records the command line that created a file, and often the command lines of its children, etc.
  - ◊ Lacks the logic that went into the commands
  - ◊ Would be very difficult to reapply the same steps to new data (or the same data)

Approach

- Create provenance ‘tags’ of the form A^B-C.
  - ◊ All 3 are md5 checksums (a 128 bit cryptographic hash function)
  - ◊ A is the checksum of the script, B is the checksum of the command line arguments and C is the checksum of an AFNI version string
  - ◊ For example: 194b56cf3a0fcb5519875f486bcce7ce^5888f95183fd1acf42dc827b5a7b3353-f98cd2b78b1f48a3538661b423b9eb5f
- Provenance tags can be chained (e.g. A_2^B_2:A_1^B_1-C)
  - ◊ Happens automatically in subscripts (i.e. a script called from another script)
    - » Files created in the subscript can thus retrieve their own script, the calling script, its calling script, etc
    - » Only one C tag, as it is assumed that the AFNI version does not change during the running of the script
  - ◊ Can be used to manually associate a file(s) with an AFNI dataset(s) (e.g. associating the covariates file to the output of 3dttest++)
- Provenance tags automatically get inserted into AFNI datasets through the use of an environment variable, whose value is automatically saved as an ‘Attribute’ of any AFNI file
  - ◊ By using environment variables, this provenance method works with practically any programming language (e.g. bash, tcsh, python)
- The actual items associated with the provenance tags are inserted into an SQL database
  - ◊ Many advantages to using a database over, for example, storing the script itself within the AFNI dataset
    - » Only 1 copy of each unique item is stored
    - » Scalable from a single computer/user to a large site
    - » Acts as a backup of all versions of all scripts used in a project, without the need to learn user-unfriendly version control systems
    - » Searchable by metadata such as user, project, date
    - » Scripts are retrievable even in the absence of the neuroimaging datasets
  - ◊ Common queries (e.g. all scripts in a project) built into the retrieval program, with the full power of SQL available for more complex queries and sophisticated users
  - ◊ Name of the database stored in an environment variable; easily set by site, user or not at all
  - ◊ Currently supports sqlite, with plans to support mysql and postgresql (using the libzdb library)
- All functionality implemented in 3 new AFNI programs
  - ◊ afni_insertscript
    - » Creates the database, computes the checksums, performs database inserts, helps to set the environment variable
  - ◊ afni_getscript
    - » Lists scripts and afni version associated with a dataset, retrieves scripts, performs simple queries
  - ◊ afni_deletescript
    - » Removes scripts from the database

Program Logic/Data Flow



References/Acknowledgement

Carp (2012) Neuroimage 63:298
MacKenzie-Graham et al. (2008) Neuroimage 42:178
Moreau et al. (2008) Concurrency and Computation: Practice and Experience 20:409

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A Complete Example

Contents of preprocess.sh (which calls the next script)

```
#!/bin/tcsh
#script needs 2 arguments: $1 = subject, $2 = run
setenv AFNI_HISTDB_SCRIPT `afni_insertscript $0 “demoproject” “perform all preprocessing steps” “$*”`
cd /demoproject/$1
to3d -epan -time:zt 39 75 0 alt+z -prefix ${1}-run$2 -save_outliers outliers.1D run${2}/*

#The following finds the minimum index of the outlier file
set base=`python -c “import numpy; print numpy.loadtxt(‘outliers.1D’)[:,0].argmin()”`

/demoproject/scripts/volreg.sh $1 $2 $base
```

The **ONE** line you need to add to your scripts

Contents of volreg.sh

```
#!/bin/bash
#script needs 3 arguments: $1 = subject, $2 = run, $3 = volreg base
export AFNI_HISTDB_SCRIPT=$(afni_insertscript $0 “demoproject” “volreg and slice timing” “$*”)

3dvolreg -base $3 -1Dfile ${1}-run${2}-motion.1D -tshift 0 \
 -prefix tempfile ${1}-run${2}+orig

#can even associate another file with the volreg output
export AFNI_HISTDB_SCRIPT=$(afni_insertscript ${1}-run${2}-motion.1D “demoproject” “motion file”)
3dcopy tempfile ${1}-run${2}-volreg
export AFNI_HISTDB_SCRIPT=$(afni_insertscript -pop)

rm *motion* tempfile*
```

Associate a text file with an AFNI file

Example commands

```
/demoproject/tom> ../scripts/preprocess.sh tom 1
/demoproject/tom> ls
run1  tom-run1+orig.BRIK  tom-run1+orig.HEAD  tom-run1-volreg+orig.BRIK  tom-run1-volreg+orig.HEAD
/demoproject/tom> afni_getscript -l tom-run1-volreg+orig
AFNI version used for this file:
Version AFNI_2011_12_21_1014
[[Precompiled binary linux_openmp_64: Jun 25 2013]]

Script number: 1
        checksum = 91455926c825a62a15a868633f171ebd
         program = tom-run1-motion.1D
         project = demoproject
            user = tross
GMT time entered = 2014-05-20 22:03:59
         comment = motion file

Script number: 2
        checksum = b1b1470d8d583d10ae320bd9a61e5154
         program = volreg.sh
         project = demoproject
            user = tross
GMT time entered = 2014-05-20 22:03:52
         comment = volreg and slice timing
            args = tom 1 37

Script number: 3
        checksum = e54b959a0a19a9ff0a99244a23093ef4
         program = preprocess.sh
         project = demoproject
            user = tross
GMT time entered = 2014-05-20 22:03:48
         comment = perform all preprocessing steps
            args = tom 1
/demoproject/tom> afni_getscript -s 2 tom-run1-volreg+orig > volreg2.sh
/demoproject/tom> diff volreg2.sh ../scripts/volreg.sh
/demoproject/tom>
```

Retrieve the AFNI version used to create the files

The scripts and file associated with the AFNI file

Can retrieve one of the scripts; it is identical to the original