RMINC Development

Chris Hammill

2016-04-17

Roadmap

- RMINC history
- CRAN
- Software development and design
- RMINC under the hood
 - representations
 - abstractions
- Getting RMINC ready for CRAN
 - building
 - testing
 - documenting
 - standardizing
- Future Directions

RMINC

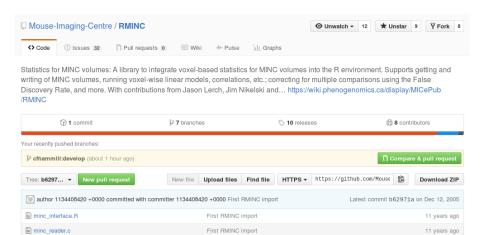
- R interface to the world of MINC
- Statistics for minc volumes
- First commit in 2005!
- Version 1.3 released February 25th, 2016



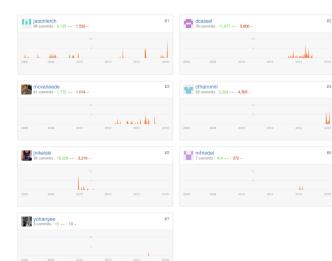
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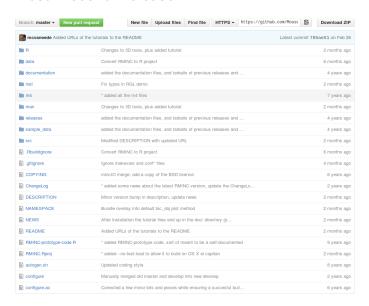
Inception



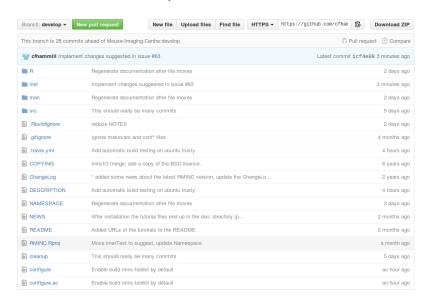
Development



Most Recent Release



Most Recent Development Branch



Visibility (be on CRAN)

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- Visibility (be on CRAN)
- Availability (be on CRAN)

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- Ease of install (be on CRAN)
- Submitted Today!

CRAN

- The Comprehensive R Archive Network
- 8287 Packages
- Holds all major R packages
- Run by the R-project
- Pretty high standards



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Package Development

• Scripting vs. Software Development

Package Development

- Scripting vs. Software Development
- getting the job done vs. building a system

Package Development

- Scripting vs. Software Development
- getting the job done vs. building a system
- comes down to design

• Rigid:

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- Rigid: tedency for code to resist modification
- Fragile: tendency for modifications to break code in unexpected places
- Immobile: tendency for supposedly modular code to not work in new situations
- Viscous: tendency for hacks to be easier to implement than robust solutions¹

Design focuses

- Design revolves around data
- Representation
- Abstraction

Barriers to good design

- Cruft
- Maintaining compatibility
- Complexity
- Managing dependencies and interfacing with external code

Refactoring

- Work to make code more understandable
- Work to make code easier to maintain
- Focus on writing small reliable functions
- Focus on composability
- Minimize global state

RMINC

Representations for minc files

Abstractions for performing statistics



Representations

- mincSingleDim: flat vector of intensities for single minc files and single value statistics tagged with metadata
- mincMultiDim: matrices with columns corresponding typically to different statistics, tagged with metadata
- mincArray: 3D array of intensities for a single minc file
- mincMultiArray?: Dimension respecting representations for results modelling

Abstraction Goals

- Facilitate movement of imaging data to and from the file system
- Facilitate the generation of useful representations
- Facilitate the fitting of statistical models
- Reduce iteration time for data exploration

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Easy Model Fitting

Modelling in R is typically direct

```
glm(binomial_response ~ covariate1 + ... + covariateN,
    data = data_source,
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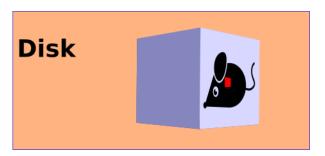
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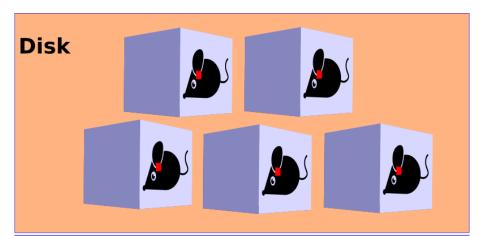
```
glm(binomial_response ~ covariate1 + ... + covariateN,
    data = data_source,
    family = binomial )
```

- Challenge: a full experiment will not fit in memory
- **Solution**: iterate through files extracting vectors of voxel values those voxel values are then fit against covariates



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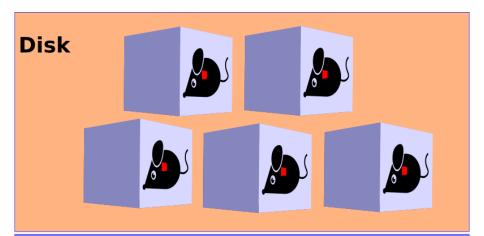
²Mouse icon made by Freepik from www.flaticon.com $\leftarrow \square \rightarrow \leftarrow \bigcirc \rightarrow \leftarrow \bigcirc \rightarrow \leftarrow \bigcirc \rightarrow \rightarrow \bigcirc \bigcirc \bigcirc \bigcirc$



$$V_{ijk} = \{m_1, m_2, ..., m_N\}$$

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$$V_{ijk+1} = \{m_1, m_2, ..., m_N\}$$

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Fitting models

- Abstractions:
 - ▶ mincLm
 - mincLmer
 - ▶ mincAnova
 - mincTtest
 - . . .
 - mincApply
 - ► mincApplyRCPP

mincApplyRCPP

R fluent interface to applying over voxels

```
str(args(mincApplyRCPP))
```

```
## function (filenames, fun,
## ..., mask = NULL, maskval = NULL,
## filter_masked = FALSE,
## slab_sizes = c(1, 1, 1),
## return_indices = FALSE,
## collate = simplify2minc)
```

mincApplyRCPP(experiment_frame\$filenames, sample, size = 5)

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Expedite fitting models

- Challenge: R is (generally) slow, fitting models can be slow
- Solution: Implement parallelism
- Abstractions:
 - pMincApply: General purpose parallelism
 - mcMincApply: Multicore parallelism
 - qMincApply: Grid computing parallelism
 - gMincApply: Open problem

Dealing with clusters

- Implements flexible support for multiple parallelism backends
- Integration with 'BatchJobs' package
- So far works with HPF and our local cluster, should work on scinet but it hasn't been tested
- New abstractions allow computation to performed in the background

New Cluster Abstractions

- qMincApply: Turnkey function
- qMincRegistry: Create shared files for parallel jobs to be coordinated, once created, registries can be loaded from another R session or even another machine
- qMincMap: Split the calculation into many peices and prepare the scripts necessary for job submission
- qMincReduce: Retrieve the job results combining them into the object of your choice, defaults to minc statistic object like mincMultiDim
- Currently only performs voxel-wise calculations, but can be extended to more complex analyses or be used to parellelize hyper-parameter search

Push for CRAN

- Must build automatically on two platforms
- Must perform as expected
- Must be well documented
- Must adhere to CRAN standards.

Building R Packages

- R uses a C-like build system
- Supports basic configure scripts and makevars
- Does not support cmake
- **Challenge**: Locating/Providing system dependencies
- **Solution(?)**: Using autoconf to generate a configure script that can flexibly locate libminc and hdf5
- if they are not found it can build minc-toolkit-v2 from source using git and cmake (fraught for automatic builds)
- Goal:

```
install.packages("RMINC")
```

Should work without issue from all supported platforms

Keeping things working

- Ensuring code performs as expected is a significant problem
- Strategies exist to ensure code performs as expected

Scale of Testing

Optimism is an occupational hazard of programming: feedback is the treatment - Kent Beck

- Optimism "this really looks like it should work"
- Hand testing "I tried a few variants of this and they work"
- Unit testing "I broke the problem into small pieces, and had the computer check that they all work"
- Property testing "I specified rules about return values, the computer explores parameter space to see if rules hold"
- Formal proof "I mathematically demonstrated the program is correct"

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Unit testing

• Unit tests are a set of assertions about the value functions return.

```
## Error: Test failed: 'My other code also works'
## Not expected: sd(1:5) not equal to 1.5
## 1.58 - 1.5 == 0.0811.
```

RMINC Testing

• RMINC includes a tool for testing the package

runRMINCTestbed()

runs a suite of tests on our code to check that all is working as expected

- runRMINCTestbed calls out to 'test_directory' which runs all tests in inst/tests
- Canonical approach is to have tests in test so that CRAN can test them automatically, but some thought is needed on how best to do the conversion

Integration testing



- Services provide automatic testing on multiple platforms
- Runs whenever code is changed on github
- Runs whenever a pull request is issued

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- Challenge: Documentation must be kept in sync with the code
- **Solution**: Documentation lives in source with the code and is autogenerated each time the package is rebuilt.
- 'roxygen2' integration with rstudio supports this

Roxygen Documentation

```
#' Retrieve Voxel Values
# '
#' Return the intensity of a given voxel in a set of minc file
# '
#' Oparam filenames paths to the minc files
#' Oparam v1 Either a 3-element vector of voxel coordinates
#' or the first
#' @param v2 the second voxel coordinate if not NULL
#' @param v3 the third voxel coordinate if not NULL
#' @return Returns a \code{mincVoxel} object containing a vec
#' of intensities and attributes specify the voxel and world
#' coordinates of the values.
#' @export
mincGetVoxel <- function(filenames, v1, v2=NULL, v3=NULL) {
```

R: Retrieve Voxel Values - Find in Topic

Retrieve Voxel Values

Description

Return the intensity of a given voxel in a set of minc files

Usage

mincGetVoxel(filenames, v1, v2 = NULL, v3 = NULL)

Arguments

filenames

paths to the minc files

Either a 3-element vector of voxel coordinates or the first

v2 the second voxel coordinate if not NULL

v3 the third voxel coordinate if not NULL

Value

v1

Returns a mincVoxel object containing a vector of intensities and attributes specify the voxel and world coordinates of the values.

[Package RMINC version 1.3.0.0 Index]

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Appeasing R CMD check

- CRAN is very particular about code quality
- Luckily R CMD check tests many requirements for you
- Highlights missed arguments in documentation, missing global variables (helpful for catching typos)
- Ensures dependencies can be loaded properly

Future directions

- Almost ready for release
- Harden parallel code
- Convert testing scheme to canonical approach
- Add abstractions for multivariate statistics

Ever need R help? Come by my desk or drop me an email Questions?