Nobody Knows What It's Like To Be the Bad Man — The Development Process for the caret Package

Max Kuhn
Pfizer Global R&D
max.kuhn@pfizer.com

Zachary Deane–Mayer Cognius zach.mayer@gmail.com

Model Function Consistency

Since there are many modeling packages in R written by different people, there are some inconsistencies in how models are specified and predictions are created.

For example, many models have only one method of specifying the model (e.g. formula method only)

Generating Class Probabilities Using Different Packages

Function	predict Function Syntax
MASS::lda	<pre>predict(obj) (no options needed)</pre>
stats:::glm	<pre>predict(obj, type = "response")</pre>
gbm::gbm	<pre>predict(obj, type = "response", n.trees)</pre>
mda::mda	<pre>predict(obj, type = "posterior")</pre>
rpart::rpart	<pre>predict(obj, type = "prob")</pre>
RWeka::Weka	<pre>predict(obj, type = "probability")</pre>
caTools::LogitBoost	<pre>predict(obj, type = "raw", nIter)</pre>

The caret Package

The caret package was developed to:

- create a unified interface for modeling and prediction (interfaces to 180 models)
- streamline model tuning using resampling
- provide a variety of "helper" functions and classes for day-to-day model building tasks
- increase computational efficiency using parallel processing

First commits within Pfizer: 6/2005, First version on CRAN: 10/2007

Website: http://topepo.github.io/caret/

JSS Paper: http://www.jstatsoft.org/v28/i05/paper

Model List: http://topepo.github.io/caret/bytag.html

Many computing sections in APM

Package Dependencies

One thing that makes caret different from most other packages is that is uses code from an abnormally large number (>80) of other packages.

Briefly, these were in the Depends field of the DESCRIPTION file which cause all of them to be loaded with caret.

For many years, they were moved to Suggests, which solved that issue,

However, their formal dependency in the DESCRIPTION file required CRAN to install hundreds of other packages to check caret. They were not pleased.

Package Dependencies

This problem was somewhat alleviated at the end of 2013 when *custom methods* were introduced into the package.

Although this functionality had already existed in the package for some time, it was refactored to be more user friendly.

In the process, much of the modeling code was moved out of caret's R files and into R objects, eliminating the formal dependencies.

Right now, the *total* number of dependencies is much smaller (2 Depends, 7 Imports, and 25 Suggests).

This still affects testing though (described later). Also:

1 package is needed for this model and is not installed. (gbm). Would you like to try to install it now?

The Basic Release Process

- create a few dynamic man pages
- use R CMD check --as-cran to ensure passing CRAN tests and unit tests
- update all packages (and R)
- run regression tests and evaluate results
- send to CRAN
- repeat
- repeat
- install passed caret version
- generate HTML documentation and sync github io branch
- profit!

Toolbox

- RStudio projects: a clean, self contained package development environment
 - No more setwd('/path/to/some/folder') in scripts
 - Keep track of project-wide standards, e.g. code formatting
 - An RStudio project was the first thing we added after moving the caret repository to github
- devtools: automate boring tasks
- testthat: automated unit testing
- roxygen2: combine source code with documentation
- github: source control

devtools

devtools::install builds package and installs it locally

devtools::check:

- Builds documentation
- Runs unit tests
- Builds tarball
- Q Runs R CMD CHECK

devtools::release builds package and submits it to CRAN

devtools::install_github enables non-CRAN code distribution or distribution of private packages

devtools::use_travis enables automated unit testing through travis-CI and test coverage reports through coveralls

Testing

Testing for the package occurs in a few different ways:

- units tests via testthat and travis-Cl
- regression tests for consistency

Automated unit testing via testthat

- testthat::use_testhat
- Unit tests prevent new features from breaking old code
- All functions should have associated tests
- Run during R CMD check --as-cran
- Can specify that certain tests be skipped on CRAN

caret is slowly adding more testthat tests

github + travis + coveralls

a little bit about travis and coveralls

Contributor submits code via a pull request

- Travis notifies them of test failures
- Coveralls notifies to write tests for new functions
- Iterate several times

You start code review once tests pass

- github supports line-by-line comments
- Usually several more iterations here

Regression Testing

Prior to CRAN release (or whenever required), a comprehensive set of regression tests can be conducted.

All modeling packages are updated to their current CRAN versions.

For each model accessed by train, rfe, and/or sbf, a set of test cases are computed with the production version of caret and the devel version.

First, test cases are evaluated to make sure that nothing has been broken by updated versions of the consistuent packages.

Diffs of the model results are computed to assess any differences in caret versions.

This process takes approximately 3hrs to complete using make -j 12 on a Mac Pro.

Regression Testing

```
$ R CMD BATCH move_files.R
$ cd \(^/\tmp/2015_04_19_09_6.0-41/\)
$ make -j 12 -i
 2015-04-19 09:13:44: Starting ada
 2015-04-19 09:13:44: Starting AdaBag
 2015-04-19 09:13:44: Starting AdaBoost.M1
 2015-04-19 09:13:44: Starting ANFIS
make: [FH.GBML.RData] Error 1 (ignored)
 2015-04-19 12:03:52: Finished WM
 2015-04-19 12:04:48: Finished xyf
```

Documentation

caret originally contained four package vignettes with in-depth descriptions of functionality with examples.

Although this functionality had already existed in the package for some time, it was refactored to be more user friendly.

However, this added time to R $\,$ CMD $\,$ check and was a general pain for $\,$ CRAN.

Efforts to make the vignettes more computationally efficient (e.g. reducing the number of examples, resamples, etc.) diminished the effectiveness of the documentation.

Documentation

The documentation was moved out of the package and to the github IO page.

These pages are built using knitr whenever a new version is sent to CRAN. Some advantages are:

- longer and more relevant examples are available
- update schedule is under my control
- dynamic documentation (e.g. D3 network graphs, JS tables)
- better formatting

It currently takes about 4hr to create these (using parallel processing when possible).

Backup Slides

roxygen2

Simplified package documentation

Automates many parts of the documentation process

- Special comment block above each function
- Name, description, arguments, etc.
- Code and documentation are in the same source file

A must have for new packages but hard to convert existing packages

- caret has 92 .Rd files
- I'm not in a hurry to re-write them all in roxygen2 format

Required "Optimizations"

For example, there is one check that produces a large number of false positive warnings. For example:

```
> bwplot.diff.resamples <- function (x, data, metric = x$metric, ...) {
+     ## some code
+     plotData <- subset(plotData, Metric %in% metric)
+     ## more code
+ }</pre>
```

will trigger a wanring that "bwplot.diff.resamples: no visible binding for global variable 'Metric'".

The "solution" is to have a file that is sourced first in the package (e.g. aaa.R) with the line

```
> Metric <- NULL
```

Judging the Severity of Problems

It's hard to tell which warnings should be ignored and which should not. There is also the issue of inconsistencies related to who is "on duty" when you submit your package.

It is hard to believe that someone took the time for this:

```
Description Field: "My awesome R package"
R CMD check: "Malformed Description field: should contain one or more complete sentences."

Description Field: "This package is awesome"
R CMD check: "The Description field should not start with the package name, 'This package' or similar."

Description Field: "Blah blah blah."
R CMD check: PASS
```