# Cross Validation techniques in $\mathbf{R}$ : A brief overview of some methods, packages, and functions for assessing prediction models.

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This month's article focuses on an initial review of techniques for conducting cross validation in **R**. Next month, a more in-depth evaluation of cross validation techniques will follow. Cross validation is useful for overcoming the problem of over-fitting. Over-fitting is one aspect of the larger issue of what statisticians refer to as shrinkage (Harrell, Lee, & Mark, 1996). Over-fitting is a term which refers to when the model requires more information than the data can provide. For example, over-fitting can occur when a model which was initially fit with the same data as was used to assess fit. Much like exploratory and confirmatory analysis should not be done on the same sample of data, fitting a model and then assessing how well that model performs on the same data should be avoided. When we speak of assessing how well a model performs, we generally think of fit measures (e.g.  $R^2$ , adj.  $R^2$ , AIC, BIC, RMSEA, etc.); but, what we really would like to know is how well a particular model *predicts* based on new information. This really gets at the goals of science and how we go about them; observation yields description, experimentation yields explanation, and all of those utilize statistical models with the goal of explanation and/or prediction. When predictions are confirmed, evidence is born for supporting a theory.

Fit measures, whether in the standard regression setting or in more complex settings, are biased by over-fitting – generally indicating better fit, or less prediction error than is really the case. Prediction error refers to the discrepancy or difference between a predicted value (based on a model) and the actual value. In the standard regression situation, prediction error refers to how well our regression equation predicts the outcome variable scores of new cases based on applying the model (coefficients) to the new cases' predictor variable scores. When dealing with a single sample, typically the residuals are a reflection of this prediction error; where the residuals are specifically how discrepant the predicted values (y-hat or  $\hat{y}$ ) are from the actual values of the outcome (y). However, because of over-fitting, these errors or residuals will be biased downward (less prediction error) due to the actual outcome variable values being used to create the regression equation (i.e. the prediction model). Cross validation techniques are one way to address this over-fitting bias.

Cross validation is a model evaluation method that is better than simply looking at the residuals. Residual evaluation does not indicate how well a model can make new predictions on cases it has not already seen. Cross validation techniques tend to focus on not using the entire data set when building a model. Some cases are removed before the data is modeled; these removed cases are often called the *testing set*. Once the model has been built using the cases left (often called the *training set*), the cases which were removed (testing set) can be used to *test* the performance of the model on the "unseen" data (i.e. the testing set).

The examples below are meant to show how some common cross validation techniques can be implemented in the statistical programming language environment  $\mathbf{R}$ . The examples below focus on standard multiple regression situations using a sample drawn from a simulated population of *true scores*. Next month's article will show how the population was generated and how each sample was drawn, as well as a more in-depth exploration of how cross validation techniques address the over-fitting problem.

### **Example Data**

The examples below were designed to be representative of a typical modeling strategy, where the researcher has theorized a model based on a literature review (and other sources of information) and has collected a sample of data. The setting for the examples below concerns a model with seven hypothesized predictors (x1, x2, x3, x4, x5, x6, & x7), each interval/ratio scaled, and one interval/ratio outcome variable (y). All variables have an approximate mean of 10. The sample contains two additional columns, one which identifies cases sequentially in the sample (s.id) and one which identifies cases sequentially in the population from which it was drawn (p.id). The sample contains 100 cases randomly sampled from a defined population of 1,000,000 individuals.

First, read in the sample data from the web, naming it 'sample1.df' (df = data.frame), and getting the ubiquitous 'head' and 'summary' to get an idea of what the data looks like.

R Console				- • ×
File Edit Misc Packages Windows Help				
<pre>&gt; sample1.df &lt;- read.table("http: + header=TRUE, sep=",", na.str &gt; head(sample1.df)</pre>			rossValidation/cv_sample1.0	df.txt",
s.id p.id y x1	x2 x3	x4 x5	x6 x7	
1 1 297497 10.239325 9.468152	10.704792 10.542263	9.014519 10.102986 10	0.29590 9.861752	
2 2 218250 10.467680 11.457565	8.870517 9.903951 1	0.312773 9.714411 11	1.32481 11.280861	
3 3 808994 11.606858 9.995756	11.690831 11.312753	9.394473 8.883531 10	0.00956 9.582854	
4 4 352628 9.565044 10.092380	8.950241 8.487879	9.634021 8.146134 9	9.99382 9.561203	
5 5 371676 9.904931 9.370441	10.906479 11.628177 1	1.768006 10.689805 10	0.84285 11.275871	
6 6 342721 9.647289 9.130054	10.284733 10.106447	8.736938 9.837188 10	0.29698 10.506574	
<pre>&gt; summary(sample1.df)</pre>				
s.id p.id	У		x2 x3	
Min. : 1.00 Min. : 33985		. : 7.651 Min.	: 6.607 Min. : 7.543	
1st Qu.: 25.75 1st Qu.:299989			.: 9.175 1st Qu.: 9.328	
Median : 50.50 Median :465996			:10.050 Median :10.069	
Mean : 50.50 Mean :510596	Mean :10.092 Mea		: 9.978 Mean :10.027	
3rd Qu.: 75.25 3rd Qu.:710626			.:10.707 3rd Qu.:10.655	
Max. :100.00 Max. :979113			:12.690 Max. :12.011	
x4 x5	x6	x7		
Min. : 7.817 Min. : 7.665		. : 6.900		
1st Qu.: 9.664 1st Qu.: 9.339		Qu.: 9.506		
Median :10.287 Median :10.032		ian :10.127		
Mean :10.176 Mean :10.015				
3rd Qu.:10.695 3rd Qu.:10.634		Qu.:10.897		
Max. :12.329 Max. :12.392	Max. :12.832 Max	. :12.401		

# The 'Design' Package

Next, we specify the model. Typically, we would use the 'lm' function from the base 'stats' package to specify an Ordinary Least Squares (OLS) regression model. However, here we will use the 'ols' function in the 'Design' package (Harrell, 2009). So, first we must load the 'Design' package, which has several dependencies.

```
R Console
File Edit Misc Packages Windows Help
> library(Design)
Loading required package: Hmisc
Loading required package: survival
Loading required package: splines
Attaching package: 'Hmisc'
The following object(s) are masked from 'package:survival':
    untangle.specials
The following object(s) are masked from 'package:base':
    format.pval, round.POSIXt, trunc.POSIXt, units
Design library by Frank E Harrell Jr
Type library(help='Design'), ?DesignOverview, or ?Design.Overview')
to see overall documentation.
Attaching package: 'Design'
The following object(s) are masked from 'package:Hmisc':
    strgraphwrap
The following object(s) are masked from 'package:survival':
    Surv
```

Now, we can use the 'ols' function to specify the model and get a summary of it. Make sure to set the optional arguments 'x = TRUE' and 'y = TRUE' as these will save a design matrix of predictors and a vector of outcome values. These two objects will be used in the cross validation techniques below. If you are not familiar with the scientific notation of **R**, the 'e-00' refers to a negative exponent and the 'e+00' refers to a positive exponent. For example, 5.234e-03 = 0.005234 and 5.234e+03 = 5234.00.

```
- • ×
R Console
File Edit Misc Packages Windows Help
> model.1 <- ols(y ~ x1 + x2 + x3 + x4 + x5 + x6 + x7, sample1.df, x = TRUE, y = TRUE)
> model.1
Linear Regression Model
ols(formula = y \sim x1 + x2 + x3 + x4 + x5 + x6 + x7, data = sample1.df,
    x = TRUE, y = TRUE)
                              d.f.
          n Model L.R.
                                           R2
                                                     Sigma
       100
              515.3
                                       0.9942
                                                 0.07509
Residuals:
                1Q Median
      Min
                                        3Q
                                                  Max
-0.154608 -0.056157 0.004808 0.045365 0.186316
Coefficients:
              Value Std. Error
                                       t Pr(>|t|)
Intercept -2.77898 0.169566 -16.389 0.000e+00
            0.86274
                       0.008341 103.429 0.000e+00
x1
            0.54708 0.007593 72.050 0.000e+00
0.23564 0.008475 27.803 0.000e+00
\mathbf{x}^2
x3
           -0.16429
                      0.009121 -18.013 0.000e+00
x4
x5
           -0.14094
                       0.009475 -14.874 0.000e+00
                      0.017262 1.093 2.771e-01
0.018421 -4.407 2.836e-05
x6
            0.01887
x7
           -0.08118
Residual standard error: 0.07509 on 92 degrees of freedom
Adjusted R-Squared: 0.9938
```

Next, we can begin exploring cross validation techniques. The 'validate' function in the 'Design' package "does resampling validation of a regression model, with or without backward step-down variable deletion" (Harrell, 2009, p. 187). Here, our examples focus on OLS regression, but the 'validate' function can hand a logistic model as well; as long as the model is fit with the 'Irm' function (Logistic Regression Model) in the 'Design' package. The key part of the output for this function is the 'index.corrected' measures of fit -- which corrects for over-fitting. We start with the default values/arguments for 'validate' which uses the 'boot' method (bootstrapped validation; Efron, 1983; Efron & Tibshirani, 1993). Bootstrapped validation takes B number of samples of the original data, with replacement, and fits the model to this training set. Then, the original data is used as the testing set for validation.

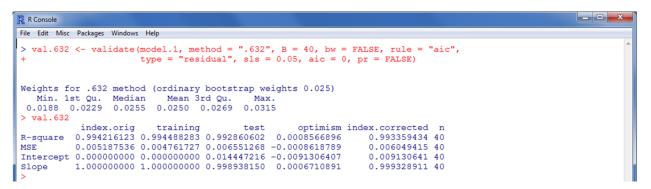
```
R Console
File Edit Misc Packages Windows Help
> val.boot <- validate(model.1, method = "boot", B = 40, bw = FALSE, rule = "aic",
+ type = "residual", sls = 0.05, aic = 0, pr = FALSE)
> val.boot
            index.orig
                           training
                                              test
                                                         optimism index.corrected
R-square 0.994216123 0.99423426
                                     0.993705437 0.0005288253
                                                                   0.993687250 ...
                                                                        0.993687298 40
           0.005187536 0.00493656 0.005645568 -0.0007090077
MSE
Intercept 0.00000000 0.0000000 -0.009016284 0.0090162843
                                                                      -0.00901628440
           1.000000000 1.00000000 1.000665178 -0.0006651782
                                                                      1.000665178 40
Slope
```

Notice in the output above the index corrected estimates are all marginally worse in terms of fit and / or prediction error. In other words, the index corrected measures do not reflect the shrinkage caused by over-fitting. The "optimism" (Efron & Tibshirani, 1993, p. 248) is the difference between the training set estimates and the test set estimates and can be thought of as the amount of optimism of each initial estimate (e.g. how much the training estimates are biased).

Next, we can explore the 'crossvalidation' method, which uses B number of observations as the testing set (testing or validating the model) and the rest of the sample for the training set (building the model).

> val.cro	ss <- validat	o (model 1 m					
+ > val.cro					", B = 40, bw = F = 0, pr = FALSE)	ALSE, rule = "aic	:",
, , , , , , , , , , , , , , , , , , , ,	S. S	training	test	optimism	index.corrected	n	
R-square	0.994216123	0.994228510	-0.06680937	1.061037880			
			0 00053004	-0 001362129	0.006549665	10	
MSE	0.005187536	0.005175911	0.00055604	-0.001302123	0.000349003	40	
MSE Intercept				-0.132408663			

Next, we can take a look at the ".632" bootstrapped method which corrects for the bias in prediction error estimates "based on the fact that bootstrap samples are supported on approximately .632*n* of the original data points" (Efron, 1983; Efron & Tibshirani, 1997, p. 552).



### The 'DAAG' package

Another package which is capable of performing cross validation is the Data Analysis And Graphing ('DAAG') package (Maindonald & Braun, 2011) which also has several dependent packages.

```
R Console
File Edit Misc Packages Windows Help
> library(DAAG)
Loading required package: MASS
Loading required package: rpart
Loading required package: randomForest
randomForest 4.6-2
Type rfNews() to see new features/changes/bug fixes.
Attaching package: 'randomForest'
The following object(s) are masked from 'package:Hmisc':
    combine
Attaching package: 'DAAG'
The following object(s) are masked from 'package:MASS':
    hills
The following object(s) are masked from 'package:Design':
    vif
The following object(s) are masked from 'package:survival':
    lung
> |
```

The 'DAAG' package contains three functions for k – fold cross validation; the 'cv.lm' function is used for simple linear regression models, the 'CVlm' function is used for multiple linear regression models, and the 'CVbinary' function is used for logistic regression models. The k – fold method randomly removes k – folds for the testing set and models the remaining (training set) data. Here we use the commonly accepted (Harrell, 1998) 10 – fold application.

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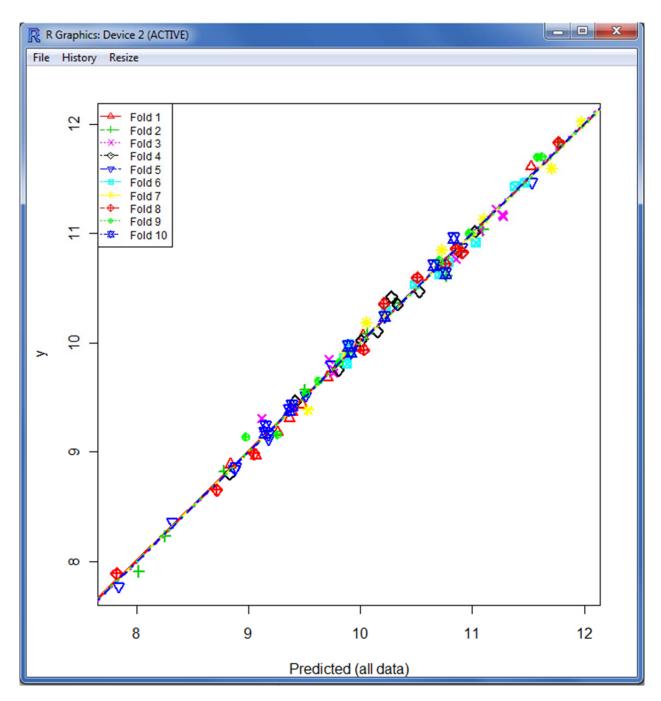
```
R Console
File Edit Misc Packages Windows Help
> val.daag <- CVlm(df = sample1.df, m = 10, form.lm = formula(y ~ x1 + x2 + x3 + x4 + x5 + x6 + x7))
Analysis of Variance Table
Response: y
          Df Sum Sq Mean Sq F value Pr(>F)
                     48.7 8631.8 < 2e-16 ***
x1
           1 48.7
               30.8
                        30.8 5471.0 < 2e-16 ***
x2
                               900.1 < 2e-16 ***
x3
                5.1
                        5.1
x4
                1.8
                         1.8
                               312.4 < 2e-16 ***
           1
                             438.3 < 2e-16 ***
x5
           1
                2.5
                         2.5
                               41.2 6.0e-09 ***
x6
                0.2
                         0.2
           1
×7
                               19.4 2.8e-05 ***
                 0.1
                         0.1
Residuals 92 0.5
                      0.0
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
fold 1
Observations in test set: 3 8 16 18 39 42 45 62 63 100
                               X16
X3 X8 X16 X18 X39 X42 X45 X62 X63 X100
Predicted 11.5141 9.9671 9.3781 8.8386 9.4042 9.7155 10.0094 9.277 9.079 9.4779
                   9.9490
                           9.3040 8.8825 9.3647 9.6782 10.0593 9.178
                                                                           8.966
                                                                                    9.4293
          11.6069
Residual 0.0928 -0.0182 -0.0741 0.0439 -0.0395 -0.0373 0.0499 -0.099 -0.113 -0.0487
                                                   n = 10
Sum of squares = 0.047
                         Mean square = 0.0047
fold 2
Observations in test set: 4 9 10 19 30 47 55 78 82 93
                                     X19
                                                                      X78
              X4
                            X10
                                             X30
                                                     X47
                                                             X55
                                                                             X82
                     X9
                                                                                     X93
Predicted 9.5047 11.785 10.0616 10.3095 10.7081 10.776 11.0915 8.2624 8.021 8.7906
          9.5650 11.829 10.0821 10.3614 10.6913 10.612 11.0314 8.2295 7.909 8.8210
Residual 0.0604 0.044 0.0206 0.0519 -0.0168 -0.163 -0.0601 -0.0329 -0.112 0.0304
Sum of squares = 0.054 Mean square = 0.0054
                                                  n = 10
fold 3
Observations in test set: 35 54 56 73 74 77 87 88 89 99
X35 X54 X56 X73 X74 X77 X87
Predicted 11.287 11.0791 9.713 11.2339 9.395 9.108 10.8626
                                                                  X88
                                                                         X89
                                                                                 X99
                                                               9.7615 11.293 9.7556
          11.169 11.0216 9.847 11.2197 9.421 9.301 10.7678
                                                               9.7507 11.155
                                                                              9.7173
Residual -0.118 -0.0575 0.134 -0.0142 0.026 0.193 -0.0948 -0.0108 -0.139 -0.0383
                                               n = 10
Sum of squares = 0.1 Mean square = 0.01
fold 4
Observations in test set: 2 21 24 41 50 64 71 75 80 95
               X2
                       X21
                              X24
                                       X41
                                             X50
                                                    X64
                                                             X71
                                                                      X75
                                                                              X80
                                                                                       X95
Predicted 10.5363 10.00998 10.274 8.8239 10.88 9.4221
                                                           9.8130 10.1583 10.3260 11.0276
y 10.4677 10.01757 10.417 8.7942 10.84 9.4606 9.7438 10.1024
Residual -0.0686 0.00758 0.142 -0.0297 -0.04 0.0385 -0.0692 -0.0559
                                                           9.7438 10.1024 10.3483 11.0132
                                                                          0 0223 -0 0144
```

Some output (folds) has been omitted.

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fold 9 Observations in test set: 6 11 22 34 37 44 51 53 65 79 X34 X6 X11 X22 X34 X37 X44 X51 X53 X65 X79 Predicted 9.6250 11.57 9.265 9.8877 10.9623 8.97 9.5057 10.6938 11.6039 9.8000 9.6473 11.70 9.154 9.9035 11.0038 9.14 9.5326 10.7534 11.6992 9.8147 Residual 0.0223 0.13 -0.111 0.0158 0.0415 0.17 0.0269 0.0596 0.0953 0.0147 Sum of squares = 0.074 Mean square = 0.0074 n = 10fold 10 Observations in test set: 1 20 29 32 38 52 69 72 81 91 X32 X1 X20 X29 X38 X52 X69 X72 X81 X91 Predicted 10.2170 10.765 9.353 9.8876 9.90237 9.1390 9.1459 9.3839 10.6522 10.824 y 10.2393 10.632 9.379 9.9687 9.90626 9.1711 9.2300 9.4207 10.7054 10.955 Residual 0.0223 -0.133 0.026 0.0811 0.00389 0.0321 0.0841 0.0369 0.0532 0.131 Sum of squares = 0.055 Mean square = 0.0055 n = 10Overall ms 0.00624

Here, at the bottom of the output we get the cross validation residual sums of squares (Overall MS); which is a corrected measure of prediction error averaged across all folds. The function also produces a plot (below) of each fold's predicted values against the actual outcome variable (y); with each fold a different color.



## The 'boot' package

Lastly, we can use the 'boot' package (Ripley, 2010) for cross validation of generalized linear models (e.g. binomial, Gaussian, poisson, gamma, etc.). Bootstrapping can be used to correct for some of the bias associated with the other cross validation techniques.

```
    R R Console

    File Edit Misc Packages Windows Help

    > library(boot)

    Attaching package: 'boot'

    The following object(s) are masked from 'package:survival':

    aml

    > |
```

First, we must fit the model. Our example below is *really* an OLS regression model, but if we specify 'family = gaussian' then it is the same as using 'lm'. If we had a logistic model, then we would specify 'family = binomial(link = logit)' to fit the logistic model.

\_ D \_X

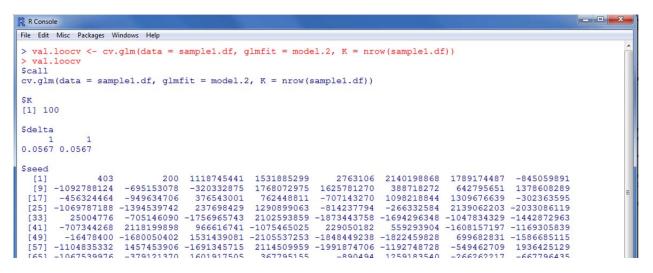
```
R Console
File Edit Misc Packages Windows Help
> model.2 <- qlm(y \sim x1 + x2 + x4 + x5 + x6 + x7, sample1.df, family = qaussian)
 > summary(model.2)
Call:
glm(formula = y \sim x1 + x2 + x4 + x5 + x6 + x7, family = gaussian,
     data = sample1.df)
Deviance Residuals:
                                 3Q
 Min 10 Median 30 Max
-0.5173 -0.1635 0.0071 0.1343 0.4584
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
 (Intercept) -0.6058 0.4589
                                    -1.32
                                            0.19006
                0.8186
                            0.0250
                                      32.78
                                              < 2e-16 ***
 x1
                                             < 2e-16 ***
\mathbf{x}^2
               0.5777
                            0.0229
                                     25.21
                                             1.0e-08 ***
x4
               -0.1748
                            0.0278
                                     -6.29
                                     -3.55 0.00061 ***
                           0.0286
              -0.1014
x5
                            0.0479
x6
                0.2171
                                       4.53
                                             1.8e-05 ***
                            0.0520
                                     -5.28
                                            8.6e-07 ***
x7
               -0.2745
Signif. codes: 0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 ` ' 1
 (Dispersion parameter for gaussian family taken to be 0.0524)
Null deviance: 89.6896 on 99 degrees of freedom
Residual deviance: 4.8774 on 93 degrees of freedom
AIC: -2.269
Number of Fisher Scoring iterations: 2
```

The 'cv.glm' function "estimates the k – fold cross validation prediction error for generalized linear models" (Ripley, 2010). If k – fold is set to the number of cases (rows), then a complete Leave One Out Cross Validation (LOOCV) is done. The LOOCV method is intuitively named; essentially, one case is *left out* as the testing set and the rest of the data is used as the training set. If this process is repeated so that each case is given a chance as the testing case, then we have the complete LOOCV method. The 'cv.glm' function returns a 'delta' which shows (first) the raw cross-validation estimate of prediction error and (second) the adjusted cross-validation estimate. The adjustment is designed to compensate for the bias introduced by not using leave-one-out cross-validation. The default for 'cv.glm' is complete LOOCV.

First, we run the common 10 - fold cross validation. Below, the majority of seed information is cut off the end of the figure.

🔀 R Console						
File Edit Misc Packages Windows Help						
<pre>&gt; val.10.fold &lt;- cv.glm(data = &gt; val.10.fold \$call cv.glm(data = sample1.df, glmfi</pre>		nodel.2, K = 1	0)			<u>^</u>
\$K [1] 10						
Sdelta 1 1 0.0572 0.0567						
\$seed         10           [1]         403         100           [9]         -1092788124         -695153078           [17]         -456324464         -949634706           [25]         -1069787188         -1394539742           [33]         25004776         -705146090           [41]         -707344268         2118199898           [42]         -1647400         -1682050402	966616741 -107546502	5 1625781270 1 -707143270 3 -814237794 9 -1873443758 5 229050182	559293904	-1047834329 -1608157197	1378608289 -302363595 -2033086119 -1442872963	E

Next, we run the complete LOOCV method, specifying k as the number of rows in the sample data (nrow). Again, below the majority of the seed numbers have been left off the figure.



Obviously the delta numbers match because we used the LOOCV method. Recall, the first delta value is the raw cross validation estimate of prediction error and the second is the adjusted cross validation estimate; which is supposed to adjust for the bias of not using the LOOCV method.

#### Conclusions

Three packages were employed to demonstrate some relatively simple examples of conducting cross validation in the **R** programming language environment. Cross validation refers to a group of methods for addressing the some over-fitting problems. Over-fitting refers to a situation when the model requires more information than the data can provide. One way to induce over-fitting is by specifying the model with the same data on which one assesses fit or prediction error. The examples here were conducted using simulated data. Rather strikingly, you may have noticed, the estimates of prediction error were not terribly different from the full sample (over-fitted) estimates, even though this sample was considerable small (n = 100) in comparison to its parent population (N = 1,000,000). These results might lead one to think cross validation and over-

fitting are not things one needs to be concerned with. However, there are a few reasons our estimates here were not more starkly different than the full sample estimates and you might be surprised to find that some of our predictor variables are not at all related to the outcome variable. Next month's article will reveal the *secrets* behind those statements. However, cross validation and over-fitting are serious concerns when dealing with real data and should be considered in each study involving modeling.

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