Project 4 Report

Analyst: Max McGrath

Investigator: Nichole Carlson

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Introduction

This study aims to investigate the efficacy of several model selection techniques for linear regression across four case scenarios. More specifically, it aims to evaluate the ability of a set of backwards selection and regularization techniques to select models that retain significant predictors and remove insignificant predictors across scenarios with varying sample sizes and correlation structures between predictors. To do so, simulation was used to create regression data sets with known underlying models, then each model selection technique was applied to each data set to build a model. Each model selection technique's performance was then be evaluated using a number of criteria that quantify the technique's overall ability to identify significant predictors and to accurately estimate those predictors' known associations with the response.

Based on these criteria, we will evaluate two hypotheses. First, backwards selection using AIC will have a higher true positive rate than BIC at the cost of a higher false positive rate, as BIC generally favors more parsimonious models than AIC. Second, backwards selection methods will generally perform "better" than regularization methods, as regularization methods are typically preferred for prediction and situations where the number of predictors is greater than the sample size rather than the situation under consideration in which inference is the goal and the set of predictors is relatively small.

Model Notation

For all case scenarios, 1000 data sets will be simulated from the model

$$y_i = \beta_1 x_{1,i} + \beta_2 x_{2,i} + \dots + \beta_{20} x_{20,i} + \epsilon_i.$$

where $\{\beta_1, ..., \beta_5\} = \{\frac{1}{6}, \frac{1}{3}, \frac{1}{2}, \frac{2}{3}, \frac{5}{6}\}, \beta_6, ..., \beta_{20}$ are equal to $0, \epsilon_j \sim N(0, 1), X_p \sim N(0, 1)$, and j = 1, 2, ..., N. The data sets for the four case scenarios then differ based on sample size, N, and correlation structure as follows: (1a) N = 250 and all predictors are independent, (1b)

N=250 and predictors have an exchangeable correlation coefficient of 0.4, (2a) N=500 and all predictors are independent, and (2b) N=500 and predictors have an exchangeable correlation coefficient of 0.4. Predictors with a non-zero known coefficient will be referred to as significant predictors, and those with a known zero coefficient will be referred to as insignificant.

Methods

For each data set, model selection techniques were applied including three backwards selection techniques and two regularization methods, and records were created of which predictors were retained in each final model along with estimated coefficients and any other relevant statistics. For backwards selection, we evaluated three techniques with differing predictor retention criteria. For the first, predictors were removed one at a time according to highest t-test p-value until all predictors have a p-value under 0.15. For the second and third, we used Akaike information criterion (AIC) and Bayesian information criterion (BIC) to iteratively reduce the model until the respective information criteria no longer decreases as predictors are removed. For p-value backwards selection the ols_step_backwards_p() function was used from the olsrr package. For AIC and BIC backwards selection, the function stepwise() was used from the RcmdrMisc R package.

For regularization, we applied LASSO and Elastic Net (ENet), each with both regularization parameter fixed at 0.2 and with regularization parameters selected using 5-fold cross-validation across a range of parameter values from 10¹⁰ to 10⁻². For Elastic Net, the penalization mixing parameter will be fixed at 0.5. Parameters will then be be considered retained if their coefficient estimate is greater than zero and removed if their coefficient estimate is equal to zero. For full details on LASSO and ENet see Tibsheranti (1996) and Zou and Hastie (2004). For LASSO and ENet, the cv.glment() and glmnet() functions were used from the glmnet package.

Simulation

For each case scenario and simulation, X_p , p = 1, ..., 20 was drawn from a N(0, 1) distribution. Then, in the cases where predictors are correlated an additional step was added where the X matrix is multiplied by the Cholesky decomposition of a 20×20 matrix with 1's along the diagonal and 0.4 everywhere else to induce exchangeable correlation. The response for each observation is then drawn from a normal distribution with the linear combination of the predictors and coefficients as the mean and 1 as the standard deviation. All data was generated using the genData() function from the hdrm R package.

Then, for each data set, a model was selected using each technique, then the model was refit using OLS using only the retained predictors. Let $I_R\{X_{p,i}\}$ equal 1 if predictor $X_p, p = 1, \ldots, 20$ was retained for simulation $i = 1, 2, \ldots, 1000$ and 0 otherwise. Then, each selection technique was evaluated for each case scenario according to the following criteria:

- 1. True positive rate for each significant predictor p = 1, ..., 5 where $TPR_p = \frac{\sum_{i=1}^{1000} I_R\{X_{p,i}\}}{1000}$
- 2. Total true positive rate where $TTPR = \frac{\sum_{i=1}^{1000} \sum_{p=1}^{5} I_R\{X_{p,i}\}}{5000}$
- 3. False positive rate where $FPR = \frac{\sum_{i=1}^{1000} \sum_{p=6}^{20} I_R\{X_{p,i}\}}{15000}$
- 4. False discovery rate where $FDR = \sum_{i=1}^{1000} \frac{\sum_{p=6}^{20} I_R\{X_{p,i}\}}{\sum_{p=1}^{20} I_R\{X_{p,i}\}}$
- 5. Coefficient bias for each significant predictor $\beta_p, p = 1, ..., 5$ where $Bias_p = \sum_{i=1}^{1000} \left[\frac{\hat{\beta_p}I_R\{X_{p,i}\}}{I_R\{X_{p,i}\}}\right] \beta_p$
- 6. Confidence interval coverage for each significant predictor $\beta_p, p = 1, ..., 5$ where $CIC_p = \sum_{i=1}^{1000} \frac{I_{CI}\{\hat{\beta}_{p,i}\}}{I_R\{X_{p,i}\}}$ where $I_{CI}\{\hat{\beta}_{p,i}\}$ equals 1 if the 95% confidence interval for $\hat{\beta}_p$ contains β_p for simulation i.
- 7. Conditional Type I error rate where $T1ER = 1 \sum_{i=1}^{1000} \sum_{p=1}^{5} \frac{I_{T1}\{X_{p,i}\}}{I_{R}\{X_{p,i}\}}$ where $I_{T1}\{X_{p,i}\}$ equals 1 if the coefficient estimate for predictor p is statistically significant according to a Wald test for simulation i

8. Conditional Type II error rate where $T2ER = \sum_{i=1}^{1000} \sum_{p=6}^{20} \frac{I_{T2}\{X_{p,i}\}}{I_R\{X_{p,i}\}}$ where $I_{T2}\{X_{p,i}\}$ equals 1 if the coefficient estimate for predictor p is statistically significant according to a Wald test for simulation i

Note that for regularization methods, evaluation metrics 5 through 8 were all calculated using the models refit with OLS following predictor selection. No data other than coefficient retention was used from the regularized model fits.

Results

Figure 1 provides plots of the TTPR, FPR, FDR, Types I and II error rates, and the average bias by case scenario and model selection technique, Figure 2 provides plots of bias, 95% confidence interval coverage, and TPR by coefficient, case scenario, and model selection technique, and Tables 1 through 4 provide a detailed look at all simulation evaluation metrics. In the discussion which follows, regularization will generally refer to LASSO with CV and ENet with CV, as regularization with fixed regularization parameters is contrary to standard practice and of secondary interest. However, all tables and figures report values for all seven model selection techniques considered.

A higher TTPR indicates that a selection technique retains known significant predictors at a greater rate, and from Figure 1 and the tables, we see that regularization generally performs better than backwards selection in terms of TTPR. LASSO with CV and ENet with CV have higher TTPR than backwards selection techniques across all case scenarios. This difference is more pronounced in scenarios where correlation is induced (1b and 2b) and when sample size is smaller (1a and 1b). Among the backwards selection techniques, p-value selection and AIC selection perform relatively the same, while BIC selection has notably lower TTPR across all case scenarios. TTPR rates are all relatively high, with the majority of methods having a TTPR above 0.95 for most or all cases scenarios. The lowest TTPR is BIC for cases scenario 1b, where it has a TTPR of 0.880. From Figure 2 we see that TPR by coefficient was nearly 1 for all predictors other than X_1 , and as such TTPR and TPR for X_1

are nearly identical.

These TTPR trends were reversed for FPR and FDR. Lower FPR and FDR generally reflects a model selection techniques ability to remove insignificant predictors, and in this regard backwards selection performed better than regularization. Across all case scenarios, backwards selection techniques had lower FPR and FDR than regularization techniques, with BIC having the lowest FPR and FDR among backwards selection techniques. However, we see far greater variation in FPR relative to TTPR, as across case scenarios BIC remains consistently near 0.025 while ENet with CV reaches a high of 0.504 for case scenario 2a.

For conditional Type I error, we see fairly consistent behavior across methods, with backwards selection using p-values and AIC generally having the lowest Type 1 error rate, followed by BIC and the regularization methods. However, for Case 2a we see regularization marginally outperforming backwards selection methods. In contrast, we see that for scenario 1b backwards selection greatly outperforms regularization, with backwards selection having conditional Type I error rates below 0.05 and regularization methods all above 0.10.

For conditional Type II error, we see that for case scenarios 1a, 1b, and 2b, regularization outperforms backwards selection. However, for case scenario 2a, we see AIC and BIC backwards selection notably outperform regularization methods (but backward selection using p-values performs worse).

For coefficient bias, we see somewhat mixed results across case scenarios and methods, but generally bias is higher for regularization selection over backwards selection, and coefficient bias was consistently small relative to coefficient size (between -0.03 and 0.03). Bias was generally greatest for $\hat{\beta}_1$ (as would be expected given its effect size), although regularization methods did have visibly higher biases for X_2, \ldots, X_5 for case scenarios 1b and 2b.

For coefficient confidence interval coverage, we see fairly consistent performance across methods and case scenarios with most estimates ranging from 0.93 to 0.97 and little in the way of discernible trends between methods and case scenarios.

Discussion

The most notable trend across methods in terms of predictor retention was the trade off between TPR and FPR. Generally, methods with higher TPR also had higher FPR. However, these tradeoffs were not always proportional. For AIC and BIC, the hypothesized trade off between true positive rate and false positive rate is as expected: AIC generally has higher for both. However, we see that across the four case scenarios the change in TPR between AIC and BIC and that of FPR is notably different. For BIC, all scenarios had a fairly consistent FPR (0.015 - 0.024) while for TTPR we see a greater range across case scenarios (0.880 to 0.980). This is noteworthy because it is indicative that the trade-off may be more beneficial for BIC in certain scenarios. Specifically, BIC sees notable improvements in FPR and only marginal disadvantages in TPR in situations with greater sample size (2a and 2b), while the difference in FPR is more pronounced in situations with smaller sample sizes (1a and 1b).

Similarly, while regularization methods all had extremely high TPR, this benefit comes at the cost of a much higher FPR. Gains in TPR for regularization over AIC selection were less than 0.025 in all scenarios, whereas FPR was more than doubled for regularization methods compared to AIC selection across cases scenarios, noting that this problem is even worse for situations without correlated predictors. This somewhat confirms our hypothesis that backwards selection generally performs "better" than regularization, but there are caveats.

Interestingly, the introduction of correlation and reduction of sample size appears to have a compounding effect in the reduction of TPR for backwards selection. However, for regularization methods, only sample size appeared to reduce TPR, as TPR was roughly the same for 1a and 1b (and 2a and 2b), indicating that regularization's ability to retain significant predictors may be more robust when predictors are correlated. This is contrasted by FPR, where backwards selection techniques had highly consistent FPR across case scenarios, whereas regularization selection had notably lower FPR for scenarios with correlated predictors. So, there is the potential that in situations with correlated predictors and in which the importance of significant predictor retention far exceeds that of insignificant predictor

removal regularization may be preferable.

Limitations and Future Work

There are several limitations to this analysis that provide insight into further cases scenarios and methodologies to consider. First, using LASSO and ENet with pre-specified regularization parameters is detached from standard practice and is unlikely to reflect real world uses of those methods. Similarly, refitting the models "selected" via regularization using OLS is likely problematic and mischaracterizes the statistical intentions of those methods. A more statistically sound method for assessing significance and CI's would be more appropriate for regularization methods and would likely alter the results obtained.

Second, as previously noted TTPR and TPR for X_1 were essentially the same stemming from the incredibly consistent TPR of 1 for all other predictors. As such, the effect sizes investigated in this analysis may have been too large, and future analysis should consider using smaller effect sizes as it may provide greater insight into the efficacy of the considered model selection approaches.

Lastly, the correlation structure induced in the predictors for case scenarios 1b and 2b was fairly simplistic and is unlikely to be representative of real world correlations. Future works should consider inducing more realistic correlation scenarios to more thoroughly elucidate the differences in model selection techniques.

Reproducibility

##

The code used to generate this analysis is available on GitHub at https://github.c om/BIOS6624-UCD/bios6624-MaxMcGrath/tree/main/Project4. The Background folder contains information pertinent to understanding the analysis but unnecessary for reproducing it. The Code folder contains thirteen files: 1_Case1a.R, 2_Case1b.R, 3_Case2a.R, 4_Case2b.R, 5_SimAnalysis1a.R, 6_MakeTables1a.R, 7_SimAnalysis1b.R, 8_MakeTables1b.R, 9_SimAnalysis2a.R, 10_MakeTables2a.R, 11_SimAnalysis2b.R, 12_MakeTables2b.R, and 13_MakePlots.R. To run the complete analysis, each script should be run in the order of the number prefixing its filename. The last directory, Report, contains the RMarkdown file report.Rmd which may be used to generate this report (note that it also depends on the aforementioned scripts).

The complete details of the R version, package versions, and machine details for the instance which generated this report are provided below.

```
## R version 4.1.1 (2021-08-10)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Catalina 10.15.7
##
## Matrix products: default
## BLAS:
           /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## locale:
  [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
                 graphics grDevices utils
## [1] stats
                                               datasets methods
                                                                    base
```

```
## other attached packages:
                                                           dplyr_1.0.7
  [1] tidyr 1.1.4
                        gridExtra 2.3
                                         ggplot2 3.3.5
  [5] janitor 2.1.0
                        kableExtra 1.3.4
##
## loaded via a namespace (and not attached):
    [1] Rcpp 1.0.7
                          svglite 2.0.0
##
                                            lubridate 1.8.0
                                                               digest 0.6.28
    [5] utf8 1.2.2
                                             cellranger 1.1.0
                                                              backports 1.2.1
                          R6 2.5.1
##
##
    [9] evaluate 0.14
                          httr 1.4.2
                                            pillar 1.6.4
                                                               rlang 0.4.12
                          readxl_1.3.1
   [13] curl 4.3.2
                                            rstudioapi 0.13
                                                               data.table 1.14.2
   [17] car 3.0-11
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                                                               broom 0.7.9
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                                                               systemfonts 1.0.2
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                          tidyselect_1.1.1
                                           tibble 3.1.5
                                                               rio_0.5.27
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                          viridisLite 0.4.0 crayon 1.4.1
                                                               withr 2.4.2
##
  [37] ggpubr 0.4.0
                                            gtable 0.3.0
                          grid 4.1.1
                                                               lifecycle 1.0.1
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                          scales 1.1.1
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                                            ggsignif 0.6.3
                                                               snakecase 0.11.0
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                          ellipsis 0.3.2
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                                            colorspace 2.0-2 rstatix 0.7.0
## [65] rvest_1.0.2
                          knitr_1.36
                                            haven_2.4.3
```

Works Cited

- Tibshirani, Robert. "Regression Shrinkage and Selection via the Lasso." Journal of the Royal Statistical Society. Series B (Methodological) 58, no. 1 (1996): 267–88. http://www.jstor.org/stable/2346178.
- Zou, H. and Hastie, T. (2005), Regularization and variable selection via the elastic net.

 Journal of the Royal Statistical Society: Series B (Statistical Methodology), 67: 301-320. https://doi.org/10.1111/j.1467-9868.2005.00503.x

Appendix - Tables and Figures

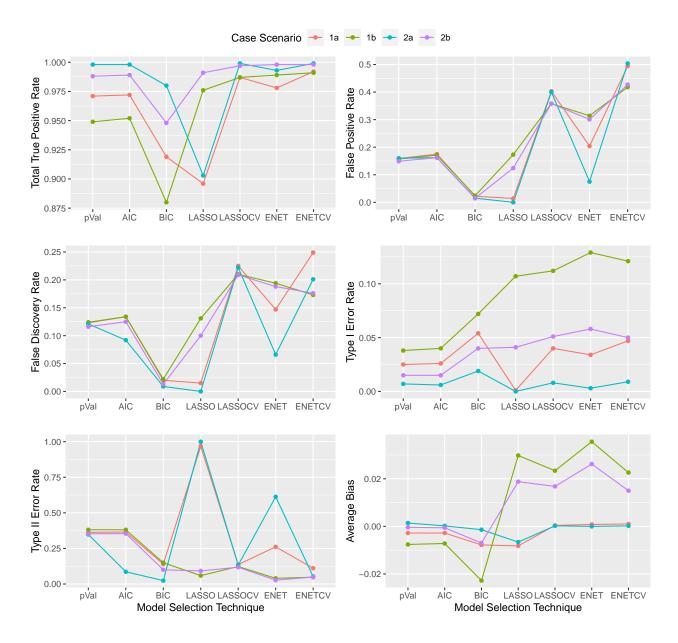


Figure 1: Grouped coefficient evaluation criteria for model selection techniques by technique and case scenario

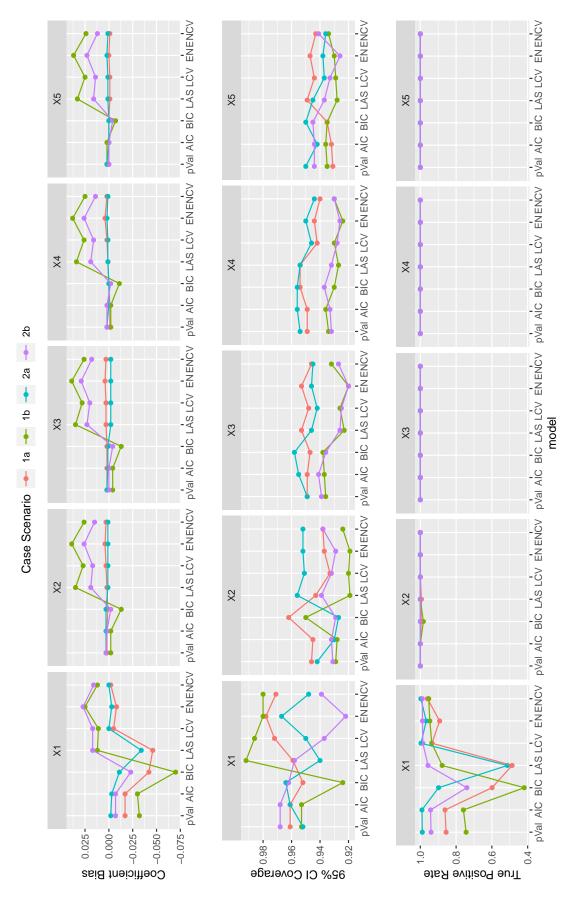


Figure 2: Known significant coefficient evaluation criteria by technique, case scenario, and coefficient. Here, pVal refers to backwards selection by p-value, LAS to LASSO, LCV to LASSO with cross-validation, EN to elastic net, and ENCV to Elastic Net with cross-validation

Table 1: Model Selection Technique Summary - Case 1a

	Backwards Selection			Regularization			
	P-Val	AIC	BIC	LASSO	LASSO with CV	Elastic Net	EN with CV
Full Model							
Total TPR	0.971	0.972	0.919	0.896	0.987	0.978	0.992
FPR	0.159	0.175	0.022	0.014	0.403	0.204	0.494
FDR	0.123	0.134	0.020	0.015	0.225	0.147	0.249
Type I Error	0.025	0.026	0.054	0.001	0.040	0.034	0.047
Type 2 Error	0.363	0.365	0.140	0.967	0.137	0.261	0.111
$\beta_1 = 1/6$							
Bias	-0.017	-0.017	-0.042	-0.046	-0.005	-0.008	-0.002
95% CI	0.961	0.961	0.952	0.959	0.972	0.978	0.971
TPR	0.856	0.862	0.599	0.487	0.935	0.892	0.960
$\beta_2 = 1/3$							
Bias	0.002	0.002	0.001	0.002	0.003	0.004	0.003
95% CI	0.946	0.945	0.962	0.943	0.933	0.937	0.938
TPR	1.000	1.000	0.995	0.994	1.000	1.000	1.000
$\beta_3 = 1/2$							
Bias	0.002	0.002	0.002	0.003	0.003	0.004	0.003
95% CI	0.949	0.949	0.947	0.953	0.948	0.953	0.946
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_4 = 2/3$							
Bias	-0.001	-0.001	0.000	0.001	0.002	0.004	0.002
95% CI	0.949	0.949	0.954	0.954	0.942	0.944	0.940
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_5 = 5/6$	'						
Bias	0.000	0.000	0.000	-0.001	-0.001	0.000	-0.001
95% CI	0.931	0.932	0.935	0.949	0.944	0.947	0.943
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 2: Model Selection Technique Summary - Case 1b

	Backwards Selection			Regularization			
	P-Val	AIC	BIC	LASSO	LASSO with CV	Elastic Net	EN with CV
Full Model							
Total TPR	0.949	0.952	0.880	0.976	0.987	0.989	0.991
FPR	0.157	0.171	0.024	0.173	0.358	0.314	0.418
FDR	0.124	0.134	0.022	0.131	0.210	0.194	0.173
Type I Error	0.038	0.040	0.072	0.107	0.112	0.129	0.121
Type 2 Error	0.381	0.381	0.150	0.059	0.123	0.040	0.048
$\beta_1 = 1/6$							
Bias	-0.032	-0.030	-0.070	0.012	0.011	0.025	0.012
95% CI	0.953	0.953	0.924	0.992	0.986	0.980	0.980
TPR	0.744	0.759	0.419	0.878	0.936	0.947	0.953
$\beta_2 = 1/3$							
Bias	-0.002	-0.002	-0.013	0.035	0.027	0.039	0.026
95% CI	0.929	0.928	0.950	0.919	0.920	0.919	0.924
TPR	1.000	1.000	0.983	1.000	1.000	1.000	1.000
$\beta_3 = 1/2$							
Bias	-0.004	-0.004	-0.013	0.035	0.028	0.039	0.026
95% CI	0.936	0.937	0.938	0.923	0.926	0.920	0.932
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_4 = 2/3$							
Bias	-0.002	-0.002	-0.011	0.034	0.026	0.038	0.025
95% CI	0.934	0.936	0.930	0.927	0.930	0.924	0.930
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_5 = 5/6$							
Bias	0.002	0.002	-0.007	0.033	0.025	0.037	0.024
95% CI	0.935	0.936	0.935	0.928	0.929	0.930	0.934
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 3: Model Selection Technique Summary - Case $2\mathrm{a}$

	Backwards Selection			Regularization			
	P-Val	AIC	BIC	LASSO	LASSO with CV	Elastic Net	EN with CV
Full Model							
Total TPR	0.998	0.998	0.980	0.903	0.999	0.993	0.999
FPR	0.160	0.162	0.015	0.000	0.400	0.075	0.504
FDR	0.121	0.092	0.009	0.000	0.222	0.066	0.201
Type I Error	0.007	0.006	0.019	0.000	0.008	0.003	0.009
Type 2 Error	0.348	0.086	0.024	1.000	0.133	0.613	0.053
$\beta_1 = 1/6$							
Bias	-0.002	-0.003	-0.011	-0.034	0.000	-0.003	0.000
95% CI	0.952	0.961	0.964	0.940	0.950	0.967	0.948
TPR	0.989	0.991	0.898	0.513	0.996	0.967	0.997
$\beta_2 = 1/3$							
Bias	0.003	0.003	0.003	0.001	0.001	0.001	0.001
95% CI	0.942	0.930	0.927	0.956	0.951	0.952	0.952
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_3 = 1/2$							
Bias	0.002	0.001	0.001	-0.002	-0.002	-0.002	-0.002
95% CI	0.949	0.955	0.958	0.946	0.942	0.946	0.945
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_4 = 2/3$							
Bias	0.002	0.000	0.000	0.001	0.001	0.002	0.001
95% CI	0.954	0.956	0.956	0.954	0.946	0.950	0.944
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_5 = 5/6$	1						
Bias	0.002	0.000	0.000	0.001	0.001	0.002	0.001
95% CI	0.950	0.942	0.950	0.945	0.937	0.938	0.936
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 4: Model Selection Technique Summary - Case 2b

	Backwards Selection			Regularization			
	P-Val	AIC	BIC	LASSO	LASSO with CV	Elastic Net	EN with CV
Full Model							
Total TPR	0.988	0.989	0.948	0.991	0.997	0.998	0.998
FPR	0.149	0.162	0.015	0.124	0.358	0.301	0.427
FDR	0.116	0.125	0.013	0.100	0.209	0.188	0.176
Type I Error	0.015	0.015	0.040	0.041	0.051	0.058	0.050
Type 2 Error	0.353	0.354	0.100	0.092	0.118	0.027	0.049
$\beta_1 = 1/6$							
Bias	-0.007	-0.007	-0.023	0.017	0.017	0.027	0.016
95% CI	0.968	0.968	0.962	0.958	0.937	0.922	0.939
TPR	0.940	0.943	0.740	0.957	0.986	0.988	0.989
$\beta_2 = 1/3$							
Bias	0.003	0.002	-0.002	0.019	0.017	0.026	0.015
95% CI	0.931	0.932	0.929	0.939	0.932	0.929	0.938
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_3 = 1/2$							
Bias	0.000	0.000	-0.004	0.023	0.020	0.029	0.018
95% CI	0.939	0.941	0.936	0.926	0.925	0.920	0.927
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_4 = 2/3$							
Bias	0.002	0.002	-0.002	0.019	0.016	0.026	0.014
95% CI	0.932	0.933	0.937	0.932	0.928	0.926	0.930
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000
$\beta_5 = 5/6$							
Bias	0.000	0.000	-0.004	0.016	0.014	0.023	0.012
95% CI	0.944	0.944	0.945	0.937	0.933	0.926	0.941
TPR	1.000	1.000	1.000	1.000	1.000	1.000	1.000