ensr: R Package for Simultaneous Selection of Elastic Net Tuning Parameters

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Abstract

Motivation:

Elastic net regression is a form of penalized regression that lies between ridge and least absolute shrinkage and selection operator (LASSO) regression. The elastic net penalty is a powerful tool for controlling the impact of correlated predictors and the overall complexity of generalized linear regression models. The elastic net penalty has two tuning parameters: λ for the complexity and α for the compromise between LASSO and ridge. The R package provides efficient tools for fitting elastic net models and selecting λ for a given α . However, glmnet does not simultaneously search the $\lambda-\alpha$ space for the optimal elastic net model.

Results:

We built the R package ensr, elastic net searcher. ensr extends the functionality of glmnet to search the $\lambda - \alpha$ space and identify an optimal $\lambda - \alpha$ pair.

Availability:

ensr is available from the Comprehensive R Archive Network at https://cran.r-project.org/package=ensr.

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Introduction

Elastic net regression (Zou and Hastie, 2005) is a penalized linear modeling approach that lies between ridge regression (Hoerl and Kennard, 1970), and least absolute shrinkage and selection operator (LASSO) regression (Tibshirani, 1996). Ridge regression reduces the impact of collinearity on model parameters and LASSO reduces the dimensionality of the support by shrinking some of the regression coefficients to zero. Elastic net does both of these. Specifically, for a linear model of the form

$$E(\mathbf{Y}|\mathbf{X}=\mathbf{x}) = \beta_0 + \mathbf{x}^{\top}\boldsymbol{\beta},\tag{1}$$

the elastic net estimates β by solving (Friedman et al., 2010)

$$\min_{(\beta_0, \boldsymbol{\beta}) \in \mathbb{R}^{p+1}} \left[\frac{1}{2N} \sum_{i=1}^{N} \left(y_i - \beta_0 - x_i^{\top} \boldsymbol{\beta} \right)^2 + \lambda P_{\alpha} \left(\boldsymbol{\beta} \right) \right], \tag{2}$$

where

$$P_{\alpha}(\boldsymbol{\beta}) = \sum_{j=1}^{p} \left[\frac{1}{2} (1 - \alpha) \beta_{j}^{2} + \alpha |\beta_{j}| \right], \tag{3}$$

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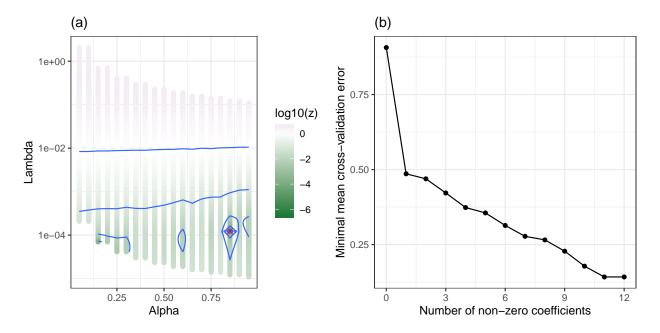


Figure 1: Plotting an ensr_obj generates two figures. The left panel (a) is a contour plot of $\lambda - \alpha$ space with the surface defined by $\log_{10}(Z)$, where Z is the number of standard deviations above the global minimum observed cross-validation error. The overall minimum error is denoted with a red dot. The right panel (b) shows the minimum cvm by the number of non-zero coefficients. This plot is provided to help users select parsimonious models with negligibly larger mean cross-validation error than the overall minimum.

N is the sample size, and there are p predictor variables. λ is a model complexity penalty that shrinks some β_i s to zero. α defines whether the elastic net model is more similar to its LASSO ($\alpha = 1$) or ridge analogs ($\alpha = 0$).

The R package glmnet (Friedman et al., 2010) provides tools for fitting elastic net regression models. The glmnet algorithms efficiently evaluate multiple possible values of λ when the user inputs a value of α (thereby choosing ridge, elastic net, or LASSO regression). glmnet can also select λ in an automated fashion using cross-validation. However, it lacks a tool to simultaneously select values of α and λ . Our package, ensr, elastic net searcher, provides a cross-validation approach to select α and λ simultaneously.

Usage

The ensr package is available from the Comprehensive R Archive Network (CRAN) at https://cran.r-project.org/package=ensr and from https://github.com/dewittpe/ensr.

After installation, load and attach the ensr namespace in an active R session. We encourage you to load and attach the data.table (Dowle and Srinivasan, 2018) namespace as well.

Users interact with the eponymous function ensr. ensr::ensr is an extension of glmnet::cv.glmnet. The two functions have the same API except that ensr has one additional argument, alphas, to define a numeric vector of specific α values to consider. In contrast, cv.glmnet will only consider a single value of α .

We included a synthetic example data set tbi in the ensr package based on Bennett et al. (2017). The following example of ensr usage aims to identify which of six procedure codes and six billing codes are associated with particular injury type. We will model the odds of injury2 as a function of the presence or absence of procedure codes pcode1, ..., pcode6 and billing codes ncode1, ..., ncode6. Additional examples using other example data sets are available in the 'ensr-examples' vignette.

As with glmnet::cv.glmnet, the end user will need to construct matrices for the response and the predictors. By default, ensr will standardize all predictors. In the below example, all predictors are

binary, 0 (false) / 1 (true). Therefore, standardization is not required. The sequence of alphas defined below has been selected to explicitly prevent either a pure ridge ($\alpha = 0$) or pure LASSO ($\alpha = 1$) model.

```
ymat <- as.matrix(tbi[, injury2])
xmat <- as.matrix(tbi[, pcode1:ncode6])
set.seed(2018)
ensr_obj <-
   ensr(x = xmat,
        y = ymat,
        alphas = seq(0.05, 0.95, length = 10),
        standardize = FALSE,
        family = "binomial")</pre>
```

Output

ensr objects (ensr_obj) are lists of cv.glmnet objects. Using an ensr_obj, a user could take one of two approaches to select a model: 1) Select the $\lambda - \alpha$ pair with the overall minimum mean cross-validation error (minimum cvm), or 2) consider the trade-off between the reduction in minimum cvm with the inclusion of additional non-zero coefficients.

A summary of the ensr_obj gives the list index, 1_index, for the cv.glmnet objects within ensr object as well as the corresponding values of λ , α , cvm, and the number of non-zero coefficients, nzero.

Selection of a preferable model can be automated or done with some analyst input. For example, consider the models with minimum cvm by number of non-zero coefficients.

```
by_nzero <-
  summary(ensr_obj)[order(cvm),
                    .SD[cvm == min(cvm)],
                   by = nzero]
by_nzero[nzero > 7]
      nzero l_index
                      lambda
                                 cvm alpha
## 1:
        11
              17 1.216e-04 0.1421 0.85
## 2:
         12
                 3 6.959e-05 0.1422
                                     0.15
        10
                19 1.675e-03 0.1781
                                     0 95
## 4:
         9
                19 3.618e-03 0.2280 0.95
             19 5.243e-03 0.2656 0.95
## 5.
```

The model with the lowest cvm has twelve non-zero coefficients and could easily be obtained using ensr::preferable.

```
pref_ensr_obj <- preferable(ensr_obj)</pre>
```

There is very little difference in cvm between the model with twelve non-zero coefficients and the model with eleven non-zero coefficients. This can been seen in the output of the summary call or from the graphic in Figure 1.

```
plot(ensr_obj, type = 1) # Generate Fig. 1a
plot(ensr_obj, type = 2) # Generate Fig. 1b
```

Discussion

As with other uses of cross-validation, selection of λ and α is subject to the number and membership of the folds. We recommend that **ensr** users select final models by bootstrapping cross-validation errors and perform sensitivity analyses varying cross-validation fold membership.

Another R package, glmnetUtils (Microsoft and Ooi, 2017), also selects λ and α using cross-validation. A major difference between ensr and glmnetUtils is that ensr evaluates a richer grid

of $\lambda - \alpha$ pairs by default. glmnetUtils uses default glmnet values of λ for each α value. This results in a unique set of λ values for each α . In contrast, ensr constructs a set of λ values such that common values of λ are evaluated for multiple values of α . The ensr contour plot method gives the user a way to visualize the grid of $\lambda - \alpha$ pairs evaluated.

Conclusion

The ensr R package extends the functionality of the glmnet package by providing users the ability to automate selection of tuning parameters for elastic net regression models.

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