Resampling Strategies for Regression

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January, 2017
Predictive Modeling with Imbalanced Distributions

- Many predictive tasks involve handling a target variable that has an imbalanced distribution in the available training data.
- Problem thoroughly explored in classification tasks.
- Similar problems occur in some regression problems.
- Important applications in real world domains (finance, ecology, meteorology)

You may check our extensive survey on existing methods for classification and regression:
Imbalanced Distributions in Regression

- Frequently occur when the main goal of the end user are extreme values of the target - e.g. unusually high(low) returns of a stock.
- These extreme values are usually rare, i.e. poorly represented in the training data.
- As within imbalanced classification, models will be biased towards the more frequent cases in the training data.
- As a result performance on the cases that matter will be disappointing.
Problem Definition

Predicting Rare Extreme Values

- Goal: obtain a good approximation of the unknown function
  \[ Y = f(X_1, X_2, \cdots, X_p) \]
- Training set: \( D = \{\langle x_i, y_i \rangle\}_{i=1}^n \)

- a subset of the range of the target variable values \( Y \) has an higher importance to the user
- the most important subset of \( Y \) is under-represented in the available training sample
Problem Definition

More formally

- Given a **relevance function**: $\phi(Y) : Y \rightarrow [0, 1]$, where 1 is maximal importance and 0 represents minimum relevance.
- Ask user for a **threshold** $t_R$ on relevance.
- $Y_R = \{y \in Y : \phi(y) > t_R\}$ and $Y_N = Y \setminus Y_R$.
- Given a training set $D$, partition it in $D_R$ where $y \in Y_R$ and $D_N = D \setminus D_R$.
- An imbalanced prediction task satisfies:
  - **non-uniform importance** of the predictive performance of the models across the domain of $Y$.
  - $|D_R| << |D_N|$.
Imbalanced Domains

Classification Example

Regression Example

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Problems created by imbalanced distributions

The combination of the specific preferences of the user with the poor representation of these situations creates problems at several levels.

Typically we need:

1. special purpose evaluation metrics that are biased towards the performance of the models on these rare cases,
2. making the learning algorithms focus on these rare events.
A Taxonomy of strategies for handling Imbalanced Domains

Strategies for Imbalanced Domains

Data Pre-processing
- Distribution Change
- Weighting the Data Space

Special-purpose Learning Methods

Prediction Post-processing
- Threshold Method
- Cost-sensitive Post-processing

Hybrid Methods

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Data pre-processing

- **Goal**: change the examples distribution before applying any learning algorithm;
- **Advantages**: any standard learning algorithm can then be used;
- **Disadvantages**: difficult to decide the optimal distribution (a perfect balance does not always provide the optimal results); the strategies applied may severely increase/decrease the total number of examples;
Special-purpose learning methods

- **Goal**: change existing algorithms to provide a better fit to the imbalanced distribution;

- **Advantages**: very effective in the contexts for which they were designed; more comprehensible to the user

- **Disadvantages**: difficult task because it requires a deep knowledge of both the learning algorithm and the target domain; often unavailable cost-benefit matrix; difficulty of using an already adapted method in a different learning system;
Strategies for Handling Imbalanced Domains

Prediction post-processing

- **Goal**: change the predictions after applying any learning algorithm;
- **Advantages**: any standard learning algorithm can be used;
- **Disadvantages**: potential loss of models interpretability;
Relevance Function

- Handling imbalanced regression requires defining the important values.
- This can be done through the definition of a relevance function, $\phi()$, that maps the domain of the target into a range of importance.
- $\phi() \in [0, 1]$ where 0 represents values of the target variable that are not relevant and 1 identifies the most important values.

Relevance Definition

Ribeiro (2011) proposed a framework for defining the relevance function of a given continuous target variable. This framework:

- includes an automatic method that allows to obtain the relevance function from the target variable sample distribution (assumes extreme rare values are the most important to the user).
- allows the user to manually specify which are the relevant and irrelevant values using a matrix.

Resampling Strategies for Regression Tasks

- Random Undersampling
- Random Oversampling
- Introduction of Gaussian Noise
- SmoteR
- WEighted Relevance-based Combination Strategy (WERCS)

The R Package UBL

- We have created an R package (UBL) that implements a large set of approaches for both classification and regression.
- We will use it for illustration purposes.
- More information about the package (and further examples) can be obtained in:
Random Undersampling

- In Random Undersampling all cases with target value with a relevance lower than the threshold are candidates for undersampling.
- User decides this threshold as well as the target proportion between normal (unimportant) and rare (important) cases in the produced data set.
- This resampled dataset is obtained by randomly removing examples from the uninteresting cases.
Random Undersampling in UBL

```r
# Using the automatic method for defining the relevance function
# This is the default behaviour
library(UBL)
# default of C.perc parameter balances the examples
bal <- RandUnderRegress(a7~., clean.algae)

extr <- RandUnderRegress(a7~., clean.algae, C.perc = "extreme")

# the automatic method for the relevance function generates only
# one "bump" with uninteresting values, thus we only need to set
# one under-sampling percentage
usr <- RandUnderRegress(a7~., clean.algae, C.perc = list(0.5))
```
Impact of different settings of Random Undersampling
Random Oversampling

- The Random Oversampling approach is simply based on the introduction of random copies of examples from the original data set.
- These replicas are only introduced in the most important ranges of the target variable, i.e., in the ranges where the relevance is above a user-defined threshold.
- User needs to define a relevance function, a relevance threshold and the percentage of oversampling to perform.
Random Oversampling using UBL

```r
## using the automatic method for defining the relevance function and
## the default threshold (0.5)
usr <- RandOverRegress(a7~., clean.algae, C.perc=list(2.5))
bal <- RandOverRegress(a7~., clean.algae, C.perc="balance")
extr0.5 <- RandOverRegress(a7~., clean.algae, C.perc="extreme")

# change the relevance threshold to 0.9
extr0.9 <- RandOverRegress(a7~., clean.algae, thr.rel=0.9, C.perc="extreme")
```
Impact of different settings of Random Oversampling

![Graph showing impact of different settings of Random Oversampling. The graph plots the density of y values across different oversampling techniques, including clean.algae, usr, bal, extr0.5, extr0.9, and a dashed line labeled φ().]
Introduction of Gaussian Noise

- This strategy combines oversampling by generating new synthetic examples with small perturbations with the random undersampling strategy.
- The relevance function and the user-defined threshold distinguish among the ranges where over and undersampling are applied.
- The target variable of the generate cases is obtained by introducing a small perturbation based on the sample standard deviation.
Introduction of Gaussian Noise in UBL

```r
# relevance function estimated automatically has two bumps
# defining the desired percentages of under and oversampling to apply
C.perc <- list(0.5, 3)
# define the relevance threshold
thr.rel=0.8
usr <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc=C.perc)
bal <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc="balance")
extr <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc="extreme")
```
Impact of different settings of Gaussian Noise

- clean.algae
- usr
- bal
- extr
- $\phi()$
Further examples with Gaussian Noise

# the default uses the value of 0.1 for "pert" parameter
bal <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel,  
                          C.perc="balance")

# try two different values for "pert" parameter
bal05 <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel,  
                          C.perc="balance", pert=0.5)
bal001 <- GaussNoiseRegress(a7~., clean.algae, thr.rel=thr.rel,  
                          C.perc="balance", pert=0.01)
The impact of changing the parameter pert
SmoteR - SMOTE for Regression Tasks

- Once again the relevance function and the relevance threshold determine which are the relevant and the unimportant cases.
- The algorithm combines an oversampling strategy by interpolation of relevant examples with a random undersampling approach.
- A similar procedure to the original Smote algorithm is used to generate new examples.
- For the target variable value of the new examples a weighted average of the values of target variable of the two seed examples is used.
- The weights are calculated as an inverse function of the distance of the generated case to each of the two seed examples.

Using the SmoteR Algorithm

```r
# we have two ranges: the first must be undersampled and the second oversampled.
# Thus, we can choose the following percentages:
thr.rel <- 0.8
C.perc <- list(0.1, 8)

# using these percentages and the relevance threshold of 0.8 with all the
# other parameters default values
usr <- SmoteRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc=C.perc, dist="HEOM")

# using the automatic method for obtaining a balanced data set
bal <- SmoteRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc="balance", dist="HEOM")

# use the automatic method for inverting the frequencies of the ranges
extr <- SmoteRegress(a7~., clean.algae, thr.rel=thr.rel, C.perc="extreme", dist="HEOM")
```
The impact of the parameters on SmoteR

![Graph showing the impact of parameters on SmoteR](image)

Legend:
- clean.algae
- usr
- bal
- extr
- $\phi()$
WEighted Relevance-based Combination Strategy (WERCS)

- WERCS key idea is to use the relevance function scores as probabilities for resampling the examples.
- Examples are selected for being either removed or added as replicas using these probabilities.
- In oversampling examples with higher relevance have higher probability of being replicated.
- In undersampling examples are randomly selected to be removed with probability $1 - \phi(y)$, i.e., the higher the relevance value of an example, the lower will be the probability of being removed.
- User is not required to set a relevance threshold.
WERCS in UBL

# using importance sampling with threshold definition
C.perc=list(0.2,6)
thrusr <- ImpSampRegress(a7~., clean.algae, thr.rel=0.8, C.perc=C.perc)
thrbal <- ImpSampRegress(a7~., clean.algae, thr.rel=0.8, C.perc="balance")
thrextr <- ImpSampRegress(a7~., clean.algae, thr.rel=0.8, C.perc="extreme")

# importance sampling without threshold
usr <- ImpSampRegress(a7~., clean.algae)
usr1 <- ImpSampRegress(a7~., clean.algae, U=0.9, 0=0.2)
usr2 <- ImpSampRegress(a7~., clean.algae, U=0.2, 0=1)
The impact of the parameters on WERCS - 1
The impact of the parameters on WERCS - 2
Experimental Analysis of the Methods

- Resampling strategies considered:
  - No resampling - original data (the baseline)
  - 2 variants of Random Undersampling (RU)
  - 2 variants of Random Oversampling (RO)
  - 2 variants of SmoteR (SMT)
  - 6 variants of Gaussian Noise (GN)
  - 4 variants of WERCS

- Several regression algorithms (31)
  - 1 LM + 8 NNET variants + 4 MARS variants + 12 SVM variants + 6 RF variants

- 15 regression data sets with different characteristics

- **A total of 7905 \((15 \times 31 \times 17)\) alternatives**

- The values of \(F_1\) for regression were estimated by means of \(2 \times 10\) - fold cross validation process and the statistical significance of the observed paired differences was measured using the non-parametric Wilcoxon Sign Rank test
A summary of the results

Total number of wins (left - blue) and losses (right - brown) of sampling strategies, against the baseline of using the original imbalanced data set.
Summary/Conclusions/Recommendations

- Random forests (RF) with either RO, GN or WERCS achieved the best performance in 10 out of 15 data sets.
- WERCS achieved the most consistent performance when compared to using the original data.
- WERCS is also more "user-friendly" as it does not require setting a relevance threshold.
- It is also computationally more efficient as it does not involve generating new cases (just replicating) and it does not increase the training set sizes.
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