Methods for handling missing and categorical data for classification with neural networks*

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Abstract

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1. Introduction

Missing data is a common problem in survey data in various domains. Several techniques for data imputation (i.e., replace missing values with plausible ones) and direct estimation (i.e., all missing data is analyzed using a maximum likelihood approach) have been proposed [?].

Random Forest and other ensembles of decision trees are the method of choice for survey data, largely because missing data and categorical variables are not easy to handle with neural networks. We investigate techniques for handling missing data and encoding categorical data such that it is appropriate to neural network classifiers. We compare six different imputation strategies: case substitution; mean or median imputation; one—hot; hot deck and cold deck; prediction model; and factor analysis. These strategies are defined in Section ??.

After briefly reviewing related works in Section ??, we experiment using neural networks on benchmark data and compare our results with the state-of-the-art in Section ??. Finally, we draw conclusions in Section ??.

2. Related work

2.1. Techniques for handling missing data

We divide proposed imputation methods into six groups listed below [?]:

- Case substitution One observation with missing data is replaced with another non-sampled observation.
- Summary statistic Replace the missing data with the mean, median, or mode of the feature vector. Using a numerical approach directly is not appropriate for nonordinal categorical data.
- **One-hot** Create a binary variable to indicate whether or not a specific feature is missing.
- Hot deck and cold deck Compute the K-Nearest Neighbors of the observation with missing data and assign the mode of the K-neighbors to the missing data. algorithm.
- **Prediction Model** Train a single prediction model (e.g., random forests) or ensemble of models to predict the missing value.
- Factor analysis Perform principal component analysis (PCA) on the design matrix, project the design matrix onto the first two eigenvectors and replace the missing values by the values that might be given by the projected design matrix.

2.2. Neural networks for classification with categorical and continuous features

Common techniques for handling categorical data in neural networks include encoding the categorical values into numeric values or using binary encoding. These techniques, however, have some drawbacks including unnecessarily increasing model complexity

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^{*}The video presentation can be viewed at youtube.com/foo. The code used for this project is available at https://github.com/jvpoulos/cs289-project.

or feature dimensionality and not preserving the similarity information embedded between categorical values [?].

More elaborate techniques include information theoretic measures [?], training separate output units for each of the allowed combination of values of the categorical independent variables [?], and using distance hierarchies [?].

In the case of categorical variables, which by definition have no direct representation or computation scheme of the distance between its values, decision trees can be useful because they do not require distance metrics. However, their training process is slow given a large enough dataset and they might not be suitable for problems where the decision boundary between classes described by a second-order polynomial,* for example [?].

3. Experiments

3.1. Benchmark data set

We experiment with the Adult dataset from the UCI Machine Learning Repository [?]. The dataset has 48,842 instances, 2/3 for training and 1/3 reserved as a final test set (i.e., train = 32,561 and test = 16,281). The dataset contains 14 features: 6 continuous and 8 categorical. The prediction task is to determine whether a person makes over \$50,000 a year. 24% of individuals in the training data make more than this amount.

Table ?? shows the test error rates obtained by the data set donor [?]. All error rates were obtained after removing samples with missing values. The state-of-the-art is a Naive Bayes classifier that achieves a 14.05% error rate.

3.2. Patterns of missing values in Adult dataset

The Adult dataset has 3,620 (7.4%) samples containing missing values. Missing values occur in three of the categorical features: Work class, Occupation, and Native country. It is unlikely that these values are missing completely at random (MCAR); it is more likely, and much less desirable that the values are not missing at random (MNAR). Since these data originate from a survey, the missing values may be due to respondents unwilling or unable to provide an

Algorithm	Error (%)
1 C4.5	15.54
2 C4.5-auto	14.46
3 C4.5 rules	14.94
4 Voted ID3 (0.6)	15.64
5 Voted ID3 (0.8)	16.47
6 T2	16.84
7 1R	19.54
8 NBTree	14.10
9 CN2	16.00
10 HOODG	14.82
11 FSS Naive Bayes	14.05
12 IDTM (Decision table)	14.46
13 Naive-Bayes	16.12
14 Nearest-neighbor (1)	21.42

Table 1. Test set error rates on Adult dataset for various algorithms, obtained after removal of samples with missing values and using the original train/test split. Source: [?].

answer.

Uncovering patterns of missing values in the dataset will help select strategies for imputing missing values. The histogram (left) in Figure ?? shows Work class and Occupation each have about 5.6% of missing values, and Native country has about 1.7% missing values. The aggregation plot (right) shows 5.5% of samples are missing values for both Work class and Occupation. Less than 2% of samples are missing just Native country and less than 1% are missing all three features.

Figure ?? shows the frequency of observed categories and missing values for *Work class* and *Occupation*. Each stacked column shows the proportion of missing values in the other feature and *Native country* for each category. The plot shows the missing values are not MCAR: individuals working in the private sector, for instance, are more likely to have missing values than those individuals in other work classes. However, missing values tend to be evenly distributed across occupational categories.

3.3. Preprocessing

We preprocess the training and test data as follows:

- Drop the string feature education because it contains identical information as its numeric counterpart education.num.
- 2. Binarize the categorical variables.
- 3. Implement imputation technique. When replacing the missing data with the mean, median, or

 $^{{}^\}star \mathrm{We}$ note, however, that a property test can be as complex as the data at hand.

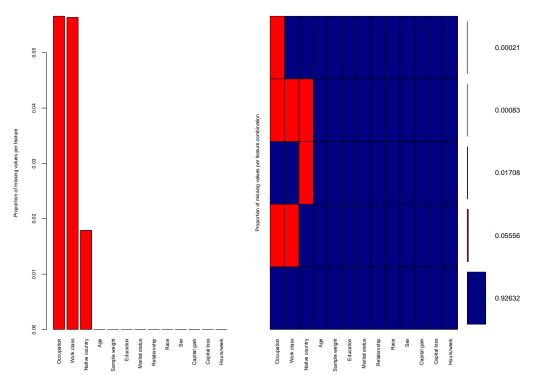


Figure 1. Histogram of proportion of missing values in each feature (Left) of Adult training set and aggregation plot of all existing combinations of missing and non-missing values in the samples (Right).

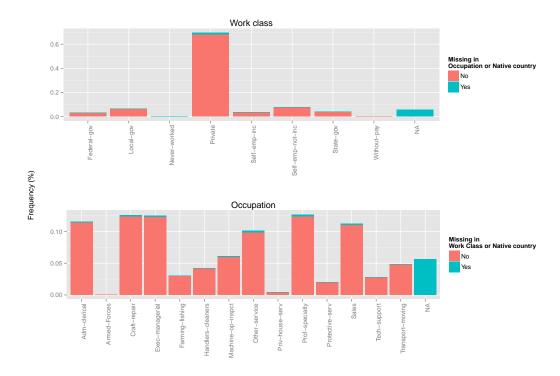


Figure 2. Barplot of proportion of observed and missing values of Work class and Occupation in Adult dataset.

mode of the feature vector, the summary statistic is computed from the training data, not from the test data.

4. Standardize each feature to midrange 0 and range 2 (i.e., minimum -1 and maximum 1). We use the training set values for range and midrange to standardize test set features.

3.4. Model selection

We implement two neural network classifiers: a simple model and a complex model. The complex model uses two hidden layers, both with the same size of hidden notes, which is computed using the formula, and root-mean-square gradient scaling for the update rule. The simple model uses one hidden layer and stochastic gradient descent for the update rule. Both models use a cross–entropy cost function and weights initialized randomly using Gaussian distribution and scaled by a factor of 10^{-2} .

formula grid search k-fold cv Table ?? Figure ??

3.5. Model assessment

Mode: 0.1684 (1 epoch) Drop: 0.1859 (1 epoch) Predict: 0.1663 (1 epoch)

4. Conclusions

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Imputation method	Model type	α	γ	Batch size	Error rate	\mathbf{Cost}	Time (min.)
Drop	Simple	9	0.1	32	0.1406	0.1525	3.7
PCA	Simple	4	0.1	32	0.1411	0.2487	8.3667
Predicted	Simple	4	0.1	32	0.1413	0.2056	6.7
Mode	Simple	9	0.1	32	0.1415	0.1829	4.2667
Replace	Simple	1	0.1	32	0.1417	0.2189	6.8
Predicted	Complex	1	0.1	32	0.1426	0.2919	9.9
PCA	Complex	1	0.01	32	0.143	0.3175	11
Drop	Complex	1	0.1	32	0.1439	0.1778	8.5
Median	Simple	4	0.1	32	0.1446	0.1924	-
Mean	Simple	4	0.1	32	0.1453	0.1915	-
Mean	Complex	1	0.1	32	0.1593	0.3118	-
Median	Complex	1	0.01	32	0.1595	0.3564	_

Table 2. Performance of models selected on the basis of cross–validated error rate on the training data. Imputation methodis how missing values in the training data are imputed; Model type is the type of neural network classifier used; α is the scaling factor used to determine the number of hidden neurons in the neural network; γ is the learning rate; Batch size is the size of the batch; Error rate is the mean 3-fold cross–validated error rate on the training data; Cost is the mean cross–entropy cost across folds; Time is the mean computational time across folds.

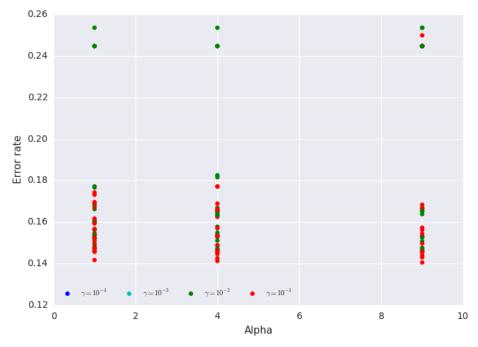


Figure 3. Performance of simple neural network on training data with missing values imputed using random forests: 3-fold cross–validated error rate versus α (x–axis) and γ (colors). See Table ?? for definitions.