Sampling Techniques in Bayesian Target Encoding

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Abstract. Target encoding is an effective encoding technique of categorical variables and is often used in machine learning systems for processing tabular data sets with mixed numeric and categorical variables. Recently an enhanced version of this encoding technique was proposed by using conjugate Bayesian modeling. This paper presents a further development of Bayesian encoding method by using sampling techniques, which helps in extracting information from intra-category distribution of the target variable, improves generalization and reduces target leakage.

1 Introduction

Target encoding technique was formulated first in [1] as a way to deal with high-cardinality categorical variables. In this technique each value of the categorical variable (which we call for simplicity a category) is mapped to a target mean conditional on the value of the variable. More precisely, for regression problem it is an expected value of the target given the category. For binary classification it is a posterior probability of the target given the category. For multi-class problem an obvious extension of the binary case would be to introduce m-1 new variables (where m is the number of classes) that are the posterior probability of the target being in a specified class.

This technique proved remarkably successful in a variety of machine learning projects and became extremely popular in data science competitions, for example, on Kaggle[1]. For several different implementations of Target Encoding see python package Category Encoders[2]. For a general discussion on categorical variable encoding see [4]. Target Encoding is also widely known as Mean Encoding because it encodes the categorical variable with conditional target mean.

One of the issues with Target Encoding is that it fails to extract information from intra-category target variable distribution apart from its mean. Even though Micci-Barreca [1] claims to use target statistics for encoding categorical variables, in fact it is using only mean, leaving variance and other target statistics out. This shortcoming is addressed in Bayesian Target Encoding techniques [5,6]. The idea is to select a conjugate prior for the conditional distribution of the target variable given the value of the categorical variable, and then update it based on training examples to obtain a posterior distribution, and encode the categorical

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1 https://www.kaggle.com
2 http://contrib.scikit-learn.org/category_encoders
variable using the first several moments of the posterior distribution. Slakey et al. [5] have the encoding of the categorical variable done in two steps or layers: the Local Layer in which the posterior distribution is computed for each value of the categorical variable, and the Encoding Layer where each category is encoded using the first Q moments of the posterior distribution.

In this paper we propose to enhance the Encoding Layer by sampling from the posterior distribution instead of taking expectations of its first Q moments. We call this method Sampling Bayesian Encoder. It puts the Bayesian Target encoding on a solid theoretical footing, opening window for more improvement of the target encoding techniques. Using this method eliminates the need to add Gaussian noise to the encoded values, as is commonly done to avoid target leakage and overfitting [2], because we are exploring the parameter space during sampling procedures. This approach was used on simulated data as well as on real world data and demonstrated better generalization for the data sets with a mixture of numeric and categorical variables with various degree of cardinality.

2 Sampling as embedding layer

Following Slakey et al. [5], we train a probabilistic model of the target variable $y$ for each categorical variable $x$, deriving a posterior distribution:

$$p_{mv} (\theta | y) \propto \mathcal{L}_{mv} (\theta | y) p(\theta), \quad (1)$$

where $v$ signifies unique values of the categorical variable $x_m$, $\theta$ is a parameter vector of the posterior distribution, $p_m (\theta)$ is a prior distribution, and $\mathcal{L}_{mv} (\theta | y)$ is a likelihood function.

Let us define $\theta_{nm}$ as a realization of the posterior distribution $p_{mv} (\theta | y)$ for categorical variable $m$ and example $n$:

$$\theta_{nm} \sim p_{mv} (\theta | y), \quad (2)$$

Let us also introduce a vector function $f_m (\theta)$ that maps the parameters of the posterior distribution to a Q-dimensional space and encode all categorical variables $x_m$ with $f_m$ and train a model $\hat{y}_\theta (\xi_n, f_1 (\theta_{n1}), .. f_M (\theta_{nM}))$ using encoded categorical variables and numeric variables $\xi_n$ that do not require encoding. We do not place any restriction on the algorithm to train the model $\hat{y}_\theta$. It could be a linear model, Random Forest, Gradient Boosted Trees, SVM, a Neural network, or any other algorithm.

Since $\theta_{nm}$ is a random variable, we will train the model $\hat{y}_\theta$ for all possible values of $\theta_{nm}$ and take an expectation of the target variable to get an expected prediction:

$$\hat{y} (x_n) = \mathbb{E}_{\theta_{nm} \sim p_{mv} (\theta | y)} \hat{y}_\theta (\xi_n, f_1 (\theta_{n1}), .. f_M (\theta_{nM})) \quad (3)$$

In the simplest case the function $f_m (\theta)$ can be an identity function, meaning that it returns $\theta$. This will be in line with all Target Encoding schemes. Additionally, it can return polynomials of $\theta$ to be more in line with the Bayesian Target Encoding method of returning multiple moments of the posterior distribution [5,6].
For all but very simple models the expectation (3) is intractable, but can be approximated by sampling from the posterior distribution. For a sample $\theta_{nm}^k$ where $k = 1..K$, the estimate is:

$$\bar{y}(x_n) \approx \frac{1}{K} \sum_{k=1}^{K} \hat{y}(x_n, f_1(\theta_{n1}^k),..f_M(\theta_{nM}^k))$$ (4)

If algorithm to derive $\hat{y}_\theta$ supports mini-batching, it is reasonable to generate a sample of the posterior distribution for every iteration or epoch. Otherwise, after sampling $K$ times we encode the categorical variables with the realizations $\theta_{nm}^k$ and concatenate the encoded data together. Thus, if the original training set contains $N$ examples, then after encoding we will get $KN$ examples on which we train the model $\hat{y}_\theta$. During prediction phase we will also sample from the posterior distribution and then average the predictions of the model $\hat{y}_\theta$. For previously unseen categories we use the value sampled from the prior distribution.

Following [5], we set the prior distribution using target statistics of the entire data set, but then scale down the parameters of the prior distribution as if they were computed on a subset of the training data. By varying the scaling factor we can better control bias-variance tradeoff for rare categories.

3 Practical implementation of the sampling techniques

Model training for regression, binary classification and multiclass classification problems will follow the same steps:

1. Finding a prior distribution $p(\theta)$ by using target statistics for the entire training data, then scaling it down to reduce excessive influence on the results.
2. Finding a conditional posterior distribution $p_{\text{mv}}(\theta|y)$ for each categorical variable and for each value of the categorical variable. If we are using conjugate priors the posterior distributions can be found analytically. This step is identical to the Local Layer in [5]
3. Generating an augmented set that contains $K$ copies of the training set with all categorical features encoded using samples from the posterior distributions
4. Training a model (Random Forest, SVM, etc.) on the augmented set
5. Finding prediction by averaging of $K$ results of the models with $K$ different encoded values $\theta$.

3.1 Binary classification tasks

Binary classification is the simplest case because of the obvious choice of the target variable distribution: Bernoulli distribution, and it also covered in details in both [5] and [6]. The conjugate prior for Bernoulli distribution is Beta distribution that has two parameters $\alpha$ and $\beta$. In Beta-Binomial model these parameters have
a simple interpretation as $\alpha - 1$ successes and $\beta - 1$ failures. So during step 1 we set the parameters of the prior distribution as follows:

$$\alpha = 1 + \gamma \sum_{n=1}^{N} y_n$$  \hspace{1cm} (5)

$$\beta = 1 + \gamma \sum_{n=1}^{N} (1 - y_n),$$  \hspace{1cm} (6)

where $\gamma$ is a non-negative scaling factor and is a hyperparameter to the model. Zero value of $\gamma$ indicates an uninformative prior that does not use any target statistics, and the greater the value is, the more the marginal target statistics influence the encoding of the categorical features.

During step 2 the parameters of the posterior distribution is updated for every category:

$$\alpha_{mv} = \alpha + \sum_{x_m = v} y_n$$  \hspace{1cm} (7)

$$\beta_{mv} = \beta + \sum_{x_m = v} (1 - y_n)$$  \hspace{1cm} (8)

More frequent categories will give us higher values of $\alpha$ and $\beta$ and result in a sharper peak in the Beta distribution, so most of the samples will be around its maximum value. For the infrequent categories the values of $\alpha$ and $\beta$ will be lower and the distribution will be wider, resulting in greater variance of the samples. For very infrequent categories the distribution will be very close to the prior. This prevents the model from overfitting on potentially extreme values for rare categories. There is also no need to add Gaussian noise to the encoded values, because by virtue of the sampling technique the target leakage is greatly reduced.

### 3.2 Multiclass classification tasks

Multiclass classification task is an extension of binary classification, and so are the probability distributions we are going to use for category encoding. The target variable is described by Categorical distribution, and the conjugate prior is Dirichlet distribution, the parameter of which is a vector $\alpha$ of the same dimension as the number of classes, where all components are greater than zero. We set the prior as:

$$\alpha^c = 1 + \gamma \sum_{n=1}^{N} I(y_n = c)$$  \hspace{1cm} (9)

and the parameters of the posterior distribution will be updated as follows:

$$\alpha_{mv}^c = \alpha^c + \sum_{x_m = v} I(y_n = c)$$  \hspace{1cm} (10)
3.3 Regression tasks

Regression case is more complicated, because the continuous target variable can rarely be modeled using the same type of distribution for all categorical variables. But in the simplest case it can be modeled as a Normal distribution. This distribution has two parameters: \( \mu \) and \( \sigma^2 \), or alternatively \( \mu \) and precision \( \tau = \sigma^{-2} \). The prior distribution is Normal-Inverse Gamma and Normal Gamma respectively. Both of them have the same set of parameters \( \mu_0, \nu, \alpha, \beta \). The parameters of the prior distribution is:

\[
\mu_0 = \bar{y} = \frac{1}{N} \sum_{n=1}^{N} y_n \tag{11}
\]

\[
\nu = 0 \tag{12}
\]

\[
\alpha = \gamma \frac{N}{2} \tag{13}
\]

\[
\beta = \frac{\gamma}{2} \sum_{n=1}^{N} (y_n - \bar{y})^2 \tag{14}
\]

The posterior distribution for each category is:

\[
\mu_{0mv} = \frac{\nu \mu_0 + N_{mv} \bar{y}_{mv}}{\nu + N_{mv}} \tag{15}
\]

\[
\nu_{mv} = \nu + N_{mv} \tag{16}
\]

\[
\alpha_{mv} = \alpha + \frac{N_{mv}}{2} \tag{17}
\]

\[
\beta_{mv} = \beta + \frac{1}{2} \sum_{n=1}^{N_{mv}} (y_n - \bar{y}_{mv})^2 + \frac{N_{mv} \nu}{\nu + N_{mv}} \frac{(\bar{y}_{mv} - \mu_0)^2}{2}, \tag{18}
\]

where \( \bar{y}_{mv} \) is the sample mean of the target values for the category \( mv \).

While it is possible to come up with more complex conditional target distributions, for example, Gaussian Mixture models, Normal is usually works pretty well and an improvement against the deterministic Target Encoding techniques.

4 Related work

The problem of target leakage was discussed in details in [7], as well as a new sampling technique called Ordered Target Statistics was proposed. The training data are reshuffled and for each example the categorical features are encoded with the target statistics of all previous entries. Thus the "earlier" examples have a higher variance than the "later" examples, and to deal with this issue several
permutations are taken, and one is picked at random for every iteration of the Gradient Boosted Trees algorithm. The idea of taking multiple permutations is similar to our idea of generating multiple samples from the posterior distribution. Indeed, a multiple permutation technique can be interpreted as a variant of Pólya urn model, that itself can be used to generate samples from distribution [3], for example, from beta distribution. With our approach the sampling from posterior distribution is done deliberately, and the technique can be used with any machine learning algorithm.

LightGBM categorical encoding also uses target statistics, but it deals with target leakage by finding the best split based on Fisher’s method of minimizing intra-category variance [9,10,11]. See Appendix A.1 for a explanation how the reduction of intra-category variance results naturally from the sampling technique proposed in this paper.

5 Experimental Studies

![Fig. 1. Model performance for make_classification() data](image1)

![Fig. 2. Model performance for make_hastie_10_2() data](image2)

The goal of the studies is to see how the category encoder hyperparameters influence performance of the model. We generated the data set using skikit-learn.
functions `make_classification()` and `make_hastie_10_2()`. In both cases the last two columns were converted to categorical variables using `KBinsDiscretizer`. We left the other variables numeric to compare the relative feature importance of the categorical and numeric variables encoded using deterministic vs. sampling approach.

For a regression problem we used a past Kaggle competition "Mercedes-Benz Greener Manufacturing" [3]. This data set has ten high-cardinality categorical variables, for which, as we know from [15], 1-hot encoding does not produce good results. This makes it a good candidate for Target Encoding and any versions of it, including our own.

Sampling approach was compared to the Target Encoding as implemented in `LeaveOneOutEncoder` class of `category_encoders` package [2]. We used identity function for $f()$. Predictions were done using `RandomForestClassifier`. We used 5-fold cross-validation and selected the best models for both baseline and sampling encoding models. After obtaining the best model from the cross-validation procedure we varied one hyperparameter of the encoder at a time to see how it influences the model performance.

![Feature importance for make_classification() data](https://www.kaggle.com/c/mercedes-benz-greener-manufacturing/)

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[3] https://www.kaggle.com/c/mercedes-benz-greener-manufacturing/
Our observations can be summarized as follows:

- Model performance does not depend on leave-one-out technique. During cross-validation the models without leave-one-out techniques actually perform better, but the difference is within statistical error.
- When we studied a regression case we had an option to include sample of $\sigma$ in addition to the sample of $\mu$. In practice, the difference is very small and is also within statistical error.
- We studied the effect of the sample size on the model performance. You can find the results of the model accuracy including $1\sigma$ confidence intervals in Figures 1 and 2. Contrary to our expectations, it seems that large samples are not required for good model performance. For `make_classification()` data the accuracy peaks at the sample size 3 and then slowly declines, although that can be considered within statistical error. For `make_hastie_10_2` the accuracy peaks at 8 draws and then stays the same.
- In a similar way, the prior distribution weight $\gamma$ has little influence on the result unless it is too big, at which point performance of the model starts declining. It is probably because the prior distribution is effective on correcting overfitting for infrequent categories, but these categories contribute little to the overall loss function.
- When checking performance on the Mercedes-Benz Greener Manufacturing data, we noticed better generalization of the model that uses sampling techniques compared with traditional target encoding on Kaggle’s public and private sets, even though during the cross-validation we saw only a modest improvement. This demonstrates that the models using Sampling Bayesian Encoder can generalize well on the unseen data.
- Many encoders of the categorical variables are causing the models to put too much importance on the categorical features, which result in poor generalization. To see how Sampling Bayesian Encoder handles this problem we compared feature importances of `RandomForestClassifier` for the models with Target Encoder and Sampling Bayesian encoder. The results are shown in Figure 3. It is indeed clear that Sampling Bayesian Encoder cause the classifier to put much less importance on the categorical variables (labeled 8 and 9), thus reducing target leakage.

6 Conclusion

In this paper we presented a new technique of categorical variable encoding by sampling from the conditional posterior distribution of the target variable given the value of the categorical variable. This method is a logical development of the target encoding methods represented in \cite{1, 4, 6} and is capable of reducing the propensity of Target Encoding and Bayesian Target Encoding to overfit due to the target leakage into the predictor data.
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A Appendices

A.1 Regularization effect of sampling techniques

In this section we consider how the loss function is modified by virtue of using sampling techniques in target encoding of the categorical variable. We will consider a regression case already discussed in section 3.3 and Mean Squared Error (MSE) loss function, which is used to optimize model $\hat{y}_\theta$:

$$
MSE = \frac{1}{N} \sum_n E_{\theta_n \sim p_{\theta_n}(\theta)} \left( y_n - \hat{y}_\theta(\xi_n, f_1(\theta_1),..f_M(\theta_M)) \right)^2 \quad (19)
$$

Expanding the square in (19) and taking expectation of each term, we can represent MSE as a sum of two terms:

$$
MSE = MSE_0 + REG, \quad (20)
$$
where $MSE_0$ is the Mean Squared Error of the point estimate:

$$MSE_0 = \frac{1}{N} \sum_n (y_n - \hat{y}(x_n))^2$$  \hspace{1cm} (21)

and $REG$ is a regularization term:

$$REG = \frac{1}{N} \sum_n \mathbb{E}_{\theta \sim p_m(\theta|y)} \left( \hat{y}_\theta(\xi, f_1(\theta_1), \ldots, f_M(\theta_M)) - \hat{y}(x_n) \right)^2$$ \hspace{1cm} (22)

It represents average difference between $\hat{y}_f$ and the average $\hat{y}_q$ under the encoding distribution $g$. This means that our optimization objective favors models that produce small variance of predictions within the categories. This is in line with LightGBM approach of minimizing intra-category variance, but we have it here as a natural consequence of the sampling technique.

### A.2 Large sample approximation

We can use the property of the large samples, that the parameters of the posterior distribution follow approximately Normal distribution around its maximum a posteriori estimation [12]:

$$(\theta - \hat{\theta}) \sim N(0, C)$$ \hspace{1cm} (23)

The covariance matrix $C$ is derived by Taylor series expansion of the logarithm of the posterior distribution and is the inverse of the information matrix. Applying Taylor series expansion to $\hat{y}_\theta$:

$$\hat{y}_\theta(\xi, \theta) \approx \hat{y}_\theta(\xi, \hat{\theta}) + \nabla_\theta \hat{y}_\theta \delta \theta + \frac{1}{2} \delta \theta^T H(\hat{y}_\theta) \delta \theta,$$ \hspace{1cm} (24)

where $\hat{\theta} = \mathbb{E}_{\theta \sim p(\theta|y)} \theta$ is an expected parameter of the posterior distribution, $\delta \theta = \theta - \hat{\theta}$ and $H(\hat{y}_\theta)$ is a Hessian matrix. Taking expectation of (24) with respect to the posterior, we get an estimate of $\hat{y}$:

$$\hat{y}(x) \approx \hat{y}_\theta(\xi, \hat{\theta}) + \frac{1}{2} \text{tr}(H(\hat{y}_\theta) \cdot C)$$ \hspace{1cm} (25)

The first term can be interpreted as a Target encoding estimate, and the second term is an estimate correction due to intra-category variance.

We can contrast this with a popular technique of adding a Gaussian noise to the maximum a posteriori estimate. Both approaches will produce the same results in large sample approximation if the intra-category variance is the same for all categories. While traditional Target Encoder requires a hyperparameter to control the Gaussian noise, the Sampling Target Encoder learns the variance from data, and can produce better results when this variance is different for different category values.