Predicting return probabilities of an online retailer by machine learning algorithms

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1 Introduction

Recently, the market share of online retailers increased drastically. The economic importance of this sector is reflected in the growth of revenues generated by online retailers: from 24.6 billion Euro in 2012 to 52.8 billion Euro in 2015 (which represents 1.5% of the German GDP at that time)[1]. This development is accompanied by huge logistic efforts. To avoid undesired shipping costs, one challenge of corporate data mining is to reduce these costs to a minimum. Several papers have outlined the importance of data mining in supporting managerial decision making Manyika et al. (2011). There is a broad literature about each step of the data mining process, from data preprocessing Crone et al. (2006) to the design of data mining algorithms Lessmann et al. (2015). The research in this area is undergoing massive transformations due to technological and methodological innovations, e.g. modern storage capacities allow to process huge amounts of data and new statistical methods evolve in order to analyze this data adequately.

In this seminar paper, a case study is presented that comprises the essential tools of corporate data mining in the context of online marketing. A raw data set of an online retailer with 150.000 observations and 13 variables is given; for two thirds of the observations exists a binary *return* variable $y \in \{0, 1\}$ that indicates if a product has been returned by the customer to the retailer (hereafter referred as `train`). The task is to train a model that predicts with high accuracy whether a product of the last third (hereafter referred as `test`) of the data set is likely to be returned or not. In order to support the managerial decision making, these predictions are then used to minimize a loss function that consists of type one error $\mathbb{P}(\hat{y} = 1|y = 0)$ and a type two error $\mathbb{P}(\hat{y} = 0|y = 1)$.

		True Value	
		item kept (0)	item returned (1)
Prediction	item kept (0)	0	$0.5 * -(3 + 0.1 * \textit{item price})$
	item returned (1)	$-0.5 * \textit{item price}$	0

Table 1: cost matrix, consisting of type one and type two errors and depending only on item price

[1]Revenues of Online Retailers in Germany 2015, source: https://de.statista.com/statistik /daten/studie/29201/umfrage/umsatz-im-online-handel-in-deutschland-seit-2008/

This seminar paper is structured as follows: *Section* 2 introduces the data. *Section* 3 provides some examples of feature engineering; *Section* 4 illustrates novel data set preparation techniques. *Section* 5 describes theory and implementation of cross validation; *Section* 6 presents the algorithms, *Section* 7 their parameter tuning and concludes with their performance scores.

2 Data

The data set has been provided by a german online retailer, more information about the retailer is not known. In total, it contains 150.000 observations, each observation reflects an order placed by a customer at the online store. For the whole data set, 13 (not very informative) variables are given, shown in Table 2. For two thirds of the data set (100.000 observations, `train`), a binary `return` variable $y \in \{0, 1\}$ is given that indicates whether the customer returned the product to the online retailer. The goal of this case study is to train various algorithms in order to predict with high accuracy if the orders of the remaining (`test`) third of the data set will be returned by the customer or not.

variable name	type	head	description
order_item_id	int	1, 2, 3, ...	ID of each order placed
order_date	chr	2012-09-04, 2012-11-03, ...	date when order has been placed
delivery_date	chr	2012-09-06, 2012-11-07, ...	delivery date
item_id	int	1507, 1745, 2588, ...	ID of each item
item_size	chr	'unsized', 10, XXL, ...	size of item
item_colour	chr	green, blue, red, ...	colour of item
brand_id	int	102, 64, 42, ...	brand ID
item_price	int	24.9, 75, 79.9, ...	price of item
user_id	int	46943, 60979, 72232, ...	customer ID
user_title	chr	Mrs, Mrs, Mrs, ...	title of customer
user_dob	chr	1964-11-14, 1973-08-29, ...	customer's date of birth
user_state	chr	Rhineland-Palatinate, Brandenburg	shipping destination
user_reg_date	chr	2011-02-16, 2011-05-21, ...	registration date of customers
return	int	0, 1, 1, ...	return variable

Table 2: first look on raw data set, containing 13 variables plus the *return* variable for the *known* data set. Abbreviations: int - integer, chr -character.

3 Feature Engineering

3.1 Definition and explanation of variables

In addition to the usual data cleaning process (treatment of missing values, outliers etc.), it is necessary to extract more information from the raw data set by creating new features. Some of the main newly created features are presented in Table 3.

Feature	**Description**	**Explanation**
item_retrate	Defined for each item as the mean of returns over the observations (in the train set) that share the same item_id (N_{item} is the number of such objects).	Very distinct for different items, for example some products will look different in picture and in real life. So just for being a specific item it will be a little more or less likely to be returned.
delivery_time	Difference in days between the delivery date and order date.	Customers do not like to wait a long time for their orders and are more likely to be unsatisfied over a certain delivery time.
price_comp	Created by assigning the percentage deviation from the average price of the specific item to each purchase.	Let's assume a customer bought an item on sale, it is more likely that he will keep the item with respect to buying it full price.
item_double	Counts when an item is ordered at least twice by the same user.	It is safe to assume the customers' behaviours follow an inductive pattern, which means they will order items that they enjoyed over and over, making those more likely to be kept. On the other hand costumers are known to order multiple items and return the ones which do not fit them.
item_type	Categorises each item through its size.	For example an item whose size is M is unlikely to be a pair of shoes.

Table 3: Overview of the main features that are used for the predictive model.

3.2 The case of `item_retrate`

Let's assume to work on `item_retrate`, the same reasoning is also valid for `user_retrate` with only minor changes and can be extended to a wide class of features.
As seen in Table 3, `item_retrate` is a numerical value for each observation whose `item_id` appears in the train set at least once. For the observations in test set with an `item_id` that does not appear in `train` set (`line 8`), the value of `item_retrate` can not be calculated, therefore the value `new` is assigned (`line 15`). Since most models can not handle mixed class variables, `item_retrate` must be turned into a factor variable.

```
1  item.k = joint.k[, list(item_nr.obs.k = .N, item_retrate = mean(return))
     , by = "item_id"]
2  c = c(0, 0.26, 0.4, 0.56, 0.71, 1.1)
3  tag = c("very low", "low", "normal", "high", "very high")
4  item.k$item_retrate_c = split(item.k$item_retrate_c, item.k$item_retrate
     , c, tag)
5  item.k$item_retrate_c[item.k$item_nr.obs.k <= 15] = "unknown"
6
7  # item_id of items that ordered ONLY in test set
8  new.item = unique(item$item_id[!(item$item_id %in% item.k$item_id)])
9
10 # combine known and general item-matrix
11 setkey(item, item_id)
12 setkey(item.k, item_id)
13 item = item.k[item]
14 item$item_retrate_c[is.na(item$item_retrate_c)] = "new"
15 item$item_retrate_c = factor(item$item_retrate_c, levels = c(tag, "
     unknown", "new"))
```

The `split` function used in `line 4` turns a numerical variable into character. It categorizes all the elements of the column `item.k$item_retrate_c` based on the values of the boundaries given by vector `c` (`line 2`), naming them by the values of `tag`.

3.2.1 Interval boundary choice

For every observation `item_retrate` $\in [0,1]$ is assigned: it is an estimator of the probability that the order will be returned from a random user. It is therefore clear that it is modelled as a Bernoulli trial with

$$P_1 := item\_retrate$$

$$P_0 := 1 - item\_retrate$$

Two questions arise naturally:

1. Is there a reliable way to choose interval boundaries when we need to turn a numerical variable into factor?
   Of course it is preferable to keep numerical variables unchanged, but problems can come up such as novel items in the `test set` for which it is impossible to infer an `item_retrate`, and items which were ordered only one time for which the proposed estimation is clearly not appropriate.

2. In which way does N_{item}, the number of times a particular item appears in the `train` set, influence the reliability and precision of our estimator `item_retrate`?
   Let's introduce a trivial example: if an item is chosen such that $N_{item} = 3$, only four values are possible
   $$item\_retrate \in \left\{0, \frac{1}{3}, \frac{2}{3}, 1\right\}$$
   In this case it would not make much sense to create a category of `item_retrate` between 0.4 and 0.5.

To start with, a first interval can be defined

$$I := \big[0.48 - \alpha, 0.48 + \alpha\big]$$

for some α. Note that I represents the items whose `item_retrate` is within average. In absence of any a priori knowledge about the theoretical distribution of `item_retrate` it is

Frequency	Estimator value
1.5 %	0
9.5 %	$\frac{1}{6} = 0.17$
23.5 %	$\frac{1}{3} = 0.33$
31.0 %	$\frac{1}{2} = 0.50$
23.5 %	$\frac{1}{3} = 0.67$
9.5 %	$\frac{1}{6} = 0.83$
1.5 %	1

Frequency	Estimator value
0.1 %	0
1.0 %	$\frac{1}{10} = 0.1$
4.4 %	$\frac{1}{5} = 0.2$
11.7 %	$\frac{3}{10} = 0.3$
20.5 %	$\frac{2}{5} = 0.4$
24.6 %	$\frac{1}{2} = 0.5$
20.5 %	$\frac{3}{5} = 0.6$
11.7 %	$\frac{7}{10} = 0.7$
4.4 %	$\frac{4}{5} = 0.8$
1.0 %	$\frac{9}{10} = 0.9$
0.1 %	1

Table 4: Classification outcomes for $N_{item} = 6$ (left) and $N_{item} = 10$ (right).

advisable to select α so that

$$\#\{x \in train \mid item\_retrate(x) \in I\} = \frac{nrow(train)}{t}$$

where t is the number of quantiles and depends on N_{item}; x represents an observation.

In this setting the mean returns calculation can be modelled as one repetition of N_{item} independent Bernoulli trials, therefore following a binomial distribution.

As a first approach the theoretical $P_1 = \frac{1}{2}$ and number of Bernoulli trials 6 are chosen, a local upper bound for the percent correct estimation of P_1 through `item_retrate` is found.

For a binomial distributed random variable X holds

$$\mathbb{P}(X = k) = \binom{n}{k} p^k (1-p)^{n-k}$$

Since the function

$$(p^n)(1-p)^n$$

has maximum for $p = \frac{1}{2}$ for every $n \in \mathbb{N}$, we have that 31% (Table 4, left) is a local maximum in a neighbourhood of $\frac{1}{2}$. This means that there is a local upper bound for percentage successful estimation of P_1 of only around 31% for an interval $[0.4, 0.6]$. Rising N_{item} to 10 can improve this result (see right side of Table 4).

This means that the local maximum success estimation of P_1 already raised to 65.6% $(= 20.5\% + 24.6\% + 20.5\%)$ of the times for the same interval $[0.4, 0.6]$.

In conclusion it is better to raise N_{item} whenever feasible, in this case until too many `item_retrate` are placed in the `unknown` category. The final choices are $N_{item} \geq 15$ (`line`

5) and $t = 5$ (+2) (`lines 2,3 and 16`) for `item_retrate` ; $N_{item} \geq 6$ and $t = 5$ for `user_retrate`.

The categories of `item_retrate` are presented in Table 5. Their distribution in Figure 2.

category	very low	low	average	high	very high	unknown	new
mean return	[0,0.26)	[0.26,0.4)	[0.4,0.56)	[0.56,0.71)	[0.71,1]	$N_{item} < 15$	item_id

Table 5: Definition of tau categories. Every order is sorted to an tau category, depending on the price of the item that got ordered.

3.3 Weight of Evidence

A method to measure the meaningfulness of a feature is the Weight of Evidence (WOE).

$$WOE(category) := ln\left(\frac{\mathbb{P}(return = 1 \mid item\_retrate = category)}{\mathbb{P}(return = 0 \mid item\_retrate = category)}\right)$$

The WOE of the variable `item_retrate` is shown in figure 1. Since the feature `item_retrate` was developed by considering the rate of return in the past, the WOE follows the anticipated logarithmic conduct for the categories `very low` to `very high`. An WOE $= 0$ denotes an average chance of return, which is especially the case for the `normal` category. Also `unknown` and `new` have an WOE around zero, since it is not possible to deduce their previous return rate.

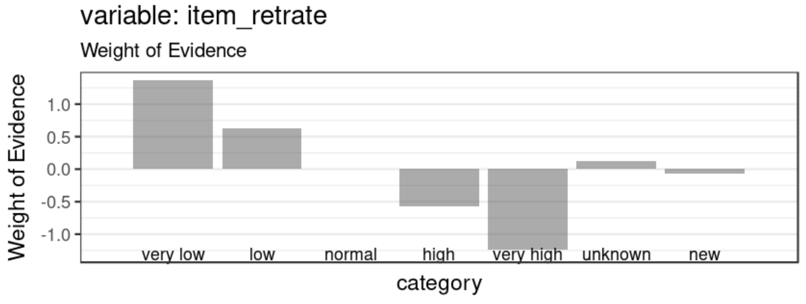
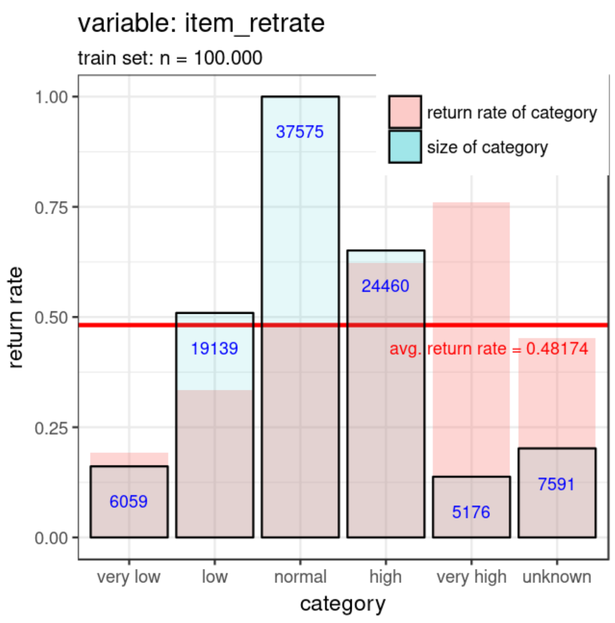
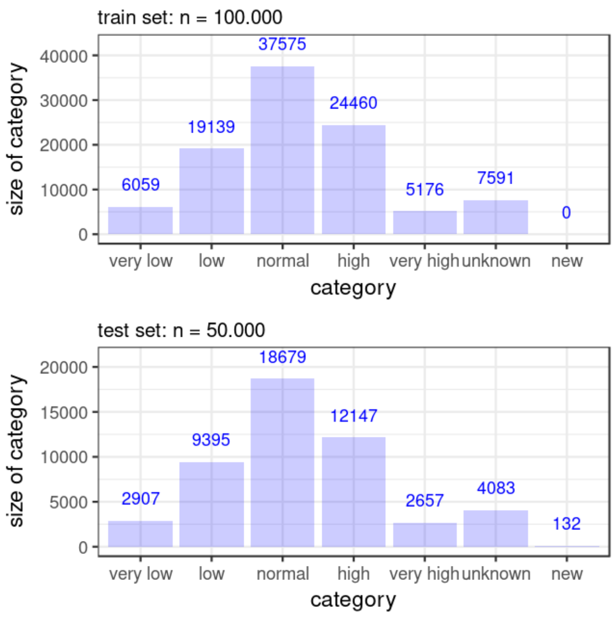


Figure 1: Weight of Evidence (WOE) of the feature `item_retrate`. Categories "very low" to "very high" were created by grouping the items according to their return rate in the training set. This created a strong feature in terms of WOE.



(a)



(b)

Figure 2: (a) Display of the artificially created feature `item_retrate`. red shading: average return rate of observations of this category with comparison to average return rate of all items in `train` set (red line, avg.returnrate = 0.48174). blue histogram: number of observations in each category. (b) Distribution of variable `item_retrate` in `train` and `test` set. In both data sets the newly created variable follows a similar distribution.

3.4 semantic grouping: the case of `item_type`

High cardinality attributes are impractical for most predictive algorithms. The original data set contained the variable `item_size`, which overall consists of more than 100 categories. Even after merging duplicate naming such as (... xs, s, m, l, ...) and (... XS, S, M, L, ...), the variable is still of high cardinality. One method of reducing the categories of a variable is semantic grouping (c.f. Moeyersoms and Martens (2015)). Categories were generated with respect to common sizing systems for shoes and clothes. Additionally the category `rest` stores items that could not be allocated to `shoes` or `clothes` and `unsized` stores items without a specific size. By using semantic grouping it was not only possible to reduce over 100 categories to only four, but also a difference in the return rate of the categories can be observed. Figure 3 shows that `unsized` has a considerably lower return rate than average (Also the return rate of `rest` is lower than average, but because of the small size of the category it will not add much information to the model.)

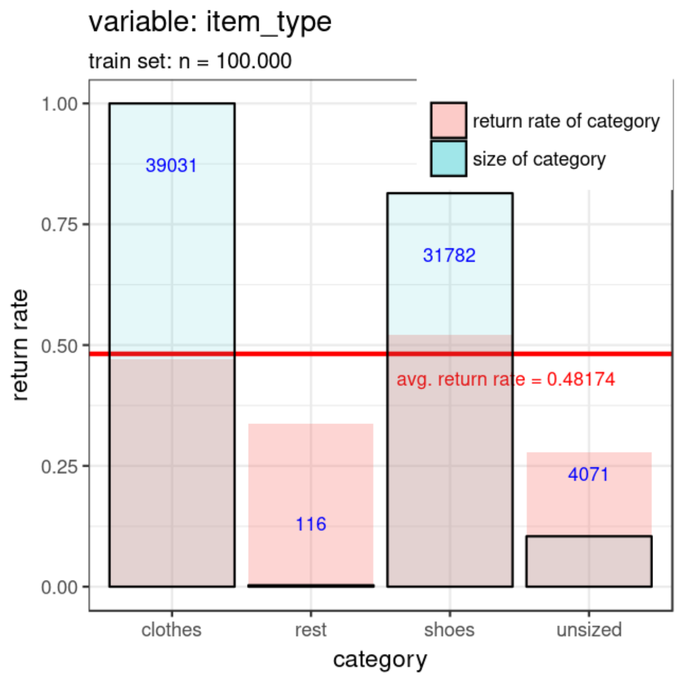


Figure 3: Display of the artificially created feature `item_type`. red shading: average return rate of orders in this categories in training set. blue histogram: number of orders of each category.

```
shoes = c(30:48, paste(35:46, "+", sep = ""),
          1:9, paste(1:12, "+", sep = ""))
clothes = c("xs", "s", "m", "l", "xl", "xxl", "xxxl",
            "XS", "S", "M", "L", "XL", "XXL", "XXXL",
            100:176)
unsized = c("unsized")

item$type                              = "rest"
item$type[item$item_size %in% shoes]    = "shoes"
item$type[item$item_size %in% clothes]  = "clothes"
item$type[item$item_size %in% unsized]  = "unsized"
```

4 Preparation of Data Set for Models

4.1 Decomposition due to uncertain categories

When creating the variables `item_retrate` and `user_retrate` (section 3.2), it is only justified to infer from items/user that occur more than 15/6 times (explanation see 3.2.1). All remaining items/user were stored in the category `unknown`. However, this category can not be treated like the categories `very low` to `very high` that are directly connected to the previous return rate of the item/user. To ensure that the predictive algorithm does not treat the category incorrectly, the data set gets decomposed into certain and uncertain subsets, as shown in Table 6. The decomposition ensures that in each subset the remaining columns are "pure" (do not contain category `unknown` or `new`). For example subset `.u` (second row) is the subset, where the column `user_retrate` got removed and `item_retrate` contains only certain categories.

```
# .u        : model without user_retrate
# remove    : "unknown" and "new" of "item_retrate"
# model     : item_retrate is clean now, can be used for model
known.u     <- known[item_retrate!="unknown" & user_retrate=="unknown",]
unknown.u   <- unknown[item_retrate!="unknown" & item_retrate!="new",]
unknown.u   <- unknown.u[user_retrate=="unknown" | user_retrate=="new",]
```

Therefore the model is trained on this subset without the feature `user_retrate` and accordingly predicts the `unknown.u` subset. Actually for training the model not only the `known.u` subset can be used, but also the `known.f` subset, since it is only important that the remaining columns are pure.

user_retrate	**item_retrate**	**rest**	**model**	**size (train/test)**
1	1	1	.f - full model	25266 / 10082
u/n	1	1	.u - without user_retrate	67143 / 35703
1	u/n	1	.i - without item_retrate	1857 / 813
u/n	u/n	1	.iu - without item_retrate and user_retrate	5734 / 3402

Table 6: Decomposition of data set due to uncertain categories. u/n stands for `unknown` and `new` categories (= uncertain categories), 1 for certain categories. Categories `unknown` and `new` in `item_retrate` and `user_retrate` are uncertain and should not be included in models. Decomposition in pure subsets ensures that model only is fed with certain categories.

In total four models get trained and used for prediction (full model, without `item_retrate`, without `user_retrate`, without `item_retrate` and `user_retrate`). This decomposition increased the performance from $loss_{full} = -243104.7$ and $AUC_{full} = 65.27\%$ to $loss_{dec} = -239499.7$ and $AUC_{dec} = 66.52\%$ (with a tuned neural network).

4.2 On multiple τ thresholds

By observing the given loss table for this specific task (see Table 1), it is evident that depending on item price, type 1 errors can be more penalising than type 2 errors and vice versa. In order to optimise the results, an analysis of its explicit dependence from item_price is due.

The essential boundaries of when type 1 and type 2 errors are equally relevant are to be assessed, resulting in a meaningful first split of the data. In most cases $\tau < 0.5$ and $\tau > 0.5$ are found to be optimal when type 2 error loss is bigger and smaller than type 1 error loss respectively.

For this particular case study only one boundary is to be found because it is the root of a grade 1 polinomial

$$\Delta := -0.5 \cdot 5(3 + 0.1 \cdot X) + 0.5 \cdot X \tag{1}$$

To decrease the loss even further, a split of the `train` and `test` sets depending on `item_price` is a natural extension of this first remarks. The difference of type 2 and type 1 error magnitudes Δ is a linear function of `item_price` so a split in a quantilelike way is recommended, but with one of the boundaries being 30 euros (see equation 1).

tau category	1	2	3	4	5	6
item_price	[0,30)	[30,59)	[59,79)	[79,90)	[90,120)	[120, max(item_price)]

Table 7: Definition of tau categories. Every order is sorted to an tau category, depending on the price of the item that got ordered.

Implementing this dependence in the cross validation code is essential not only to be able to estimate accuracy through AUC (and other measures) and tune parameters , but also to

obtain an estimate of the specific total loss of a prediction.
Running the cross validation for each of

$$T_k := \{observation \in Split.Train \mid \tau = k\}$$

produces significantly different optimal values for τ, which is a confirmation of what was expected from the above reasoning.

5 Cross Validation

5.1 Theory

Let's assume to be in one of the following situations:

- the prediction algorithm of choice has a variety of parameters that need to be tuned, which means optimised in order to improve accuracy (or any other measure of goodness)
- performances of a group of completely different models need to be assessed and ranked for selection purposes

Cross validation is a widely (if not the most) used class of methods to assign to each different model an estimate of their "goodness". A great asset of cross validation is that it offers the flexibility to choose the most appropriate measure of goodness, depending on the situation. Such measures can be the very intuitive accuracy, the ever popular AUC or, as in this paper's case study, a customised function depending on a loss matrix (in this case Table 1).
The class of Cross Validation (CV) methods contains, among others:

- K-fold CV
- leave-one-out CV (limit case of K-fold for $K := \#\{training\ \ set\}$)
- stratified K-fold CV
- N-repeated stratified K-fold CV

The method that was chosen for this study is a 6-repeated stratified 3-fold CV, which offers a good balance between accuracy and computational intensity.

N-repeated stratified K-fold C.V.

Suppose a training set T is given so that every $(v_i, y_i) \in T$ is of the form $(v_{1,i}, .., v_{u,i}, y_{1,i}, .., y_{v,i})$ where u is the number of explanatory variables, v is the number of outcomes.

Definition 5.1. *A subset $T_k \subset T$ is called a stratified K-fold of T if*

1. *their cardinalities follow relation*

$$\#T_k = \left\lfloor \frac{\#T}{K} \right\rfloor$$

2. *is picked randomly from the family of subsets of T such that*

$$\mathbb{E}_{T_k}[y] = \mathbb{E}_T[y]$$

First of all $\forall k \in 1, .., K$ a stratified K-fold T_k of T is taken. A model prediction will be called $\hat{M}(\cdot, \theta)$ for simplicity and in order to stress its dependence from the parameter θ to be tuned. Note that $\hat{M}(\cdot, \theta)$ could be interpreted as a total different model prediction $\hat{M}_\theta$ as well.
The second step consists in training the model on $T \backslash T_k \ \ \forall \theta_i \in \Theta$ the parameter candidates set (from now on we use the simplified notation $\hat{M}_k(\cdot, \theta) := \hat{M}_{T \backslash T_k}(\cdot, \theta)$). Finally $\forall (v_j, y_j \in T_k$

$$L(\hat{M}_k(v_j, \theta_i), y_j)$$

is calculated and the results summarised in the following way (C.f. Tibshirani and Tibshirani (2009))

$$CV(\theta) := \frac{1}{\#T} \sum_{k=1}^{K} \sum_{j \in C_k} L(\hat{M}_k(v_j, \theta), y_j)$$

For minimisation and maximisation reasons the multiplication by $\frac{1}{\#T}$ is irrelevant so it can be omitted.

5.2 Implementation

Script `00-1-kfold.R` performs k-fold cross validations for n variations of settings for a neural network. In order to perform a k-fold cross validation, the dataset is randomly split into k

subsets folds(`line 5`). For every run i of the k-fold cross validation subset `folds==i` is left out for prediction, which means that the model is trained on the subset without `folds==i` and the prediction is performed on subset `fold==i`. This split is performed in `lines 17-22`, followed by training the model (`line 24`) and prediction (`line 29`). Note that the second index n indicates the settings for the neural network (`line 27+28`). This index n is changed by the outer foreach-loop (`line 11`).
To evaluate the performance of the model, the loss **??** is used as a measure (`line 30`).

In order to decrease run time, the script uses the package `"doParallel"` for parallel computing. `Lines 7-9` define the settings for parallel computing. In line 14 the nesting operator `%dopar%` starts parallel computing, so that different runs of the foreach-loop can be performed by a different cores at the same time.
The output of the k-fold cross validation is a k*n matrix (k: k-fold cross validation, n: number of variations of settings for model), where every element consists of a list of the measure and the settings of the model (`line 36`).

```
1  # 00-1-kfold_cv.R
2  k = k                # dimension of cv is choosen in parent script
3  sample.idx = sample(nrow(tr.v))
4  train.rnd  = tr.v[sample.idx,]
5  folds      = cut(1:nrow(train.rnd), breaks = k, labels = FALSE)
6  # settings for parallel computing
7  nrOfCores = detectCores()
8  cl         = makeCluster( max(1,detectCores()-1))
9  registerDoParallel(cl)
10 # loops for cross validation and tuning
11 results.par = foreach(n = 1:nrow(parameters), .combine = cbind,
12                       .packages = c("caret", "nnet", "data.table")) %:%
13     foreach(i = 1:k,
14             .packages = c("caret","nnet", "data.table")) %dopar%{
15         set.seed(1234) # set seed for reproducibility
16         # Split data into training and validation
17         idx.val   = which(folds == i, arr.ind = TRUE)
18         cv.train = train.rnd[-idx.val,]
```

```
        cv.train = cv.train[order(cv.train$order_item_id),]
        cv.val   = train.rnd[idx.val,]
        cv.val   = cv.val[order(cv.val$order_item_id),]
        price    = real_price$item_price[cv.val$order_item_id]
        # train nnet and make prediction
        nnet     = nnet(return~. -order_item_id - tau,
                        data  = cv.train,
                        trace = FALSE, maxit = 1000,
                        size  = parameters$size[n],
                        decay = parameters$decay[n])
        yhat.val = predict(nnet, newdata = cv.val, type = "raw")
        loss     = helper.loss(tau_candidates = tau_candidates,
                               truevals       = cv.val$return,
                               predictedvals  = yhat.val,
                               itemprice      = price)
        pars     = data.table("size"  = parameters$size[n],
                              "decay" = parameters$decay[n])
        res      = list("loss"        = max(loss),
                        "parameters"  = pars)
        }
stopCluster(cl) # stop parallel computing
```

Since the performance of the model also depends on the 'quality' of the training data and the training data is determined randomly, it is crucial to change the randomness of the splits. By varying the seed `set.seed(1234*t)` in the mother script `00-2-rep_cv.R` , the randomness of the training set tr is changed (`line 11-16`).

Further this script `00-2-rep_cv.R` splits the dataset according to the six tau-categories (see Table 7). The k-fold cross validation from the previous section is then performed for every of these subsets. The results for each tau-category `v` are then stored in a list `tau_c` (`line 22`).

The output of the m-times repeated cross validation is a list of m times the same cross validation procedure (only with different randomness). Each element of the m-sized list is a list of the k*n matrix for the six tau-categories v.

(m : number of repeated cross validations (same procedure but different randomness), v : six tau-categories, k : k-fold cross validation, n : number of variations of settings for model)

```r
tau_c   = list()
cv.list = list()

for (t in 1:m){
    set.seed(1234*t)
    # Splitting the data into a test and a training set
    idx.train = caret::createDataPartition(y = known$return, p = 0.8, list = FALSE)
    # Actual data splitting
    tr = known[idx.train,  ] # training set
    ts = known[-idx.train, ] # test set
    for (v in 1:6){
        # call script for each tau-class
        tr.v = tr[tr$tau == v, ]
        print(paste("tau =", v, "rep = ", t))
        source(file = "./nnet/00-1-kfold_cv.R")
        tau_c[[paste("tau_c ==", v)]] = results.par
  }
  cv.list[[t]] = tau_c
}
```

Section 4.1 explains the importance of decomposing our dataset into four subsets according to the explanatory power of the features for training. In script `01-par-tuning.R` the whole tuning-process is performed for the different subsets. The following explains the preparation of the `.u` subset exemplarily.

The known dataset consists of the subsets where a full model can be trained (`.f`) and the subset where the model without `user_retrate` can be trained (`.u`). These two subsets are combined to the known data set (`line 51`). For training a neural network additional data preparation as described in section 6.3.2 is necessary (`line 54`). Then the columns of the feature `user_retrate` get removed and the set is named according to the requirements of the script for cross validation (`lines 55-59`).

After performing the m times repeated k-fold cross validation for the n variations of settings for the model, the results are stored in a the list `cv.list.u` for further evaluation (`line 71`).

```
known   = rbind(known.f, known.u) # can also use .f for training,
  variables are pure
unknown = unknown.u               #
# additional data preparation for nnet
source(file = "./nnet/00-3-nnet_DataPrep.R")
known.n$user_retrate   = NULL     # remove user_retrate (uncertain
  categories)
unknown.n$user_retrate = NULL     #
                                  #
known   = known.n                 # output of additional data
  preparation
unknown = unknown.n               #

# perform repeatet cross validation
source(file = "./nnet/00-2-rep_cv.R")
cv.list.u   = cv.list             # store result of repeated cross
  validation
```

6 Classification Alogrithms

6.1 Extreme Gradient Boosting

Extreme Gradient Boosting is a gradient boosting decision tree algorithm, which may be implemented in R via the package `xgboost` by (Chen and Guestrin, 2016) Boosting refers to an additive training technique where starting with some base classifiers $\hat{y}^{(0)} = f_0(x_0)$, an objective function $F(y, f_k)$,

$$F = \sum_{i=1}^{N} l(y_i, \hat{y}_i) + \sum_{k=1}^{K} \Omega(f_k)$$

that consists of a training loss term $l(y_i, \hat{y}_i)$ and a regularization term $\Omega(f_k)$ gets optimized by adding at each iterative stage a term to the classifier function that compensates for the errors of the previous model.

$$
\begin{aligned}
\hat{y}^{(0)} &= 0 \\
\hat{y}^{(1)} &= \hat{y}^{(0)} + f_1(x_1) = f_1(x_1) \\
\hat{y}^{(2)} &= \hat{y}^{(1)} + f_2(x_2) = f_1(x_1) + f_2(x_2) \\
&\vdots \\
\hat{y}^{(t)} &= \sum_{k=1}^{K} f_k(x_k) = \hat{y}^{(t-1)} + f_t(x_t)
\end{aligned}
$$

This sequential procedure stops when no further improvements can be made, e.g. when the reduction of the loss term is smaller then the change in the regularization term.

Various parameters can be tuned [2], :

1. `n_rounds`: number of trees that were sequentially created. Several values were tested, e.g. 50, 100 or 500
2. `eta`: learning rate - how far we go into the direction of the gradient (the gradient is used in the Taylor approximation of the objective function). Values used for tuning: 0.01, 0.1, 0.15
3. `min_child_weight`: minimum number of observations in a node to make a split. Ususally set to 1.

6.2 Random Forest

A random forest is an ensemble of tree classifiers with implemented randomisation procedures. Random forest tends to be good out of the box and apt for parallelization. The model default parameters are (c.f. Breiman (2001))

1. `m_tree`: $(\#features) \cdot \frac{1}{3}$ for regression, $(\#features)^{1/2}$ for classification
2. `n_tree`: 500
3. `nodesize`: 1 (for classification), 5 (for regression)

[2]https://cran.r-project.org/web/packages/xgboost/index.html

Definition 6.1. *A tree-structured classifier $h_{\theta_k}(\boldsymbol{x})$ is a generalised step function $h_{\theta_k} : \boldsymbol{X} \to F \subset \mathbb{R}$ where $\boldsymbol{X}$ is the data set and F is a finite cardinality set. This function has constant values on a partition of the data set consisting of hyper-rectangles.*

Note that θ_k indicates how to create such a partition by determining

1. predictors to split on
2. values of the splits
3. depth of the tree

where the first is a randomly chosen subset of the parameters of cardinality equal to `m_tree` in the `random.Forest` package, the second is chosen in order to maximize information gain, the third corresponds to `n_tree` in `random.Forest`.
The concept of generalization error for a random forest was first presented in Breiman (2001). The following passage represents a selection of theory introduced in that article.

Definition 6.2. *Let $\{h(\boldsymbol{x}, \theta_k) \mid k \in \overline{n}\}$ be a collection of tree-structured classifiers where θ_k are i.i.d. random vectors. A random forest is the classifier for which each tree casts a unit vote for the most popular class at input $\boldsymbol{x}$.*

For notation simplicity purposes, from now on, $h(\mathbf{x}, \theta_k)$ can be replaced with $h_k(\mathbf{x})$ and viceversa.

Definition 6.3. *Given $\{h_k(\boldsymbol{x}) \mid k \in \overline{K}\}$, with training set drawn at random from the distribution $\boldsymbol{X}$ and realisation Y through $h(\cdot)$, the margin function is*

$$mg(\boldsymbol{X}, Y) = \sum_{k=1}^{K} \frac{I(h_k(\boldsymbol{X}) = Y)}{K} - \max_{j \neq Y} \sum_{k=1}^{K} \frac{I(h_k(\boldsymbol{X}) = j)}{K}$$

where $I(\cdot)$ is the indicator function.

The margin measures the proportion of the average votes for the right class and the average vote for any other class. Larger margin values mean a more reliable classification.

Definition 6.4. *We will call generalization error*

$$\mathbb{P}(mg(\boldsymbol{X}, Y) < 0)$$

where the probability is over the $(\boldsymbol{X}, Y)$ *space.*

For a large number of trees the following result hold:

Theorem 6.1. *As the number of trees* K *increases, the generalization error converges almost surely to*

$$\mathbb{P}_{\boldsymbol{X},Y}(\mathbb{P}_\theta(h(\boldsymbol{X}, \theta) = Y) - \max_{j \neq Y} \mathbb{P}_\theta(h(\boldsymbol{X}, \theta) = j) < 0)$$

which assures the method does not overfit for big ensembles of trees.

Proof. By definition of almost sure convergence, it suffices to show that there is a set of probability zero C on the sequence space $\{\theta_k \mid k \in K\}$ such that outside of C, $\forall x$,

$$\sum_{k=1}^{K} \frac{I(h(\mathbf{x}, \theta_k) = j)}{K} \to \mathbb{P}_\theta(h(\mathbf{x}, \theta) = j)$$

For a fixed training set and fixed θ , $\{x \mid h(x, \theta) = j\}$ is a union of hyper-rectangles. This follows from the definition of tree-structured classifier. Moreover, $\forall\ h(x, \theta)\ \exists!\ T < \infty$ number of such unions of hyper-rectangles, denoted by $S_1, ..., S_T$. Define $\phi(\theta) = t$ iff $\{x \mid h(x, \theta) = j\} = S_t$. Let K_t be the number of times that $\phi(\theta_k) = t$ in the first K trials. Then

$$\sum_{k=1}^{K} \frac{I(h(\mathbf{x}, \theta_k) = j)}{K} = \sum_{t} \frac{K_t I(x \in S_t)}{K}$$

By the Strong Law of Large Numbers, $\exists\ \theta$ such that

$$K_t = \sum_{k=1}^{K} \frac{I(\phi(\theta_k) = t)}{K} \to \mathbb{P}_\theta(\phi(\theta) = t)$$

almost surely. By definition of a.s. convergenceTaking unions of all the sets on which convergence does not occur for some value of k gives a set C of zero probability such that outside of C,

$$\sum_{k=1}^{K} \frac{I(h(\mathbf{x}, \theta_k) = j)}{K} \to \sum_{t} \mathbb{P}_\theta(\phi(\theta) = t) I(x \in S_t)$$

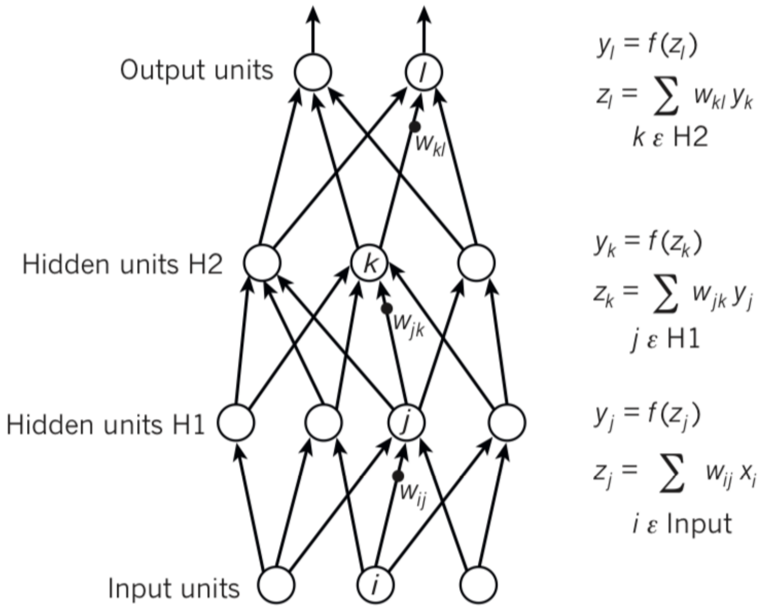


Figure 4: An example of a neural network structure map. In this particular case there are three input variables, two hidden layers consisting of four and three neurons respectively and two output variables. Note that in the *nnet* R-package there is only one hidden layer. Source: LeCun et al. (2015)

The right hand side is $\mathbb{P}_\theta(h(\mathbf{x}, \theta) = j)$ $\square$

6.3 Neural Network

Neural networks were first developed in the middle of the twentieth century, had great importance for a few decades and then overshadowed by other algorithms such as support vector machines in the later decades of the last century until they were discovered to be great in performance when paired with backpropagation for unsupervised learning. The idea behind this category of algorithms is that most real life problems are highly non linear, and therefore standard models such as linear regression will not be suited for approximation of reality. The way this class of algorithms work is calculating numerous weighted linear combinations of the input variables and applying a non linear function to it. This procedure is repeated multiple times depending on the design of the network, each of these basic operation is called a neuron. The group of neurons on a same level is called hidden layer, there can be multiple hidden layers each performed taking the outputs of the previous one (altough the *nnet* package uses only one, see Figure 4). Neural networks not only depend on the number of neurons for each hidden layer (this is called *size* in *nnet* package), number of layers and definition of input variables for each neuron. In fact they are defined also by which nonlinear function is applied in each neuron: the traditionally used are sigmoid functions such as hyperbolic tangent and logistic function,

$$f_1(t) := \tanh(t) \quad f_2(t) := \frac{1}{1+e^{-t}}$$

the latter being used in the *nnet* package. The reason for the application of such functions for each elementary step is an attempt to linearise the boundary of highly nonlinear sets.

6.3.1 Backpropagation

Backpropagation is one of the milestones of the development of neural networks and plays a fundamental role especially for deep networks, which consist of multiple hidden layers. This process aims to find out the most appropriate weights $w_{i,j}$ for the construction of each neuron in the net (see Figure 4). To start with an objective function, generally a loss function, is differentiated and used as in Figure 5 together with the chain rule to find partial derivatives of the error function with respect to the weights $w_{i,j}$ for each stage and using gradient descent method with learning rate η (which is often associated with the parameter *decay* in *nnet*) to define new weights

$$\hat{w}_{i,j} := w_{i,j} - \eta \frac{\partial E}{\partial w_{i,j}}$$

One might think that local minima might be a problem, luckily *"Regardless of the initial conditions, the system nearly always reaches solutions of very similar quality. Recent theoretical and empirical results strongly suggest that local minima are not a serious issue in general."* (C.f. LeCun et al. (2015)). Once the weights and structure of the network are determined it is a mere substitution that will produce the results for each different input.

6.3.2 Additional Data Preparation

The performance of neural networks increases, when the data is numerical (instead of categorical). Different techniques can be used to convert a categorical variable to a numerical, but not every technique is suitable for every case.
Since item_retrate and user_retrate are based on their connection to the target variable, assigning the Weight of Evidence (WOE) to each category does not aggravate overfitting even more. The WOE is also used for the categories of delivery_time and price_comp, but to prevent overfitting, the WOE was calculated on a small subset of the train set, that is

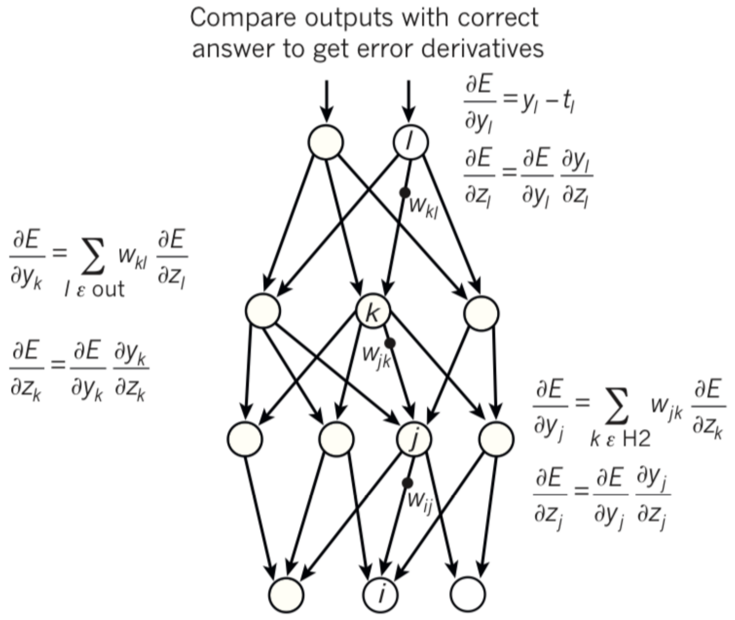

Compare outputs with correct answer to get error derivatives
$\frac{\partial E}{\partial y_l} = y_l - t_l$
$\frac{\partial E}{\partial z_l} = \frac{\partial E}{\partial y_l}\frac{\partial y_l}{\partial z_l}$
$\frac{\partial E}{\partial y_k} = \sum_{l \in \text{out}} w_{kl}\frac{\partial E}{\partial z_l}$
$\frac{\partial E}{\partial z_k} = \frac{\partial E}{\partial y_k}\frac{\partial y_k}{\partial z_k}$
$\frac{\partial E}{\partial y_j} = \sum_{k \in \text{H2}} w_{jk}\frac{\partial E}{\partial z_k}$
$\frac{\partial E}{\partial z_j} = \frac{\partial E}{\partial y_j}\frac{\partial y_j}{\partial z_j}$
w_{kl}
w_{jk}
w_{ij}
l
k
j
i

Figure 5: Diagram on how the backpropagation procedure is carried out. Starting from the error $y_l - t_l$, the chain rule of derivatives is used to explicit a variation in the error as function of variations in the input variables. Note that the error is taken as the differentiation of a loss function: in this case $\frac{1}{2}(y_l - t_l)^2$. Source: LeCun et al. (2015)

not going to be used for training anymore (c.f.Moeyersoms and Martens (2015)):
If the variable only has few categories, it is beneficial to introduce dummy variables. Instead of having one variable item_type with four categories, there will be four binary dummy variables that indicate whether the item is of this category.
The advantage of dummy variables is, that they are independent of the target variable but since every category requires a new dummy variable, they should only be used for lower dimensional variables (c.f. Moeyersoms and Martens (2015)).

7 Parameter Tuning

7.1 Parameters of Neural Network

To increase the performance of a model it is vital to use the optimal parameter depending on the input data. Since the data set is decomposed into four subsets, that differ in the composition of predictive variables (see section 4.1), the tuning needs to be performed on every subset separately. In the following the subset test.u (model without the variable user_retrate) is evaluated exemplarily.
The results of the parameter tuning are shown in Figure 6. The data set was divided into six subsets according to their tau-categories (see section 4.2). The tuning parameters are as follows: size of the hidden layer: [3, 5, 7, 9, 11, 13, 15] and decay: [0.01, 0.1, 0.5, 0.8, 1.0].

index	1 - 7	8 - 14	15 - 21	22 - 28	29 - 35
decay	0.01	0.1	0.5	0.8	1.0
size	3, 5, 7, 9, 11, 13, 15	3, 5, 7, 9, 11, 13, 15	3, 5, 7, 9, 11, 13, 15	3, 5, 7, 9, 11, 13, 15	3, 5, 7, 9, 11, 13, 15

Figure 6 shows that for every tau-category the loss is more stable for larger decay values. For higher decay values, the size of the hidden layer has only marginal influence on the loss. Hence it is not necessary to find the exact optimal parameter for every tau-category and train a separate model on this category (within a certain range of parameters). Further it is even beneficial to refrain from splitting into tau-categories, and instead training only one model with almost optimal parameters on the whole dataset. Then the training data carries sixfold as many observations which enables a better training of the neural network.
The sum of the six normed tuning graphs of Figure 6 is shown in Figure 7. The almost optimal parameters are extracted from the maximum of the loss. (index 25 $\rightarrow$ size of hidden layer: 9, decay: 0.8).
In order to increase the reliability of the tuning results, they were calculated of a 3-fold cross validation, that got repeated 6 times (ensuring that the datasets are sampled differently).

7.1.1 optimal τ for loss function

With the parameters from the previous section (7.1), the neural network has optimal performance for our needs. As a last step the threshold value τ (which is the threshold that decides if the predicted probability is big enough to be assigned as 1 (item is returned) or stays 0 (item is not returned)) needs to be tuned to minimize the loss function. As described in section 4.2, the loss depends on the item price and therefore the data set is split into six subset according to the price (subsets are called tau-categories).
Figure 8 displays the loss function for the six tau-categories. In each category the loss is calculated for each possible τ value. The function reaches its maximum in the range between $\tau = 0.45$ and $\tau = 0.65$, depending on the category. The maximum of the function is the optimal τ that minimizes the loss of the subset. It is not surprising that for categories 1 to 6 (where 1 are cheapest and 6 most expensive items (see 4.2)) the optimal τ increases.

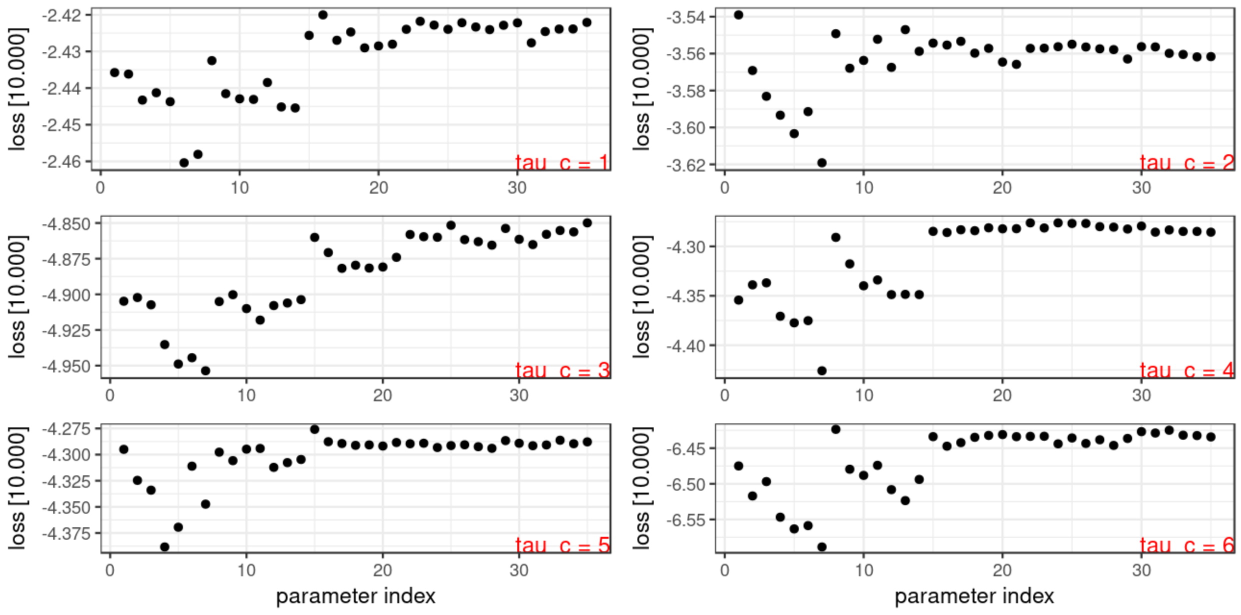


Figure 6: Tuning graph for the six different subsets (according to tau categories). For every subset 35 different models were trained and the loss of each prediction calculated. The settings change as follows: size = 3, 5, ... , 15 then dacay = 0.01, 0.1, 0.5, 0.8, 1.0. Stable loss values for bigger decays, size does not have much influence for high decay values.

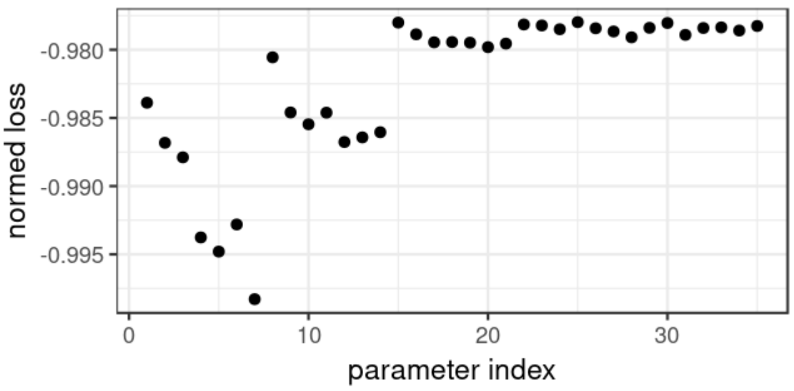


Figure 7: Sum of normed tuning graphs of the six subsets from graph 6. Loss is the highest for bigger decay values. Size only has little influence on loss values for high decay values.

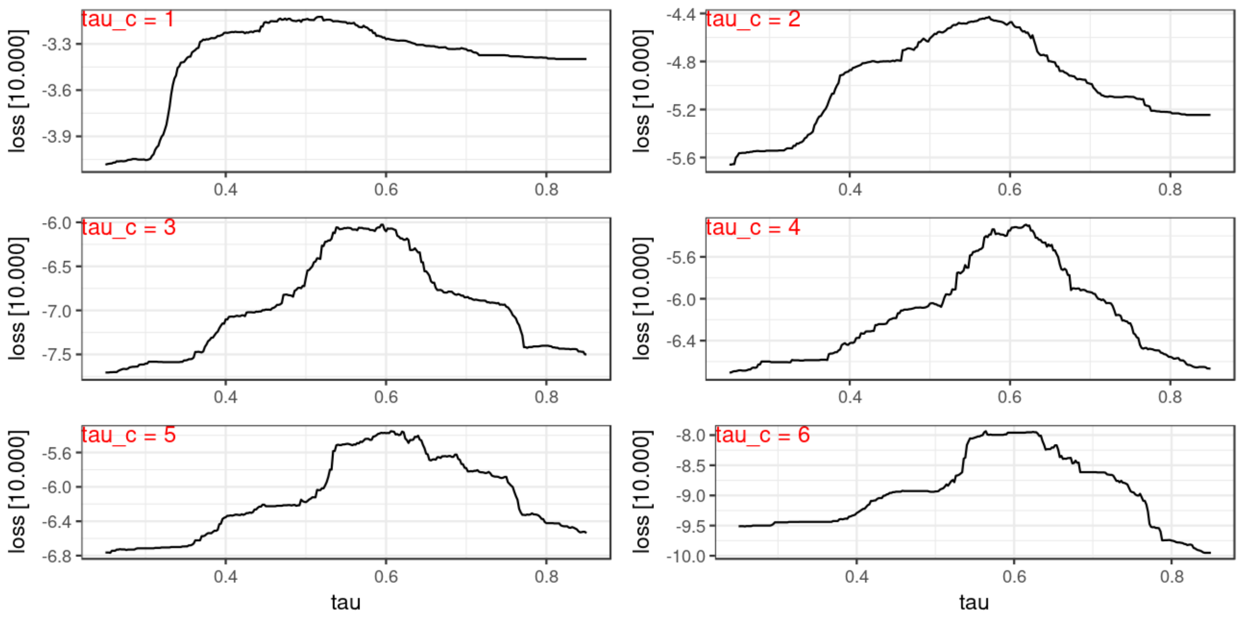


Figure 8: Loss function for the six tau-categories. In each category the loss is calculated for each tau-candidate. The negative loss shows its maximum in the range between $\tau = 0.45$ and $\tau = 0.65$.

(Interpretation of τ in connection to item price and return probability in section 4.2.)

7.2 Performance Benchmark

The following table shows how neural network outperformed random forest and xgboost in this problem for a set of 25000 observations. Double values are expected in the test set, which contains 50000 observations.

Prediction	**Estimated total loss**
trivial 1 (vector consisting of ones only)	-415415.6
trivial 0 (vector consisting of zeros only)	-321240.2
random 01 vector with *mean* $= 0.48$	-365703.9
first randomForest ($\tau = 0.5$)	-321420.5
tuned randomForest (optimised multiple τ)	-260608.5
tuned xgboost (optimised multiple τ)	-290419.9
tuned nnet (optimised multiple τ)	-239499.7

Table 8: Estimated total loss of random forest, xgboost and nnet in comparison to trivial predictions. Performed on 25000 observations (25% of train set.

7.3 Prediction

In order to construct values for a comparison of the performance on the `test` dataset, the prediction is run on the `train` dataset. Therefore the `train` dataset is randomly split (with stratification, see section 5.1) into a new training and test dataset. After training and predicting with the four models (`.f, .u, .i` and `.iu`), the loss is $loss_{dec} = -238879.0$ and the average return rate of the prediction lies at 39.9%.
On the test dataset the predicted average return rate is $39,4\%$, which is similar to our test-run. The loss can not be computed, since the true return is unknown.

8 Conclusion

In this case-based analysis, we developed two predictive models from start to finish. Starting with the data cleaning process through training and tuning several classifiers up to the incorporation of the loss function into the cross validation. The work presented in this paper only reflects the two models (RF and NN) that we considered in the end as the most accurate ones (based on their impact on the loss function). Not reported in this paper is the development of other models that we built, e.g. extreme gradient boosting (XGBoost)[1].
However, there is definitively space for improvements and further work, e.g. other ensemble models like stacking may help to reduce bias and variance as they make use of multiple base models (c.f.Yu et al. (2006)).
One (in-)evitable error occurred during the creation of the variables user_retrate and item_retrate: the whole training data set has been used for creating these variables, because otherwise there were not enough observations in each category (since only around one third of the users have placed six or more orders). As we have used the whole training data set for creating the variables and trained the models on the same data set, it may be likely that some overfitting occurred.
Besides predicting return probabilities, there should be other actions taken into account when minimizing shipping costs. For example, online retailers can prevent return of orders by implementing a rating system on their websites such that costumers are able to assess

[1]The related code is available on GitHub https://github.com/Humboldt-BADS/bads-ws1718-group07

items and thereby receive a peer-review for the products. Furthermore, conversion tables for clothing sizes that are individualized for each brand may also reduce returns. Along with these marketing actions is a more informative data collection (in close coordination with online-privacy policies) recommended. More data is not the unique solution for data mining problems, but more informative variables can help to increase predictive accuracy.

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