The TDMR Tutorial: Examples for Tuned Data Mining in R

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1 Overview

The TDMR framework is written in R with the aim to facilitate the training, tuning and evaluation of data mining (DM) models. It puts special emphasis on tuning these data mining models as well as simultaneously tuning certain preprocessing options.

This document (TDMR-tutorial.pdf)

- describes the TDMR installation
- shows example usages: how to use TDMR on new data mining tasks
- provides a **FAQ-section** (frequently asked questions)

This document should be read in conjunction with the companion document TDMRdocu.pdf [Konen and Koch, 2012a], which describes more details and software concepts of TDMR.

Both documents are available online as CIOP Reports (PDF, Konen and Koch [2012a,b]) from http://www.gm.fh-koeln.de/ciopwebpub.¹

Both documents concentrate more on the software usage aspects of the TDMR package. For a more scientific discussion of the underlying ideas and the results obtained, the reader is referred to Konen et al. [2010, 2011], Konen [2011], Koch et al. [2012], Koch and Konen [2012], Stork et al. [2013], Koch and Konen [2013], Koch et al. [2014].

¹The precise links are http://www.gm.fh-koeln.de/ciopwebpub/Kone12a.d/Kone12a.pdf and http://www.gm.fh-koeln.de/ciopwebpub/Kone12b.d/Kone12b.pdf. The same files are available as well via the index page of the TDMR package (User guides and package vignettes).

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2 Installing TDMR

Once you have R (http://www.r-project.org/), > 2.14, up and running, simply install TDMR with

install.packages("TDMR");

Then, library TDMR is loaded with

library(TDMR);

```
## Loading required package: SPOT
## Warning: package 'SPOT' was built under R version 3.2.5
## Loading required package: twiddler
## Loading required package: tcltk
```

3 Lessons

NOTE: Many, but not all TDMR demos and functions will run under RStudio. That some demos are not running under RStudio is due to some incompatibilities in RStudio's graphic device(s). All demos and functions will however run under RGui.

To start a demo, e.g. demo/demo00-0classif.r, type

```
demo("demo00-0classif")
```

or

demo("demo00-0classif",ask=F)

3.0 Lesson 0: A simple TDMR program

demo/demo00-0classif.r
demo/demo00-1regress.r

This demo shows the most simple TDMR program. It does not need any external files.

3

```
data(iris)
response.vars="Species"  # names, not data (!)
input.vars=setdiff(names(iris),"Species")
result = tdmClassifyLoop(iris,response.vars,input.vars,opts)
print(result$Err)
```

Here, tdmOptsDefaultsSet will construct a default list opts with all relevant settings. See TDMR-docu.pdf Konen and Koch [2012a], Appendix B, for a complete list of all elements and all defaults for list opts. After initializing graphics and log file, the dataset iris is loaded and the target (Species) as well as the input variables (all other column names from iris) are defined.

Now the classification DM task is started with tdmClassifyLoop.

Inside tdmClassifyLoop the following things happen:

Data partitioning: The dataset will be divided by random sampling in a training set (90%) and validation set (10%), based on opts\$TST.kind="rand", opts\$TST.valiFrac=0.1.

Variable selection: Since you do not specify anything from the opts\$SRF-block (sorted random forest importance), you use the default SRF variable ranking (opts\$SRF.kind ="xperc", opts\$SRF.Xperc=0.95). This means that the most important columns (containing in sum at least 95% of the overall importance) will be selected.

Modeling and evaluation: Since you do not specify anything else, function tdmClassifyLoop builds an RF (randomForest) model (opts\$MOD.method="RF") using the training data and evaluates it on training and validation data. It returns an object result. The object result of class TDMclassifier is explained in more detail in Table 3 of TDMR-docu.pdf Konen and Koch [2012a].

Repeated runs: Since the default setting opts\$NRUN=2 is used, the whole procedure (random partitioning into training and validation set, RF-based selection of the most important variables, model building, and model evaluation) is repeated 2 times in 2 runs with different random seeds (yielding different data partitions & different split decisions in RF). The different runs are aggregated (usually by averaging).

We now take a look at the output generated by tdmClassifyLoop. Since we do not change the default opts\$VERBOSE=2, TDMR will print a lot of diagnostic output:

```
## default.txt : Stratified random training-validation-index with opts$TST.valiFrac = 10 %
##
## default.txt : Importance check ...
## Clipping sampsize to 135
## default.txt : Train RF (importance, sampsize= 135 ) ...
## default.txt : Saving SRF (sorted RF) importance info on opts ...
## Variables sorted by importance (4 ):
## [1] "Petal.Width" "Petal.Length" "Sepal.Length" "Sepal.Width"
## Dropped columns (0 [= 0.0% of total importance]):
```

```
## Proc time: 0.02
## Run 1 / 2 :
## default.txt : Train RF with sampsize = 135 ...
## Proc time: 0.07
## default.txt : Apply RF ...
## Proc time: 0.02
## default.txt : Calc confusion matrix + gain ...
##
## Training cases ( 135 ):
##
     predicted
## actual setosa versicolor virginica
## setosa 45 0 0
                 0
## versicolor
                            42
                                      3
## virginica 0
                          3
                                      42
## total gain: 129.0 (is 95.556% of max. gain = 135.0)
##
## Validation cases (15):
    predicted
##
## actual setosa versicolor virginica
## setosa 5 0 0
                 0
## versicolor
                            5
                                      0
## virginica 0
                            1
                                     4
##
    setosa versicolor virginica Total
## gain.vector 5 5 4 14
## total gain : 14.0 (is 93.333% of max. gain =
                                                 15.0)
##
##
   Relative gain on training set
                                     95.55556 %
##
   Relative gain on validation set
                                   93.33333 %
##
## default.txt : Stratified random training-validation-index with opts$TST.valiFrac = 10 %
##
## default.txt : Importance check ...
## Clipping sampsize to 135
## default.txt : Train RF (importance, sampsize= 135 ) ...
## default.txt : Saving SRF (sorted RF) importance info on opts ...
## Variables sorted by importance (4 ):
## [1] "Petal.Length" "Petal.Width" "Sepal.Length" "Sepal.Width"
## Dropped columns (1 [= 0.5% of total importance]):
## [1] "Sepal.Width"
## Proc time: 0.02
## Run 2 / 2 :
## default.txt : Train RF with sampsize = 135 ...
## Proc time: 0.06
## default.txt : Apply RF ...
## Proc time: 0.02
```

```
## default.txt : Calc confusion matrix + gain ...
##
## Training cases ( 135 ):
##
            predicted
## actual
             setosa versicolor virginica
                 45
                                      0
##
   setosa
                            0
                 0
##
    versicolor
                             42
                                       3
##
    virginica
                 0
                             3
                                      42
## total gain: 129.0 (is 95.556% of max. gain =
                                                 135.0)
##
## Validation cases (15):
##
   predicted
            setosa versicolor virginica
## actual
##
                 5
                             0
                                       0
   setosa
                   0
                              5
                                       0
##
   versicolor
##
    virginica
                 0
                             0
                                       5
##
             setosa versicolor virginica Total
              5
## gain.vector
                            5
                               5
                                           15
## total gain : 15.0 (is 100.000% of max. gain =
                                                   15.0)
##
##
    Relative gain on
                    training set
                                     95.55556 %
##
    Relative gain on validation set
                                     100 %
##
##
## Average over all 2 runs:
## cerr$train: (4.44444 +- 0.00000)%
## cerr$vali: (3.33333 +- 4.71405)%
## gain$train: ( 129.00 +- 0.00)
## gain$vali: ( 14.50 +- 0.71)
## rgain.train: 95.556%
## rgain.vali:
               96.667%
##
        cerr.trn gain.trn rgain.trn ntrn cerr.tst gain.tst rgain.tst
## [1,] 0.04444444 129 95.55556 135 0.066666667
                                                   14 93.33333
## [2,] 0.04444444
                      129 95.55556 135 0.0000000
                                                       15 100.00000
##
        cerr.tst2 gain.tst2 rgain.tst2 ntst
## [1,] 0.06666667
                        14
                             6.222222
                                       15
## [2,] 0.0000000
                     15
                             6.666667
                                       15
```

The first line tells us that TDMR has set aside 10% of the data (15 records in the case of **iris** with 150 records) for validation, the remaining 135 are for training. A random forest is trained to assess the importance of the input variables. We get with

[1] "Petal.Width" "Petal.Length" "Sepal.Length" "Sepal.Width"

the variables sorted by decreasing importance. It depends on the importance of the least important variable (here: Sepal.Width) whether it will be dropped or not. In the first run it is not dropped, because its importance is above the threshold 1-0.95 = 5%. In the second run it is dropped, because due to statistical fluctuations now its importance is with 0.5% below

In the next step the DM model (here: RF) is trained with the selected variables and then the trained model is applied to the training data and to the validation data. In each case the confusion matrix (actual vs. predicted) is shown. The confusion matrices are below the lines Training cases (135) and Validation cases (15), resp. In the case of RF, the prediction on the training data is the OOB prediction.

Next, the total gain is reported as the sum of the element-wise product "gain matrix \times confusion matrix" where the gain matrix denotes for every classification outcome "actual vs. predicted" the associated gain.² If nothing else is said, the gain matrix is the identity matrix. In this case, relative gain is equivalent to the classification accuracy (percent of correctly classified records). The relative gain is defined as

$$\texttt{rgain} = \frac{\sum_{ij} G_{ij} C_{ij}}{\sum_{ij} G_{ij} C_{ij}^{(ideal)}}$$

with G = gain matrix, C = confusion matrix and where $C^{(ideal)}$ is the perfect confusion matrix (all records appear on the main diagonal).

As the final output from tdmClassifyLoop, below the line Average over all 2 runs, all runs (2 in this example) are averaged and the average classification error cerr, the average gain, and the average relative gain rgain are reported for training and validation set.

A similar information, but now for each run separately, is provided with the last statement in the demo program

print(result\$Err)

the threshold of 5%.

which gives for each run separately classification error (cerr), gain (gain), and relative gain (rgain) on the training set (.trn) with ntrn=135 training records and on the test set (.tst) with nst=15 records.³

cerr.trn gain.trn rgain.trn ntrn cerr.tst gain.tst rgain.tst ## [1,] 0.04444444 129 95.55556 135 0.06666667 14 93.33333 ## [2,] 0.04444444 129 95.55556 135 0.00000000 15 100.00000 ## cerr.tst2 gain.tst2 rgain.tst2 ntst ## [1,] 0.06666667 14 6.222222 15 ## [2,] 0.0000000 15 6.666667 15

If you add the line

 $^{^{2}}$ In this toy problem, the gain on the validation set is statistically not very meaningful since the validation set has only 15 records.

 $^{^3}$ The columns with .tst2 refer to a test set with special postprocessing, see TDMR-docu.pdf and the TDMR manual pages for details.

```
opts$VERBOSE <- opts$SRF.verbose <- 0</pre>
```

before calling tdmClassifyLoop, then tdmClassifyLoop is completely silent. The only output you get is the printout of result\$Err.

A similar demo program for regression is found in demo/demo00-1regress.r.

3.1 Lesson 1: DM on task SONAR

demo/demo01-1sonar.r demo/demo01-2cpu.r

Now we want to conduct a data mining process with a pre-defined parameter set different from the defaults (sonar_00.apd).

This lesson demonstrates the usage of TDMR for a somewhat bigger DM task: data are read from file and the information for controlling TDMR is distributed over several files. This may look complicated at first sight, but it is useful for two reasons:

- **Separate function file:** As a preparation for the tuning process in subsequent lessons: It is very useful if we can package the whole data mining process (from training-validation-data generation over model building up to model evaluation) into one function or file. It will be easily callable by the tuner.
- Separate parameter file: For conducting slightly different variants, runs or experiments, it is useful to package the parameter setting part in one (or several) files as well.

In this lesson we will look at four relevant files:

- 1. sonar_00.apd (the parameter settings)
- 2. main_sonar.r (the DM function main_sonar)
- 3. start_sonar.r (starter file)
- 4. demo01-1sonar.r (demo starter only needed for TDMR-package demo)

Suppose that you have a dataset and want to build a DM model for it. To be concrete, we consider the classification dataset SONAR⁴. The data file sonar.txt should be in the subdirectory myDir/data relative to the other files.

If you want to build a DM classification model with TDMR, you need to provide two files, sonar_00.apd and main_sonar.r.⁵ The first file, sonar_00.apd (.apd = algorithmic problem design), is already in preparation for later tuning (see Lesson02 and Lesson03), it defines in list opts all relevant settings for the DM model building process. The second file, main_sonar.r, contains this DM model building process. It gets with list opts the settings and returns in

⁴see UCI repository or package mlbench for further info on SONAR)

⁵Templates for sonar_00.apd and main_sonar.r are available from <inst>/demo02sonar where <inst> refers to the installation directory of package TDMR as returned by find.package("TDMR").

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list **result** the evaluation of the DM model. The list **result** is either inspected by the user or by the tuning process.

```
## sonar_00.apd
##
## set the basic elements of list opts for task sonar. See ?tdmOptsDefaultsSet
## for a complete list of all default settings and many explanatory comments
    opts = tdmOptsDefaultsSet();
    opts$dir.data <- "data/";
    opts$filename <- "sonar.txt"
    opts$READ.TrnFn <- readTrnSonar
    opts$NRUN <- 1
    opts$data.title <- "Sonar Data"</pre>
```

Here, tdmOptsDefaultsSet() will construct a default list opts with all relevant settings. See TDMR-docu.pdf Konen and Koch [2012a], Appendix B, for a complete list of all elements and all defaults for list opts. You need to specify only those things which differ from tdmOptsDefaultsSet(): in this case most importantly the filename and directory of the SONAR dataset and a function opts\$READ.TrnFn containing the data-reading command.

The file main_sonar.r contains two functions main_sonar and readTrnSonar:

```
main_sonar <- function(opts=NULL, dset=NULL, tset=NULL) {</pre>
  if (is.null(opts)) source("sonar_00.apd", local=TRUE);
  opts <- tdmOptsDefaultsSet(opts);</pre>
                                      # fill in all opts params not yet set
  gdObj<-tdmGraAndLogInitialize(opts); # init graphics and log file
  ######## PART 1: READ DATA
                                if (is.null(dset)) {
      cat1(opts,opts$filename,": Read data ...\n")
      dset <- tdmReadData2(opts);</pre>
  names(dset)[61] <- "Class" # 60 columns V1,...,V60 with input data, one</pre>
                              # response column "Class" with levels ["M"/"R"]
  response.vars <- "Class"</pre>
                                       # which variable(s) are target
  # which variables are input variables (in this case all others):
  input.vars <- setdiff(names(dset), c(response.variable))</pre>
  ####### PART 2: Model building and evaluation #########
  result <- tdmClassifyLoop(dset,response.vars,input.vars,opts,tset);</pre>
  # print summary output and attach certain columns
```

To start the whole procedure, there is a small starter file **start_sonar.r**:

source("main_sonar.r");
result <- main_sonar(opts);</pre>

This file is invoked by demo01-1sonar.r:

```
## ------ demo/demo01-1sonar.r -----
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");
source(paste(path,"main_sonar.r",sep="/")); # needed to define readTrnSonar
source(paste(path,"sonar_00.apd",sep="/"),local=TRUE); # set opts, needs readTrnSonar
source(paste(path,"start_sonar.r",sep="/"),chdir=TRUE,print.eval=TRUE);</pre>
```

The reason why we have the file chain

demo01-1sonar.r $\xrightarrow{\text{source}}$ start_sonar.r $\xrightarrow{\text{call}}$ main_sonar.r

is that main_sonar needs to perform certain file I/O in the directory path. Sourcing start_sonar.r with source(..., chdir=TRUE) tells R that it changes to the directory path prior to sourcing (and automatically returns to the actual working directory at the end of sourcing⁶).

The distinction between start_sonar.r and demo01-1sonar.r is only needed for the TDMR-package demo. If you write your own application, you can have main_sonar.r together with the .apd file in the same directory myDir. Then you only need one starter script in myDir which simply reads like this:

```
source("main_sonar.r");
source("sonar_00.apd");
result <- main_sonar(opts);</pre>
```

⁶Even in the case of an error inside start_sonar.r R will correctly return to the actual working directory.



res.SRF

Figure 1: Some plots from demo01-1sonar.r



Sonar Data: The five most important inputs

Figure 2: Some plots from demo01-1sonar.r



True/false classification on Validation set

Figure 3: Some plots from demo01-1sonar.r

3.2 Lesson 2: SPOT tuning on task SONAR

demo/demo02sonar.r

In this lesson we not only want to run the data mining process for a fixed parameter set as in Lesson 01 (Sec. 3.1), but we want to *tune the parameters*, i. e. to find good or optimal parameters within a certain range, the *region of interest* (.roi-file).

If you want to do a SPOT tuning [Bartz-Beielstein, 2010] on task SONAR, you should follow the steps described in TDMR-docu.pdf (see Konen and Koch [2012a], Sec. 2.2 *TDMR Workflow, Level 2*) and create in addition to main_sonar.r from Lesson 01 the three small files sonar_01.conf, sonar_01.apd and sonar_01.roi. The content of these files may look for example like this:

sonar_01.conf

```
alg.func = "tdmStartSpot"
alg.resultColumn = "Y"
alg.seed = 1235
io.apdFileName = "sonar_01.apd"
io.roiFileName = "sonar_01.roi"
spot.seed = 120 # 125
io.verbosity = 3;
auto.loop.steps = 50; # number of spot metamodels to be generated
```

```
auto.loop.nevals = 50; # concurrently, max number of algo evaluations
init.design.func = "spotCreateDesignLhd";
init.design.size = 10; # number of initial design points
init.design.repeats = 1; # number of initial repeats
seq.merge.func <- mean;
seq.design.size = 100;
seq.design.retries = 15;
seq.design.maxRepeats = 2;
seq.design.oldBest.size <- 1;
seq.design.new.size <- 3;
seq.predictionModel.func = "spotPredictRandomForest";
report.func = "spotReportSens"
```

```
sonar_01.apd
```

sonar_01.roi

name low high type CUTOFF1 0.1 0.80 FLOAT CLASSWT2 5 15 FLOAT XPERC 0.90 1.00 FLOAT %0

The three parameters CUTOFF1, CLASSWT2 and XPERC are tuned within the borders specified by sonar_01.roi. Usually you should set opts\$GRAPHDEV="non" and opts\$GD.RESTART=F to avoid any graphic output and any graphics device closing from main_sonar.r, so that you get only the graphics made by SPOT.

To start the whole procedure, there is a small starter file **start_bigLoop.r**:

```
#*# ------ start_bigLoop.r -----
envT <- tdmEnvTMakeNew(tdm);
opts <- tdmEnvTGetOpts(envT,1);
dataObj <- tdmSplitTestData(opts,tdm);
envT <- tdmBigLoop(envT,spotStep,dataObj);</pre>
```

This file is invoked by demo02sonar.r:

```
#*# ------ demo/demo02sonar.r -----
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");
tdm=list(mainFile="main_sonar.r",runList="sonar_01.conf");
spotStep = "auto";
source(paste(path,tdm$mainFile,sep="/"));
source(paste(path,"start_bigLoop.r",sep="/"),chdir=TRUE);</pre>
```

The reason why we have the file chain

demo02sonar.r $\xrightarrow{\text{source}}$ start_bigLoop.r $\xrightarrow{\text{call}}$ tdmEnvTMakeNew

is the same as in Lesson 1: tdmEnvTMakeNew may need to perform certain file I/O in the directory path. Sourcing start_bigLoop.r with source(...,chdir=TRUE) tells R that it changes to the directory path prior to sourcing (and automatically returns to the actual working directory at the end of sourcing⁷).

Again, as in Lesson 1, the distinction between start_bigLoop.r and demo02sonar.r is only needed for the TDMR-package demo. If you write your own application, you can have main_sonar.r together with the .apd, .roi and .conf files in the same directory myDir. The data file sonar.txt should be in the subdirectory myDir/data. Then you only need one starter script in myDir which simply reads like this:

```
tdm=list(mainFile="main_sonar.r",runList="sonar_01.conf");
source(paste(path,tdm$mainFile,sep="/"));
envT <- tdmEnvTMakeNew(tdm);
opts <- tdmEnvTGetOpts(envT,1);
dataObj <- tdmSplitTestData(opts,tdm);
envT <- tdmBigLoop(envT,"auto",dataObj);</pre>
```

In any case, what happens in this demo is the following:

- The first command sets the minimal tdm.
- The second command sources the main file.
- With the command tdmEnvTMakeNew(tdm) we construct an environment with all necessary TDMR data and functions for this lesson. Inside tdmEnvTMakeNew the minimal tdm is filled with all defaults (see tdmDefaultsFill).

 $^{^{7}}$ Even in the case of an error inside start_bigLoop.r R will correctly return to the actual working directory.

• The command tdmBigLoop is the main workhorse. It reads in the DM data, splits them in a train/vali and a test part. Then it calls the desired tuner(s) (in this case only SPOT, since the default for tdm\$tuneMethod is "spot", but tdm\$tuneMethod could be a vector of tuners as well). Each tuner performs multiple DM runs in order to find the best values for the tunable parameters defined in the .roi file. The results of the whole tuning process are returned in envT, more details on envT are in the manual / help section for tdmBigLoop.

3.3 Lesson 3: "The Big Loop" on task SONAR

demo/demo03sonar.r demo/demo03sonar_B.r demo/demo03newdata.r

3.3.1 Multiple .conf Files

To start "The Big Loop", you configure a file similar to demo/demo03sonar.r:

```
#*# ----- demo/demo03sonar.r -----
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");</pre>
tdm <- list( mainFile="main_sonar.r"</pre>
            , runList = c("sonar_04.conf","sonar_06.conf")
            , umode="CV" # { "CV" | "RSUB" | "TST" | "SP_T" }
            , tuneMethod = c("lhd")
            , filenameEnvT="demo03.RData" # file to save envT (in dir "path")
            , nrun=3, nfold=2 # repeats and CV-folds for the unbiased runs
            , nExperim=1
            , parallelCPUs=1
            , parallelFuncs=c("readTrnSonar")
             optsVerbosity = 3
                                     # the verbosity for the unbiased runs
           );
spotStep = "auto";
source(paste(path,tdm$mainFile,sep="/"));
source(paste(path, "start_bigLoop.r", sep="/"), chdir=TRUE, local=TRUE);
# change dir to "path" while sourcing
```

This is very much the same as in Lesson 2, we reuse the small starter file start_bigLoop.r from there. The only difference is that now multiple tuning runs can be performed with respect to the following three dimensions:

- configuration files (elements of tdm\$runList)
- tuners (elements of tdm\$tuneMethod)
- repeated experiments with different random seeds (number tdm\$nExperim).

The function tdmBigLoop realizes a triple for-loop over these dimensions. With k = length(runList), m = length(tuneMethod), and n = nExperim we have in total kmntuning runs.

Here, the script demo03sonar.r will trigger the following sequence of experiments:

- sonar_04.conf is started with tuner lhd
- sonar_06.conf is started with tuner lhd.

This sequence of 2 tuning experiments is repeated nExperim=1 time. The corresponding 2 result lines are written to data frame envT\$theFinals:

print(envT\$theFinals);

CLASSWT2 CONF TUNER NEXP CUTOFF1 XPERC NEVAL RGain bst ## 1 sonar_04 lhd 1 0.06907716 13.637625 0.8581948 10 91.66667 97.22222 ## 2 sonar_06 1 0.45476980 5.536813 0.6545237 lhd 10 ## RGain.avg Time.TRN NRUN RGain.TRN sdR.TRN RGain.CV sdR.CV Time.TST ## 1 77.66667 0.96 3 82.47619 5.1428706 82.66667 1.5275252 0.35 ## 2 88.55556 0.99 3 98.66667 0.5773503 96.66667 0.5773503 0.36

Here CUTOFF1, CLASSWT2, and XPERC are the tuning parameters, the other columns of the data frame are defined in Table 2 of TDMR-docu.pdf Konen and Koch [2012a]. In the case of the example above, the tuning process had a budget of NEVAL=10 model trainings, resulting in a best solution with class accuracy RGain.bst (in %). The average class accuracy (mean w.r.t. all design points) during tuning is RGain.avg. When the tuning is finished, the best solution is taken and NRUN=3 unbiased evaluation runs are done with the parameters of the best solution. The mean classification accuracy RGain.TRN from the 3 training runs is returned.⁸ Additionally, NRUN=3 trainings are done with cross validation (CV) with new randomly created folds in each run, resulting in an average class accuracy RGain.CV. For each measure RGain.* there is also an accompanying column sdr.* giving the standard deviation with respect to the NRUN runs.

Tuning runs are rather short, to make this example run quickly. Do not expect good numeric results. See demo/demo03sonar_B.r for a somewhat longer tuning run, with two tuners SPOT and LHD.

Single .conf File 3.3.2

If you have only a single CONF file it is recommended that you use tdmTuneIt instead of tdmBigLoop. tdmTuneIt has dataObj as a mandatory calling parameter. This makes it easier to build up your task since it has a clearer data flow concept behind.

See Lesson 3.9 (Tuning with fewer data) for a fully worked-out example with tdmTuneIt.

Alternatively you may look at the demo demo03newdata for another example:

⁸Since the classification model in this example is RF (Random Forest), RGain.TRN refers to the OOB-error.

```
#*# ------ demo/demo03newdata.r -----
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");
#path <- paste("../inst", "demo02sonar",sep="/");
oldwd <- getwd(); setwd(path);
envT <- tdmEnvTLoad("demo03.RData");
source(envT$tdm$mainFile);
source("sonar_06.apd")  # opts
opts$READ.NROW=-1;
dataObj <- tdmSplitTestData(opts,envT$tdm);
envT <- tdmBigLoop(envT,"rep",dataObj);
setwd(oldwd);</pre>
```

Here we use tdmBigLoop (and not tdmTuneIt), since we have two CONF files in envT of demo03.RData. tdmBigLoop will retrieve the best tuning parameters from each tuning run and perform with it a re-training and re-evaluation on the new data.⁹

The results of the new unbiased evaluation runs are recorded in envT\$theFinals:

print(envT\$theFinals);

```
##
        CONF TUNER NEXP
                           CUTOFF1 CLASSWT2
                                                 XPERC NEVAL RGain.bst
## 1 sonar_04
               lhd
                      1 0.06907716 13.637625 0.8581948
                                                         10 91.66667
## 2 sonar 06
              lhd
                      1 0.45476980 5.536813 0.6545237
                                                         10 97.22222
##
    RGain.avg Time.TRN NRUN RGain.TRN sdR.TRN RGain.CV
                                                          sdR.CV Time.TST
                          3 57.53205 1.468774 57.05128 0.2775722
## 1
     77.66667
                  0.02
                                                                     1.14
                  0.01 3 80.12821 2.001602 76.12179 4.8634586
## 2 88.55556
                                                                     0.99
```

3.4 Lesson 4: Regression Big Loop

```
demo/demo04cpu.r
```

The same as Lesson 3, but applied to a regression task (dataset CPU).

3.5 Lesson 5: Interactive Visualization

demo/demo05visMeta.r

Once a Lesson-3 experiment is completed, the return value envT from tdmBigLoop() contains the result of such an experiment and may be visually inspected. Alternatively, envT may be loaded from an appropriate .RData file. The call

⁹ Note that the dataset dataObj, when specified in tdmBigLoop, is used for every run (every CONF file) in the big loop. If dataObj were not specified in the call to tdmBigLoop, each CONF file would construct its own dataObj inside tdmBigLoop.

🤋 twiddler 📃 🗖 🔀				
showMeta(tuner, nExp = 1, report				
	tuner	spot	*	
xAxis		CUTOFF1	*	
yAxis		CLASSWT2	*	
r	reportFunc spotReport3d		*	
	modelFit	spotPredictRa	ndomFore 💌	
nSkip 4				
0	3	6	9	
	Eval		ose	

Figure 4: The user interface in tdmPlotResMeta. The user may select the tuner, the design variables to show on x- and y-axis, the display function (spotReport3d or spotReportContour) and the metamodel function (modelFit). Two optional sliders are nExper and nSkip (see text).

tdmPlotResMeta(envT);

allows to visually inspect all RES data frames contained in envT.

The user interface is shown and explained in Fig. 4. An additional combo box confFile appears only, if envT\$runList has more than one element. An additional slider nExper appears only, if envT\$tdm\$nExperim>1.

The user selects with tuner, confFile and nExper a certain RES data frame from envT. This data frame contains a collection of function evaluations for certain design points selected by the tuner. With one of the metamodel construction functions (see package SPOT for further details)

- spotPredictGausspr
- spotPredictRandomForest
- spotPredictMlegp

a metamodel is fitted to the RES data frame and the result is shown as shaded surface in the plot. The RES data points are shown as black points in Fig. 5. Since certain "bad" RES point may dominate the plot as outliers and hinder the user to inspect the region near the optimum, there are two options to suppress "bad" points:

- 1. If the slider nSkip has a value > 0, then the nSkip RES data points with the worst y-value are discarded.
- 2. If the checkbox "Skip incomplete CONFIGs" is activated, then design points belonging



Figure 5: Two example outputs from tdmPlotResMeta with reportFunc=spotReport3d. Left: modelFit = spotPredictGausspr, right: = spotPredictRandomForest.

to a configuration which was not evaluated maxRepeats times are discarded (relevant for SPOT only).

Note that both options will reduce the number of RES data points. This will also affect the metamodel fit, so use both options with care, if the number of RES data points is small.

The plots created with spotReport3d make use of the rgl-package. They can be interactively manipulated with the mouse. They can be selected and saved as PNG images with commands like

rgl.set(7); rgl.snapshot("myFile.png");

A complete demo example is invoked with:

demo(demo05visMeta);

3.6 Lesson 6: Performance Measure Plots

demo/demo06ROCR.r

With the help of package ROCR Sing et al. [2005], several area performance measures can be used for binary classification. The file demo/demo06ROCR.r shows an example:

```
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");
source(paste(path, "main_sonar.r",sep="/"),chdir=TRUE);
opts = tdmOptsDefaultsSet();
opts$filename = "sonar.txt"
opts$READ.TrnFn = readTrnSonar  # defined in main_sonar.r
opts$data.title <- "Sonar Data";
opts$rgain.type <- "arROC";
source(paste(path, "start_sonar.r",sep="/"),chdir=TRUE);
```



Figure 6: (a) ROC curve on validation set with tdmROCRbase(result); (b) Lift chart on training set with tdmROCRbase(...,typ="lift"). The bar on the right side shows a color coding of the cutoff parameter.

As explained in Lesson 1 in more detail, the file start_sonar.r contains the line

result <- main_sonar(opts);</pre>

Once the variable result contains an object of class TDMclassifier, we can infer from it with tdmROCRbase the area under the ROC curve and – as a side effect – plot the ROC curve (Fig. 6(a)). The **ROC curve** is a plot 'false positive rate' vs. 'true positive rate', which is obtained by varying the cutoff. Each record is rated by the model and if the model output is above cutoff, then this record is marked 'positive'. The bigger the area between ROC curve and main diagonal, the better the model.

```
cat("Area under ROC-curve for validation data set: ",
    tdmROCRbase(result),"\n"); # side effect: plot ROC-curve
```

Area under ROC-curve for validation data set: 0.92

Equally well we can infer with typ="lift" the area under the lift curve and plot a lift chart (Fig. 6(b)). A lift chart is constructed in the following way: The records are sorted according to model output. If a high cutoff is choosen only a small portion of the data is marked 'positive' (we have a low rate of positive predictions), but within this portion the rate of true positives is much higher than the overall 'true' rate. The ratio 'true rate in portion'/'overall true rate' is the lift. If we move to lower cutoff values, the 'positive' portion becomes bigger, it is eventually the whole dataset, but at the same time the lift reduces to 1.0. The bigger the area between the lift curve and the horizontal line at 1.0, the better the model.

```
cat("Area under lift curve for training data set: ",
    # side effect: plot lift chart:
    tdmROCRbase(result,dataset="training",typ="lift"),"\n");
```

Area under lift curve for training data set: 0.5552925

The curves in Fig. 6(a) and 6(b) are colorized according to the cutoff, whose range is shown in the colorbar to the right. That is, if the color is blue, the cutoff is 0.1 in the left plot. This is a very low value, leading to the acceptance of every record. The true positive rate will be 1.0, but of course the false positive rate will be 1.0 as well.

Once the variable result contains an object of class TDMclassifier, it is also possible to inspect such an object interactively with the following command:

tdmROCR(result);

A twiddler interface for object result shows up (Fig. 7) and allows to select between

- different performance measure plots (ROC-, lift- or precision-recall-chart)
- different data sets (training set or validation set)
- different runs stored in object result.

NOTE: The twiddler interface of tdmROCR(result) does sometimes not launch successfully when issued from RStudio. If started a second or third time, it will normally launch, but even then the interaction between RStudio's graphics device and twiddler may have the problem, that the next lift chart only shows after a second hit on the Eval button. If you observe such problems, then start tdmROCR(result) from the normal R console (RGui under Windows), this works always correctly.

🍽 twiddler		
tdmROCR_	_(dataset, nRun, ty	o)
dataset	validation	*
typ	ROC	*
nRun		2
Eval	Close	

Figure 7: Twiddler interface for tdmROCR(result). The user may select the dataset (training or validation), the type of plot (ROC, lift, or precision-recall) and the number of the run (only if Opts(result)\$NRUN>1).

3.7 Lesson 7: Tuner CMA-ES (rCMA)

demo/demo07cma_j.r
demo02sonar/sonar_03.conf

This demo conducts for tuner cma_j (Java version of CMA-ES Hansen [2006] interfaced to R via package rCMA) a complete tuned data mining process (TDMR, level 3). Other settings are the same as in demo03sonar.r, except that we use sonar_03.conf as configuration file. rCMA uses rJava for the R-to-Java-interface.

3.7.1 Fixing problems with the rJava installation

On some operating systems, especially Windows 7, it may happen that the command require(rJava) in demo07cma_j.r issues an error of the form

Error : .onLoad failed in loadNamespace() for rJava, details: ...

This means that **rJava** was not installed properly on your computer. Try then the following:

1. Define the environment variable JAVA_HOME: Explorer - RightMouse on "Computer" - Properties - Environment Variables, and add there

JAVA_HOME = C:\Program Files\Java\jdk1.7.0_11\jre7

and **restart R**. (The path is the correct one on my computer, on others it might be slightly different.)

Package rJava needs to find the Java DLL jvm.dll. To enable this, expand the environment variable Path: Explorer - RightMouse on "Computer" - Properties - Environment Variables - Path - Edit, and add at the end of the Path string

C:\Program Files\Java\jdk1.7.0_11\jre\bin\server

and **restart R**. (The path is the correct one on my computer, on others it might be slightly different. It must be the directory of the current Java installation containing jvm.dll.)

Note that the above remarks are for 64-bit-Java and 64-bit-R. If you use 32-bit-Java, the locations might be slightly different as well.

On some Linux/UNIX systems there might be also problems with the installation of rJava because R cannot locate the Java installation. In that case, fix it permanently by issuing the command

```
sudo R CMD javareconf -e
```

at the UNIX prompt (needs admin rights). If you do not have admin rights, you may invoke

R CMD javareconf -e

in each session where you need rJava.

3.8 Lesson 8: Parallel TDMR

```
demo/demo08parallel.r
demo02sonar/sonar_04.conf
```

This demo does the same as demo03sonar.r, but it runs 4 experiments on 4 parallel cores (if your environment supports parallel clusters with the R core-package parallel).

3.9 Lesson 9: Tuning with fewer data

```
examples/ex-winequality/start-wine.r
examples/ex-winequality/final-wine.r
```

3.9.1 Tuning

We add an extra feature to this demo lesson: Suppose you have a large dataset and you want to do quick tuning runs. To reduce the tuning time (of course at the price of a somewhat reduced tuning quality) you may specify the parameter opts\$READ.NROW to a value smaller than the size of the dataset.¹⁰ Then only this number of records is read and used for training and validation during tuning. After tuning has finished, you may want to use the best parameters found by tuning and to perform a high-quality training and evaluation on the full dataset to assess the real strength of the tuning result.

Tuning is started with the function tdmTuneIt:

¹⁰Alternatively, you may reduce opts\$RF.samp, the sampsize parameter in case of Random Forest, to a small value. These settings are all done in the APD-file wine_01.apd, as specified in wine_01.conf.

```
#*# -----ex-winequality/start_wine.r -----
path <- paste(find.package("TDMR"), "examples/ex-winequality",sep="/");</pre>
oldwd=getwd(); setwd(path);
tdm=list(mainFile="main_wine.r"
         ,runList="wine_01.conf" # in "wine_01.apd": optsfREAD.NROW=600
         ,umode="SP_T"
         ,U.saveModel=F
         ,optsVerbosity=1
         ,nrun=2
);
source(tdm$mainFile);
#
# perform a complete tuning, but only with the first 600 records
envT <- tdmEnvTMakeNew(tdm); # construct envT from the TDMR settings in tdm
opts <- tdmEnvTGetOpts(envT,1);</pre>
dataObj <- tdmSplitTestData(opts,tdm);</pre>
envT <- tdmTuneIt(envT, "auto", dataObj); # start the tuning loop
## Warning in randomForest.default(x, y): The response has five or fewer unique
values. Are you sure you want to do regression?
```

setwd(oldwd);

As usual, the file main_wine.r containts the function main_wine with the template for the data mining proc to read the data. This tuning experiment is repeated nExperim=1 time. The corresponding 1 result line is written to data frame envT\$theFinals:

print(envT\$theFinals);

CONF TUNER NEXP XPERC NEVAL RGain.bst RGain.avg Time.TRN NRUN
1 wine_01 spot 1 0.9330384 11 65.0463 64.26768 5.74 2
RGain.TRN sdR.TRN RGain.SP_T sdR.SP_T Time.TST
1 63.88889 1.964186 57.91667 0.5892557 1.01

Tuning runs are rather short, to make this example run quickly. Do not expect good numeric results.

3.9.2 Retrain on bigger data set

The tuning results are saved in wine_01.RData. The following code from final_wine.r shows how to retrain with these tuning results.

We load this file, then set opts READ.NROW = -1. This means that we now read all data with tdmSplitTestData and split them into 10% test data (the default) and 90% training

data (since we specify with tdm\$TST.valifrac=0 that we want no validation data).

```
Note the bracketing lines with
opts <- tdmEnvTGetOpts(envT,1)
```

and

tdmEnvTSetOpts(envT,opts).

Between these lines we first retrieve all opts-settings from envT and then modify specific opts-values for the retraining. Here we set for example opts\$RF.samp to a larger value.

Now we enter tdmTuneIt with the new dataset dataObj, the new opts, and with spotStep="rep" indicating that we shall grab the best tuning result and perform training and evaluation on the new dataset:

```
#*# -----ex-winequality/final_wine.r -----
path <- paste(find.package("TDMR"), "examples/ex-winequality",sep="/");</pre>
oldwd <- getwd(); setwd(path);</pre>
tdm=list(mainFile="main_wine.r"
         ,runList="wine_01.conf"
         ,umode="SP_T"
         ,TST.valiFrac=0
         ,U.saveModel=F
         ,optsVerbosity=1
         ,nrun=2
);
source(tdm$mainFile);
# re-use prior tuning result (spotStep="rep"); do only spot-report and
# unbiased eval on best tuning result.
# But do so by training a model on 80% of all 4898 records.
tdm <- tdmDefaultsFill(tdm)</pre>
load(tdm$filenameEnvT); # envT
opts <- tdmEnvTGetOpts(envT,1);</pre>
opts$READ.NROW=-1;
                          # read all 4898 records of winequality-white.csv
opts$RF.samp=5000;
envT$tdm$optsVerbosity <- 1;</pre>
envT$tdm$U.saveModel <- tdm$U.saveModel;</pre>
envT$tdm$TST.valiFrac <- tdm$TST.valiFrac;</pre>
dataObj <- tdmSplitTestData(opts,envT$tdm);</pre>
envT <- tdmEnvTSetOpts(envT,opts);</pre>
envT <- tdmTuneIt(envT, "rep", dataObj);</pre>
setwd(oldwd);
```

The result of the new unbiased training + evaluation runs is again recorded in envT\$theFinals:

print(envT\$theFinals);

CONF TUNER NEXP XPERC NEVAL RGain.bst RGain.avg Time.TRN NRUN
1 wine_01 spot 1 0.9330384 11 65.0463 64.26768 0.03 2
RGain.TRN sdR.TRN RGain.SP_T sdR.SP_T Time.TST
1 67.81067 0.884109 71.1951 0.1444549 9.94

Note that we get a higher gain (lower error) on RGain.TRN and RGain.SP_T than we had after tuning in Sec. 3.9.1. This is due to the increased number of data used during the unbiased training and evaluation runs.

A Appendix A: Frequently Asked Questions (FAQ)

A.1 I have already obtained a best tuning solution for some data set. How can I rerun and test it on the same / other data?

As an example, we assume that demo03sonar.r has been run, so that demo03.RData is available. You may look at the demo demo03newdata already presented in Lesson 3.3:

```
#*# ------ demo/demo03newdata.r -----
path <- paste(find.package("TDMR"), "demo02sonar",sep="/");
oldwd <- getwd(); setwd(path);
envT <- tdmEnvTLoad("demo03.RData");
source(envT$tdm$mainFile);
source("sonar_06.apd")  # opts
opts$READ.NROW=-1;
dataObj <- tdmSplitTestData(opts,envT$tdm);
envT <- tdmBigLoop(envT,"rep",dataObj);
setwd(oldwd);</pre>
```

This will reload the tuning results from demo03.RData. Then all data will be read with tdmSplitTestData into dataObj (Since envT\$tdm\$umode="CV", we will have all 208 data records in the train-validation set. The split into 2 cross-validation folds with 104 records each is done later in tdmClassifyLoop, for each seed differently.)

tdmTuneIt will use the best tuning parameters previously found, train it on the CVtrain data and test it on the CV-validate data. The results are reported, as usually, in envT\$theFinals.

A.2 How can I make with a trained model new predictions?

Run your Lesson-3 script or Lesson-4 script to produce an environment envT, which is an object of class TDMenvir. There is an element lastModel defined in envT which contains the model trained on the best tuning solution during the last unbiased run.¹¹ TDMR defines a function predict.TDMenvir, which makes it easy to do new predictions:

```
newdata=read.csv2(file="cpu.csv", sep="", dec=".")[1:15,];
z=predict(envT,newdata);
print(z);
```

Remarks:

• If the new data contain factor variables (e.g. vendor in case of CPU data), it is necessary that levels(newdata\$vendor) is the same as during training. Therefore we read in the above code snippet first all CPU-data to get the levels right. Only then we shorten them with [1:15,] to the first 15 records.

¹¹The last model lastModel is available, if tdm\$U.saveModel=TRUE, which is the default.

- lastModel will be saved to .RData file only if tdm\$U.saveModel=TRUE. This is however the default.
- See also the examples in demo/demo04cpu.r and in predict.TDMenvir.

Why do I get sometimes "Warning in randomForest.default(x, x)A.3y): The response has five or fewer unique values. Are you sure you want to do regression?"

This comes from the report step in SPOT. If we have the setting

seq.predictionModel.func = "spotPredictRandomForest";

then the metamodel used in SPOT is Random Forest. If this model gets only a few data points for training, it issues this warning, because the data could come also from a classification task.

You can safely ignore this warning, we want to do regression at this point. (This is also true if your data mining task is a classification.)

A.4Why are there two similar functions tdmTuneIt and tdmBigLoop? Which function should I use when?

If you only have a single CONF file, then tdmTuneIt is the recommended choice. It has a clearer syntax, dataObj is a mandatory calling parameter and this makes the data flow more easy to understand.¹²

If you want to process multiple CONF files in one TDMR experiment, then tdmBigLoop is the recommended choice. If each CONF file works with the same dataObj, it is recommended to pass dataObj as argument to tdmBigLoop. The argument dataObj is however optional in a call to tdmBigLoop. This is for the cases where each CONF file needs different data: If dataObj is not an argument to tdmBigLoop then dataObj is constructed anew on each loop-pass inside tdmBigLoop.

A.5My .RData files for saving envT are pretty big. Is there a way to make them smaller?

It is the default, that the last DM model is saved in envT\$result\$lastRes\$lastModel. Such a DM model can be pretty big. If you do not want this, set tdm\$U.saveModel=FALSE.

Note however, that it is then not possible to reload the .RData file with envT and do directly new predictions. You would have to re-train a model first with appropriate training data.

 $^{^{12}}$ If you pass to tdmTuneIt a list of CONF files, only the first one will be taken.

A.6 How can I add a new tuning parameter to TDMR?

• As a user: Add a new line to userMapDesign.csv in directory tdm\$path. If such a file does not exist yet, the user has to create it with a first line

roiValue; optsValue; isInt

Suppose you want to tune the variable <code>opts\$SRF.samp</code>: add to file <code>userMapDesign.csv</code> a line

SRF.SAMP; opts\$SRF.samp; 0

This specifies that whenever SRF.SAMP appears in a .roi file in directory tdm\$path, the tuner will tune this variable. TDMR maps SRF.SAMP to opts\$SRF.SAMP. The last 0 means that SRF.SAMP is not an integer but a continuous variable.

- As a developer: Add similarly a new line to tdmMapDesign.csv. This means that the mapping is available for all tasks, not only for those in the current tdm\$path.
- Optional, as a developer: For a new variable opts\$Z, add to tdmOptsDefaultsSet() a line specifying a default value for opts\$Z. Then all existing and further tasks will have this default for opts\$Z.

A.7 How can I add a new tuning algorithm to TDMR?

See Sec. 10.1.2 "How to integrate new tuners" in TDMR-docu.pdf Konen and Koch [2012a].

A.8 How can I add a new machine learning algorithm to TDMR?

See Sec. 10.2 "How to integrate new machine learning algorithms" in TDMR-docu.pdf Konen and Koch [2012a].

A.9 How can it happen that some variables have an importance that is exactly zero?

Well, the importance for variables with low importance can be zero or even slightly negative (as a consequence of some statistical fluctuations). All those zero or negative importance values will be clipped to zero, therefore a variable with apparently exactly zero importance can happen more frequently than expected. CIOP Report 03/2012

B Appendix B: Overview TDMR Demos

demo/00Index

demo00-0classif	Simple, self-contained classification with tdmClassifyLoop on task iris
demo00-1regress	Simple, self-contained regression with tdmRegressLoop on task cpu
demo01-1sonar	TDMR, level 1: Simple TDMR classification on task sonar (one run / no tuning)
demo01-2cpu	TDMR, level 1: Simple TDMR regression on task cpu (one run / no tuning)
demo02sonar	TDMR, level 2: SPOT tuning for task sonar
demo03sonar	TDMR, level 3: Tuning for TDMR classification task sonar (multiple runs / short tuning)
demo03sonar_B	TDMR, level 3: same as demo03sonar, but with parameters for a longer tuning run
demo03newdata	TDMR, level 3: apply the result of demo03sonar to new data (redo training on new data with best-tuned parameters)
demo03newpredict	TDMR, level 3: apply the result of demo03sonar to new data (use last trained model in envT)
demo04cpu	TDMR, level 3: Tuning for TDMR regression task cpu (multiple runs / short tuning)
demo05visMeta	Interactive visualization of RES data frames generated by demo04cpu and their metamodels
demo06R0CR	Visualization of classification results using package ROCR
demo07cma_j	Tuning demo for tuner cma_j (CMAES, Java version through rCMA, runs on all platforms)
demo08parallel	Demo for parallel execution (8 experiments of type demo03sonar on 4 cores)

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